Division of Agricultural and Food Chemistry of the ACS Fall 2023

CORNUCOPIA

including the AGFD program and abstracts for the

266th American Chemical Society (virtual & live) National Meeting on

August 13 - 17, 2023

in

SAN FRANCISCO

Jonathan Beauchamp, Jason Soares
Program Chairs

Going to San Francisco?
Join the AGFD Awards Banquet at FOGO DE CHAO
Tuesday, August 15, 6:00 - 8:00pm
(tickets available at the AGFD information table)

Two minute walking directions to Fogo de Chao from Moscone Center –
exit the Center onto Howard Street. Turn right. Cross 3rd Street at the corner. Turn right.
Fogo de Chao (201 3rd St., Suite 100) is on your left.

Visit our website - www.agfoodchem.org - for a pdf of Cornucopia, job postings, awards and much more.
Check out our Facebook page - www.facebook.com/agandfood
We're on LinkedIn, too!

MESSAGE FROM THE CHAIR

It seems that barely any time has passed since we enjoyed the engrossing AGFD symposia and wider program of ACS Spring 2023 in Indianapolis, yet here we are again, with the next ACS National Meeting – ACS Fall 2023 in San Francisco – just around the corner (or already on our doorstep, if you have just picked up this copy of the AGFD Cornucopia on site at the meeting). As with previous national meetings, the work of putting together the divisional program commences long before the actual meeting takes place. Indeed, a provisional list of AGFD symposia for this conference was submitted to ACS early December 2022, with the call for abstracts launched early January and closing early April; thus, even as we attended ACS Spring 2023 at the end of March, efforts were underway towards creating the program for this meeting. Following the submission deadline, the symposium orgs. were tasked with evaluating abstracts and scheduling accepted contributions, with subsequent format assignment and formal programming by the Program Chairs, coordinated by Jason Soares. As in past years, but more so for this meeting, AGFD session requirements greatly exceeded the slots allocated by ACS, forcing the organizing team – program chairs and symposium orgs. – to streamline and merge sessions. This resulted in some unavoidable session cuts and consolidations, including virtual-only talks for speakers attending the meeting in person; I apologize to anybody affected by this most unfortunate situation, but hope that the comprehensive on-site technical program and non-technical events compensate for this inconvenience. I take my hat off to Jason for managing the unthankful and challenging task as interlocutor to resolve these issues as best possible. Jason, you have done a formidable job in putting together a fantastic AGFD program for this meeting, as all attendees will no doubt agree with once the conference kicks-off.

Looking back at the ACS Spring 2023, the AGFD technical program featured a wide range of topics with 119 paper contributions across 19 sessions in 12 symposia, including two panel discussions and the general papers oral and poster sessions, the latter featuring the undergraduate poster competition. The outstanding quality of all poster entries presented a challenge for the judges, but ultimately the panel shortlisted the most exceptional contributions and conferred three awards, with first prize jointly awarded to Celina Paoletta (Christopher Newport University) and Christopher Prajogo (UC Davis), second prize being received by Jordon Scalia and Bret Watson (Shippensburg University of Pennsylvania) for their co-authored paper, and third place secured by Kourtney Collier (Purdue University). See page 12 of this Cornucopia for details. Congratulations to these winners; we look forward to future contributions from these young researchers and their fellow competitors as they embark on their scientific careers.

Looking ahead, ACS Fall 2023 promises an even richer and comprehensive AGFD program, with 21 symposia encompassing 39 half-days sessions (13 in-person, 18 hybrid, and 8 virtual) covering topics that range from the chemistry of wine to artificial intelligence, amongst many more. Notable mentions should be made to the inaugural symposia of two ACS Convergent Chemistry Community initiatives spearheaded by AGFD – Food Security: Tackling Hunger and the ACS Microbiome Research Consortium; these represent important cross-divisional endeavors addressing pressing societal issues. This fall meeting sees another first: the Virtual Graduate Students Symposium in Asia-Pacific Region. This symposium is organized by the ACS Shanghai Chapter and showcases the latest activities in the field from emerging research leaders from our international colleagues. Traditionally, AGFD uses the ACS Fall meetings as an opportunity to recognize exceptionally talented and dedicated members of the division for their contributions to the field, with this meeting being no exception. Accordingly, I congratulate Liangli (Lucy) Yu for receiving the Award for the Advancement of Application of Agriculture and Food Chemistry and invite you all to attend the symposium in her honor, taking place on Tuesday. Likewise, I congratulate Xiaonan Sui and Zhuohong (Kenny) Xie as deserving recipients of the AGFD Young Scientist and Young Industrial Scientist Awards, respectively, who will similarly be honored in a dedicated symposium, also on Tuesday, together with the Journal of Agricultural and Food Chemistry Best Paper Award. It is my great pleasure to formally confer these awards during the Chair's Awards Banquet on Tuesday evening, which I invite you to attend (spaces are limited; see the cover page of this Cornucopia for details on securing tickets).

I conclude this message with my express gratitude to everybody who has worked tirelessly behind the scenes, not just in creating an exciting technical program, but also organizing non-technical events, with dedicated support and promotion of our division. In addition to the many symposium orgs. and presiders (too many to name here), special thanks go to Mike Appell, Elyse Doria, Carl Frey, Alyson Mitchell, Mike Morello, Steve Toth and Mike Tunick. Finally, Jason Soares deserves a second and especial mention here for his tireless efforts in putting together an amazing program for us to enjoy this week. It has been a great pleasure and honor to have served the

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division as AGFD Chair this year and I am exceptionally grateful to the AGFD Executive Committee for their unrelenting support. The division can look forward to a progressive year ahead when I hand over the baton to Jason.

I am looking forward to seeing old friends, making new acquaintances and broadening my horizons in San Francisco and wish you all a socially enjoyable and scientifically enriching ACS Fall 2023. See you there!

Jonathan Beauchamp
AGFD Chair 2023
July 2023, Freising, Germany

CORNUCOPIA EDITORIAL STAFF & CONTACT INFORMATION	
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General Manager	P. White
Staff	C. Kent, L. Lane, J. Olsen

FUTURE PROGRAMS

NEW ORLEANS March 17-21, 2024

ACS Meeting Theme - The Many Flavors of Chemistry
note – call for abstracts open August 7

Chemistry of Alcoholic Beverages Nick Flynn nflynn@wtamu.edu (YCC)

Sensory Beyond Earth: The Relevance of Flavor Chemistry in Space Exploration Julia Low julia.low2@rmit.edu.au Scott McGrane scott.mcgrane@effem.com Jonathan Beauchamp jonathan.beauchamp@ivv.fraunhofer.de Neil Da Costa neil.dacosta@iff.com

Extraction & Biotechnology: A Natural and Sustainable Future for Flavors Elizabeth Kreger elizabeth.kreger@sensient.com Lewis Jones lewis.jones@sensient.com Xiaofen Du xdu@twu.edu

Mycotoxins: Challenges and Future Perspectives Hans-Ulrich Humpf humpf@uni-muenster.de Lauren Jackson Lauren.Jackson@fda.hhs.gov

Flavor Preferences of Companion Animals Scott McGrane scott.mcgrane@effem.com Jonathan Beauchamp jonathan.beauchamp@ivv.fraunhofer.de

Agnes Rimando Memorial International Student Symposium Michael Tunick mht39@drexel.edu Roberta Tardugno roberta.tardugno@uniba.it

Michael Granvogl Memorial Symposium Jonathan Beauchamp jonathan.beauchamp@ivv.fraunhofer.de Yu Wang yu.wang@ufl.edu Xiaoting Zhai xiaotingzhai@ahau.edu.cn Roberta Tardugno roberta.tardugno@uniba.it

Food Security: Tackling World Hunger - CCC highlighting chemistry across AGRO, ANYL, ENVR divisions Kenny Xie kyx@usp.org Mike Morello mjmorello226@gmail.com

Toward Precision Nutrition – A Holistic View of Relationships Between Food, Food Components Contributing to Taste, Aroma, Color and the Gut Microbiome in Health Promotion Tom Wang tom.wang@usda.gov LinShu Liu linshu.liu@usda.gov Karley Mahalak karley.mahalak@usda.gov

General Papers (oral) Jason Soares Jason.w.soares.civ@army.mil Elizabeth Kreger elizabeth.kreger@sensient.com

General Posters/Undergraduate Poster Competition Jason Soares Jason.w.soares.civ@army.mil Elizabeth Kreger elizabeth.kreger@sensient.com Kathryn Deibler kdd3@cornell.edu

Pairing Flavors with Health and Wellness Food Products Xiaofen Du xdu@twu.edu Danhui Wang dwang4@twu.edu

Food Allergen Characterization, Modification and Detection Qinchun Rao qrao@fsu.edu Chris Mattison chris.mattison@usda.gov

Withycombe-Charalambous Graduate Student Symposium Kathryn Deibler kdd3@cornell.edu Jason Soares Jason.w.soares.civ@army.mil Elizabeth Kreger elizabeth.kreger@sensient.com

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DENVER August 18-22, 2024 | ACS Meeting Theme – Elevating Chemistry

Honoring Professor Chi-Tang Ho on the Occasion of his 80th Birthyear Fereidoon Shahidi fshahidi@mun.ca Ronald B. Pegg rpegg@uga.edu Liangli (Lucy) Yu lyu5@umd.edu Shengmin Sang ssang@ncat.edu

Chemistry and Health of Highly Processed Foods Alyson Mitchell aemitchell@ucdavis.edu Fereidoon Shahidi fshahidi@mun.ca

Processing and Storage Induced Toxins Lauren Jackson Lauren.Jackson@fda.hhs.gov Liangli (Lucy) Yu lyu5@umd.edu Alyson Mitchell aemitchell@ucdavis.edu

Cellular Agriculture Jianping Wu jwu3@ualberta.ca

Alternative Foods or Plant-based & Alternative Food Protein Lingyun Chen lingyun.chen@ualberta.ca

Chemistry of Aroma and Taste Modification Robert McGorrin robert.mcgorrin@oregonstate.edu

Micro/Nanoplastics in Food and the Need for Developing Biodegradable Polymers Changqing Wu changwu@udel.edu Xuetong Fan Xuetong.fan@usda.gov

CCC – ACS Microbiome Research Consortium Tom Wang tom.wang@usda.gov LinShu Liu linshu.liu@usda.gov Karley Mahalak karley.mahalak@usda.gov

JAFC Best Paper Award Thomas Hofmann jafc@jafc.acs.org William King WKing@acs-i.org Jason Soares Jason.w.soares.civ@army.mil

Young Scientist Award Youngmok Kim youngmok.kim@finlays.net

Spencer Award Michael Appell michael.appell@gmail.com Michael Morello mjmorello226@gmail.com

SAN DIEGO March 23 – 27, 2024 | ACS Meeting Theme – TBD

3rd Global Symposium on the Chemistry and Biological Effects of Maple Food Products Hang Ma hang_ma@uri.edu Navindra Seeram nseeram@uri.edu

James Seiber Memorial Symposium Alyson Mitchell aemitchell@ucdavis.edu

Executive Committee Meeting Minutes

Sunday, 3/26, 3:00-5:00 PM Indianapolis, Indiana and Zoom

Attendees: Alyson Mitchell, Jonathan Beauchamp, Elyse Doria, Michael Appell, Nick Flynn, Lucy Yu, Neil Da Costa, Jun Hu, Fereidoon Shahidi, Robert McGorrin, Michael Morello, Mike Tunick, Jane Lealand, Liz Kreger, Jason Soares, Michael Qian, Natasa Poklar, Lingyun Chen, LinShu Liu, Lauren Jackson, Jianping Wu, Joulain ??, Stephen Toth, Jianping Wu, Kenny Xie, Keith Cadwallader

Jonathan Beauchamp called the meeting to order at 3:11 PM (EST
The **minutes** of the previous Executive Committee meeting were approved with no changes and are published in the Spring 2023 Cornucopia.

Michael Tunick summarized the **Special Topics** meeting**.** A proposal by Michael Tunick and LinShu Liu for organizing a Board of Advisors (senate) of long-term AGFD members (ex-officers) was discussed. The Board should provide advice to the AGFD Executive Committee and the Subdivisions, but will have no formal governance over the Division. Michael Tunick and LinShu will work on clarifying and further establishing the membership, terms and objectives of the Board. MPGG announced that beginning 2025, the Spring meetings will emphasize in-person attendance, whereas the Fall meetings will emphasize international and virtual attendance, with inter-divisional co-organized symposia being encouraged by ACS.

Stephen Toth gave the **Treasurer's Report**. The division has had little activity over the past year. The Division has four major investment accounts totaling $744,753. In addition, there is a little over $200,000 in cash assets, which include allocations for the Indianapolis's meeting ($25,000), the CCC grants, and the Strategic Planning meeting ($67,000). The

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Division usually spends $110,000 annually and strives to keep $500,000 in reserve to be fully operational for three consecutive years (based on approximately $150,000 expenditure per year). The Division has $986,640 in total assets and is financially healthy. A budget of $40,000 was set and approved for the 2023 fall meeting in San Francisco.

The **Awards Committee Report** was given by Mike Morello. Awards are published in Cornucopia. Mike indicated that the Division needs to identify an individual to be responsible for award solicitations as the Division is not getting enough nominations for awards. For example, there were no nominations for the **Young Industrial Scientist Award**, which was initiated prior to the COVID-19 pandemic. The committee agreed to keep giving this award, but recognizes the need to engage more members with publicizing the award. Anybody interested in helping with award solicitation should let Michael Morello know. The committee agreed that in order for an individual to qualify for the **Young Industrial Scientist Award** they will need to have been a full member of ACS and AGFD Division member for a minimum of 3 years. The committee also agreed that nominations for the award would be carried over for 1 year after submission (similar to other Division awards). Michael Morello also suggested that we add an agenda item for the Fall meeting to focus on ways to re-engage the industry member base. The 25-year service awards were last given in 2017 due to the COVID-19 pandemic. The Division currently has over 100 members that have reached the 25-year service milestone, and many that have reached their 50-year service anniversary. Michael Morello will reach out to ACS membership and will work with Michael Qian to get our honored 25-year members pins. Ball caps or scarfs will be given to our members with 50-year service anniversaries. Congratulations were extended to **Liangli (Lucy) Yu, Ph.D**., Distinguished University Professor, Department of Nutrition and Food Science, University of Maryland in receipt of the **Award for the Advancement of Application of Agricultural and Food Chemistry**; to **Xiaonan Sui**, PhD Professor, Associate Head, Department of Cereals, Oils and Vegetable Protein Engineering, College of Food Science, Northeast Agricultural University, China in receipt of the **Young Scientist Award**; and to **Kaidi Wang**, Department of Food Science and Agricultural Chemistry, Macdonald Campus McGill University in receipt of the **Roy Teranishi Graduate Fellowship in Food Chemistry**. The committee also warmly congratulated **Fereidoon Shahidi**, Ph.D., FACS, FAGFD-ACS, FAOCS, FCIC, FCIFST, FIAFoST, FIFT, FISNFF, FRSC (UK), University Research Professor and Distinguished Scholar, Department of Biochemistry, Memorial University of Newfoundland for receiving the **IFT: Lifetime Achievement Award in honor of Nicolas Appert**.

The **Journal Report** was given by Lucy Yu. The chosen JAFC-AGFD best article of the year was titled "Sweet Biotechnology: Enzymatic Production and Digestibility Screening of Novel Kojibiose and Nigerose Analogues" by authors Shari Dhaene, Amar Van Laar, Marc De Doncker, Emma De Beul, Koen Beerens, Charlotte Grootaert, Jurgen Caroen, Johan Van der Eycken, John Van Camp, and Tom Desmet. This paper will be presented at the Fall 2023 meeting in San Francisco. The first author has already submitted their abstract to the meeting.

The Division's 2023-2025 new student representative to the Executive Committee, Elyse Doria was introduced and gave the **Student Committee Report**. Elyse is planning a lunch with the student membership during the meeting in Indianapolis and will be engaging with all student presenters at the poster session. Elyse had AGFD stickers made to hand out to students during the poster session. She will reach out to Kathryn Diebler regarding reinitiating the Twitter account, and will post pictures taken during the meeting.

LinShu Liu gave the **Program Report**. The Division featured 20 AGFD hybrid symposia on a broad range of topics that included 207 oral presentations and 89 posters at the Fall 2022 national meeting in Chicago, Il. The Spring meeting was also a great success featuring 12 symposia comprising 19 sessions (6 in-person, 6 hybrid and 7 virtual), two of which were interactive virtual panel discussions. There were 119 oral presentations and 57 posters.

The **Future Programs Report** was given by Jonathan Beauchamp. The Division has 22 symposia planned for the Fall 2023 meeting in San Francisco, and 103 abstracts have already been submitted. There are currently 16 symposia scheduled for the 2024 Spring Meeting, in New Orleans, LA. The theme of the NOLA meeting is *The Many Flavors of Chemistry (*Neil Da Costa is the Thematic Program Chair). Division programming is well aligned with this theme. Alyson Mitchell will reach out to Gavin Sacks to see if he is planning on holding the C4 competition. There are 10 symposia currently planned for the Fall 2024 meeting in Denver, CO including the Agnes Rimando Memorial International Student Symposium. The Spring 2024 meeting will include the Michael Granvogl Memorial Symposium and AGFD will also be featuring two ASC Convergent Chemistry Community (CCC) symposia at this meeting in alignment with the U.N. Sustainable Development Goals (SDG-2) of Zero Hunger. Kenny Xie and Michael Morello are coordinating a symposium in collaboration with the AGRO, ANYL, and ENVR Technical Divisions titled: **CCC- Food Security:**

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Tackling Hunger, and Tom Wang, LinShu Liu, and Karley Mahalak will be hosting a workshop and symposium titled

CCC-ACS Microbiome Research Consortium. Michael Qian indicated that the International Flavor Conference will be held in New Zealand sometime in 2024 (no date is yet set). Contact Michael Qian for more information.

No reports were given for the **Flavor, Functional Foods & Natural Products, Food Bioengineering** or **Food Safety, Diet and Gut Microbiome, or Nutrition Subdivisions** at the meeting. Jonathan Beauchamp will reach out to subdivision leaders to get email reports and to remind them that they are required to present a Subdivision Report at both the Spring and Fall Executive Committee meetings.

Karley Mahalak gave the **Nutrition and Gut Microbiome Subdivision Report**. The subdivision had a very successful symposium last year, and will be hosting a kick-off symposium for this next year.

Wunmi Omowun gave the **Sustainability & Green Technology Subdivision Report**. The Subdivision held a symposium with over 60 participants as well as a webinar last year. They have three sessions on Food Sustainability at this meeting and have plans for symposia next year.

The **Councilors Report** was given by Michael Tunick and Lauren Jackson. Michael indicated that ACS is moving towards harmonizing between all Divisions. ACS leadership is proposing change beginning Spring 2025. Proposed changes include having half of the Divisions' allotment contingent upon joint programming; and having the Spring meeting emphasize in-person symposia and the Fall meeting emphasize virtual and international participation. Items that will be considered at this year's Council meeting will include: Converting one of the six *Director at Large* positions into an *International District Director*, and dropping the age requirement for Emeritus members and basing it on service only (35+ years).

The **Nominations Report** was given by LinShu Liu. The nomination committee recommends Professor Coralia Rosa Osario, University of Columbia as the 2024 Vice-Chair. Alyson Mitchell and Stephen Toth were both nominated to continue in their roles as Division Secretary and Division Treasurer for 2024. The Division will need to vote for two Councilors as Alyson Mitchell and Lauren Jackson's terms end December 31, 2023. Both have indicated a desire to serve an additional term. The Division will also need an Alternate Councilor as Keith Cadwalladers term is also ending in December 2023. Keith has indicated that he does not want to continue in this role. Brian Guthrie will be put forward as a candidate for the position. The Division bylaws allow for electronic balloting. The deadline for the voting is November. Alyson asked that another Executive Committee member run the balloting to avoid any potential conflict of interest. The deadline for identifying Subdivision chairs and new leadership is July 15, 2023. LinShu will reach out to current Subdivision Chairs and help them meet this deadline.

The **Cornucopia Report** was given by Alyson Mitchell. An electronic version of the Cornucopia was sent out to members via email and 100 hard copies were printed for the Spring meeting.

The **Hospitality/Public Relations Report** was given by Alyson Mitchell who indicated that a Chair's Reception was

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From the Spring 2023 AGFD Chair's Reception (photo credit G. Tunick)

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being held at Buca Di Beppo on Tuesday, March 28, 2023 from 6:00-8:00 PM and all are encouraged to join.

Michael Qian gave the **Membership Report**. Although membership has declined from our pre-Covid peak of over 3,000, the membership decline seems to have stabilized. Current Division membership is 1923.

Mike Appell gave the **Communications Report** and indicated that our website is primarily accessed from individuals across North America (based upon website hits). Alyson will be working with Michael to migrate our email list to the new website as it has better email capabilities for mail-outs. There was discussion regarding the best way to achieve a seamless transition. A membership list will be obtained from ACS and used as the new email list as it is current. Once everything is migrated, Alyson will send out a notice via the old Listserv letting recipients know that the Listserv will be discontinued and reminding them to update membership so they will still get monthly Division emails. Alyson Mitchell asked that everyone send her updates for the newsletter at least one week in advance of the end of the month.

In **New Business**, Kenny Xie discussed how to enhance awareness of the Convergent Chemistry Community (CCC) initiative, and how to link it to Facebook, and other channels to broadcast the event. Michael Morello indicated that this program fits well with the goals of the Sustainability & Green Technology Subdivision, and that the Division should work more with our partner Divisions (AGRO, ENVR) and promote co-programming symposia. The ACS initiative is in support of the U.N. Sustainable Development Goals, and includes goal #2 of Zero Hunger. ACS has a new Center for Sustainability, and wants to highlight the work chemists are involved in to reduce hunger. Our Division is well positioned to support this effort. Michael Qian included his experience with the ACS campaign on a Sustainable Future, which addressed reducing waste through sustainable packaging. Wunmi Omowun indicated that the Sustainability & Green Technology Subdivision is very interested in supporting the wider ACS efforts on sustainability.

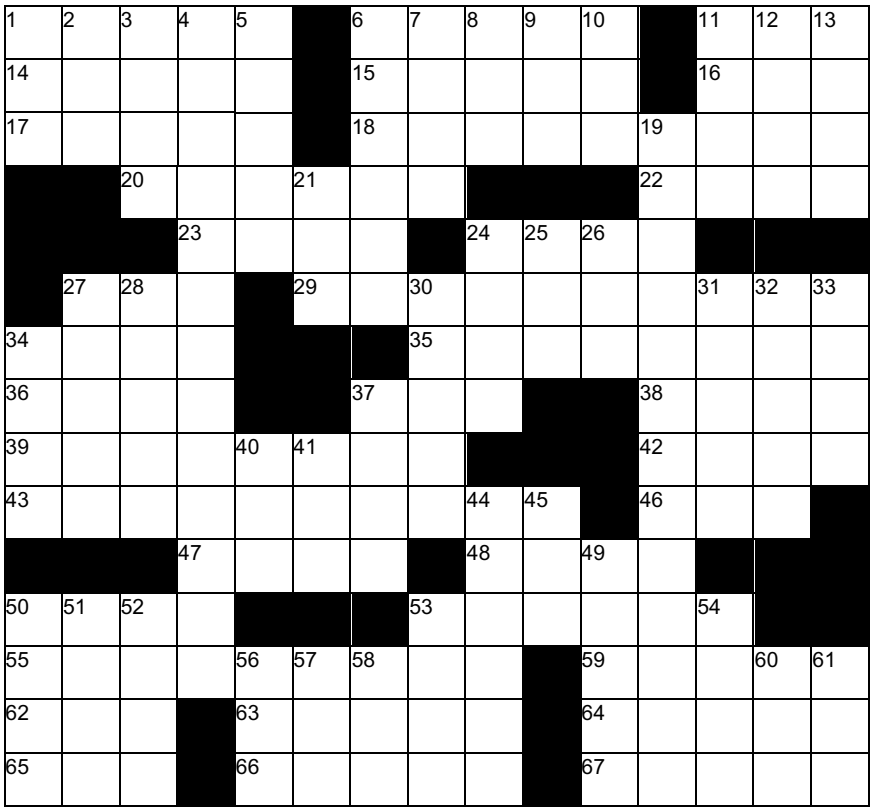
The meeting adjourned at 5:05 PM (EST). *Minutes submitted by Alyson Mitchell*

In Memorium

Jim Seiber
1940 – 2023

James N. Seiber, Jim, born in 1940, passed away peacefully at home surrounded by his loving family while leaving behind a long list of accomplishments, friends and colleagues. He began his studies, earning a B.S. in Physics at Bellarmine College in Louisville, Kentucky. He continued with an M.S. in Chemistry at Arizona State and obtained his Ph.D. in Analytical Chemistry at Utah State University. He worked at Dow Chemical in Michigan and California before joining the University of California at Davis faculty in 1969, eventually becoming Professor of Environmental Toxicology. He led the Departments of Environmental Toxicology and Food Science and served as Associate Dean for Research for the UC Davis College of Agricultural and Environmental Sciences (CA&ES). His significant and impressive research on pesticides, their use, analysis and environmental impact led to over 280 publications, 3 ACS Symposium Series books, numerous presentations as part of AGFD and other technical symposia and participation on expert committees around the world. Dr. Seiber served as a leading expert for the World Health Organization addressing the impact of pesticides on the health of both youths and adults. He served as Editor of the Journal of Agricultural and Food Chemistry (1999-2014) successfully stewarding it into one of the most respected scientific journals in the field. Along with his academic efforts at UC Davis, Jim led the Center for Environmental Sciences and and Engineering at the University of Nevada, Reno and served as Director of the USDA Western Regional Research Center from 1998-2010. Jim and his wife Rita have three sons, Chuck, Chris, and Kenny and seven grandchildren. Jim received a long list of awards reflecting the impact of his work, including – Fellow of ACS Agrochemicals Division (1988), AGFD Fellow (2006), ACS Fellow (2010), AAAS Fellow (2013), Kenneth A. Spencer Award (2012), USDA Sterling B. Hendricks Memorial Lecture (2018) and the CA&ES Award of Distinction (2018). He served on the UC Davis Foundation Board of Trustees and funded the James and Rita Seiber Fellowship for Innovation in International Agricultural Research and the James, Rita Seiber International Graduate Student Award and the James and Rita Seiber Agricultural and Environmental Chemistry Fellowship. He is remembered as an optimistic, kind and thoughtful friend, mentor and colleague. His many co-workers, collaborators and friends at AGFD miss him and extend condolences to his family. *(thanks to Wally Yokoyama for preparing this memorium)*

FRISCO FUN



A prize to the first send a correct solution to Carl Frey (via smartphone photo/e-mail) at - cfreyenterprise@gmail.com

ACROSS

1 Hey, listen to this!
6 R2-D2 or C-3PO
11 Scanning pros
14 Target of Salk vaccine
15 __ *of Two Cities*
16 *Nightmare on __ Street*
17 Show jubilation
18 End of semester test
20 NL team of Oracle Park
22 Doubled
23 Board game with a rope
24 Dudley Do-Right org.
27 Theater candy: __-Caps
29 Realistic
34 Chicken Chow __
35 Chromosome protein support or greeting to Jagger and Richards
36 Aired via the tube
37 Word-based 'Dad' joke
38 Harvest wheat or rye
39 Definitely before.
42 Pretentious cultured air
43 Fluent in three languages
46 Sporty Audi 2 seaters
47 We should definitely do it
48 __-tiller or __-Rooter
50 Wile Coyote's suppier
53 Levi's Stadium NFL team
55 Classic peanut butter taffy or black strapped shoes
59 What the middle letter of 41 DOWN stands for
62 A holiday's night before
63 Just love to bits
64 More confident
65 '98 flim:*Waking__Devine*
66 Mount, as a horse
67 Portray emotion on stage

DOWN

1 EMT safety equipment
2 Red or White of MLB
3 Slimy shell-less mollusk
4 High tech home to Apple, Google & Meta
5 Complete. Sum up.
6 Huck Finn or Tom Sawyer
7 Elisha of ups and downs
8 Outlaw. Forbid.
9 Motor__ or Victr__
10 Business card abbrev.
11 Don't do this while you drive
12 BBQ side dish
13 BBs or snowballs
19 Science, technology and arts museum on Pier 15
21 Pecan or almond
24 Horse control leather strap
25 100th parts of dols
26 Parisian witticism: bon __
27 Tijuana gentlemen address
28 Al Capone associate Frank__
30 Highest point of Mt. Kilimanjaro
31 Like xenon, neon or argon
32 Acts of strength and skill
33 Annual award from ESPN
34 High end pen: __ Blanc
37 Cribbage board inserts
40 Old expression of disgust
41 Explosive $C_7H_5N_3O_6$
44 Out of bed
45 'Man of 1000 Faces' Chaney
49 Present or past for example
50 You said it, Brother
51 Spelunker's realm
52 Droll TV horse of the '60's
53 He fiddled while Rome burned
54 AL MLB player from 'oustan
56 TV show about USN court prosecutors
57 Gator __
58 Do or do __. There is no try!
60 Phrase on some beverage bottles: No DEP, No __
61 Miner's quest

AGFD DIVISION MEMBERSHIP APPLICATION

The Agricultural and Food Chemistry Division (AGFD) of the American Chemical Society (ACS) is a non-profit organization dedicated to the technical advancement of all aspects of agricultural and food chemistry. AGFD encourages technical advancement in the field by -
- organizing symposia/workshops on agricultural/food chemistry at ACS national meetings and other venues
- publishing proceedings of AGFD symposia
- publishing the *Cornucopia* newsletter
- updating members several times a year via e-mail blasts
- hosting social and networking gatherings at ACS national meetings
- providing cash awards and recognition to leading undergraduate and graduate students, young scientists and established scientists in the field of agricultural and food chemistry

At ACS National Meetings you can discuss division activities at the AGFD information table located near the AGFD technical session rooms. Join >1900 AGFD members via the application form (below) or on-line at www.agfoodchem.org or www.acs.org (click on Communities, Technical Divisions, Technical Division List) or call ACS (800)333-9511 (in US) or 616-447-3776 (outside US). Payment by Visa/MasterCard or AmEx.

Check out AGFD on You Tube: https://www.youtube.com/watch?v=CyBMAnOuFKE

	APPLICATION FOR AGFD DIVISION MEMBERSHIP (7623P)
Title	
Name	
1st address line	
2nd address line	
City	
State	
Zip code	
Country	
e-mail address	
Phone	
check one	**MEMBERSHIP FEE**
[ ]	I am an ACS member and wish to join AGFD ($10.00)
[ ]	I am not an ACS member and wish to join AGFD ($15.00)
[ ]	I am a full-time student and wish to join AGFD ($10.00)
Be cool **J O I N** **A G F D**	Return application, with payment (payable to American Chemical Society), to AGFD Membership Chair: Michael Qian, Professor Department of Food Science and Technology Oregon State University Corvallis OR 97330

ROSTER OF AGFD OFFICERS & COMMITTEE LEADERSHIP

Chair - Serves 1 year. Preside over Division meetings & appoint committees
Jonathan Beauchamp
Fraunhofer Institute
jonathan.beauchamp@ivv.fraunhofer.de

Chair-Elect - Serves 1 year. Substitute for the Chair as needed
Jason W. Soares US Army DEVCOM Soldier Ctr Jason.w.soares.civ@army.mil

Vice-Chair - Serves 1 year. Assist Chair-elect. Develop future technical programs.
Liz Kreger Sensient Flavors & Extracts
Elizabeth.Kreger@sensient.com

Secretary - Responsible for Division correspondence and meeting minutes.
Alyson Mitchell
University of California, Davis
aemitchell@ucdavis.edu

Treasurer - Responsible for Division finances.
Stephen Toth III
International Flavors & Fragrances R&D
Union Beach NJ stephen.toth@iff.com

Cornucopia Editor - Edit newsletter.
Carl Frey cfreyenterprise@gmail.com

Councilors - Represent Division for 3 years on ACS council.
Alyson Mitchell (thru '23)
aemitchell@ucdavis.edu
Lauren Jackson (thru '23)
lauren.jackson@fda.hhs.gov
Michael Tunick (thru '24)
mht39@drexel.edu

Website - Maintain web site.
Michael Appell
michael.appell@ars.usda.gov

Student Activities - Attract and retain graduate/undergraduate student membs.
Elyse Lauren Doria, eldoria@ucdavis.edu

Nominations - Develop officer slate. Served by immediate past chair.
LinShu Liu USDA-ARS-ERRC
linshu.liu@ars.usda.gov

Finance - Monitor Division's finances. Served by immediate past chair.
LinShu Liu USDA-ARS-ERRC
linshu.liu@ars.usda.gov

Hospitality - Organize receptions and banquets. Alyson Mitchell
aemitchell@ucdavis.edu

Alternate Councilors - Substitute for Councilors. Serves 3 years.
Keith Cadwallader (thru '23)
cadwlldr@uiuc.edu
Kathryn Deibler (thru '24)
kdd3@cornell.edu
Michael Qian (thru '24)
Michael.qian@oregonstate.edu

At-Large Executive Committee Members - Assist in Div. management. Serves 3 years.
Jane Leland (thru '23)
JLelandEnterprises@gmail.com
Robert McGorrin (thru '23)
robert.mcgorrin@oregonstate.edu
Bosoon Park (thru '24)
bosoon.park@usda.gov
Brian Guthrie (thru '24)
Brian_Guthrie@cargill.com

Awards - Oversee awards process.
Chair Michael Morello
mjmorello226@gmail.com
Fellow Awards Fereidoon Shahidi
fshahidi@mun.ca
Young Scientist Award
Youngmok Kim
youngmok.kim@finlays.net
Teranishi Fellowship
Liangli (Lucy) Yu lyu5@umd.edu
Student Awards
Kathryn Deibler kdd3@cornell.edu
Canvassing
Stephen Toth, stephen.toth@iff.com
Young Industrial Scientist Award
Michael Morello
mjmorello226@gmail.com

Multidisciplinary Program Planner
Help coordinate nat'l mtg programs
Neil Da Costa International Flavors & Fragrances neil.dacosta@iff.com

Public Relations – Publicize Div.
Alyson Mitchell,
aemitchell@ucdavis.edu

Membership - Recruit and retain Division members. Michael Qian
michael.qian@oregonstate.edu

Agriceutical Sub.Div.
Chair, Daxi Ren dxren@zju.edu.cn
Ch-elect, Hyunsook Kim
Hyunsk15@henyang.ac.kr
V-Chair, Yuzhu Zhang
yuzhu.zhang@usda.gov
Secretary, Ying Wu ywu@Tnstate.edu

Food Bioengineering Sub.Div.
Chair, Majher Sarker
Majher.Sarker@usda.gov
Chair-Elect, Kwang-Guen Lee
kwglee@dongguk.edu
Vice-Chair, Hongsik Hwang
hongsik.hwang@usda.gov
Secretary, Changqin Wu,
changwu@udel.edu

Flavor Sub.Div.
Chair, Gal Kreitman
Gal.Kreitman@ejgallo.com
Chair-Elect, Xiaofen Du xdu@twu.edu
Vice-Chair, Coralia Osorio Roa
cosorior@unal.edu.co
Secretary, Joonhyuk Suh J.Suh@uga.edu
Yun Yin, yunyin2@vt.edu (2024)

Food Safety Sub.Div.
Chair, Reuven Rasooly
rueven.rasooly@ars.usda.gov
Chair-Elect, Xiaonan Lu
xiaonan.lu@mcgill.ca
V.Chair, Boyan Gao
gaoboyan@sjtu.edu.cn
Secr'y, Vivian Wu, vivian.wu@usda.gov

Functional Food/Nat. Product SubDiv
Chair, Jianping Wu Jwu3@ualberta.ca
Chair-Elect, Kenny Xie KYX@usp.org
Vice-Chair, Yingdong
Zhu,yzhu1@ncat.edu
Secretary, Khizar Hayat
khizaraura@gmail.com

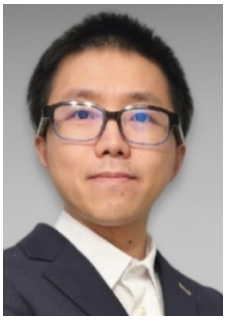
Nutrition & Gut Microbiome Sub.Div.
Chair, Karley Mahalak
Karley.mahalak@usda.gov
Chair-elect, Laurel Doherty
Laurel.a.doherty.civ@mail.mil
Vice-Chair Ida Pantoja-Feliciano
Ida.g.pantojafeliciano.civ@mail.mil
Secretary Tom Wang,
Tom.wang@usda.gov

Sustainability/Green Tech. Sub.Div.
Chair, Vinka Oyanedel-Craver,
craver@uri.edu
Chair-Elect, Yufeng Jane Tseng
yjtseng@csie.ntu.edu.tw
Vice-Chair, Lingyun Chen
lingyun.chen@ualberta.ca
Secretary, Omowunmi "Wunmi" Sadik
sadik@njit.edu

AWARD NEWS

Liangli (Lucy) Yu, Ph.D., Distinguished University Professor, Dept. of Nutrition and Food Science, University of Maryland won the 2023 **Award for the Advancement of Application of Agricultural and Food Chemistry**. This award (sponsored by International Flavors and Fragrances, Inc.) recognizes outstanding contributions to pure and applied agricultural and food chemistry. The award celebrates Prof. Yu's research in three areas: nutraceuticals and functional foods, chemical aspects of food safety, and analytical technologies to ensure food integrity. Dr. Yu's leadership resulted in her group reporting for the first time: the free radical scavenging components in wheat grain, natural antioxidants and anti-inflammatory components from seed flours – previously a waste stream, free radical properties of conjugated linoleic acids (CLA) - different reactions of CLA isomers with DPPH radicals, prevention of peroxidation of ω-3 fatty acids EPA and DHA during procession and storage by extracts of Chardonnay grape and back raspberry seeds, free radical generation and mediation 3-MCPD diesters from diacylglycerol under high temperature and low moisture conditions, and Fe^{2+}/Fe^{3+} catalysis of 3-MCPD ester formation reactions. Lucy and her team also devised new methodology for detecting milk adulteration by combining chromatographic fingerprints with statistical analysis, and devised a novel approach to detect unknown food toxicants by combining cultured kidney cells and hepatocytes with chemometric analyses. Professor Yu has mentored 17 Ph.D. and 12 MS students, 1 junior faculty, 24 visiting professors/scholars/Ph.D. students and 12 undergraduate students. She has authored 289 peer reviewed journal articles, 18 book chapters, 2 edited 5 books, translated 1 book, holds 3 patents, 9 patent applications, 6 Invention disclosures and delivered >100 invited or peer reviewed presentations. Dr. Yu is a Fellow of the ACS, AGFD and IFT. Among her many other awards are the 2008 AGFD Young Scientist Research Award and the 2020 Stephen S. Chang Award for Lipid or Flavor Science from IFT.

Xiaonan Sui, Ph.D. Professor, Associate Head, Dept. of Cereals, Oils and Vegetable Protein Engineering, College of Food Science, Northeast Agricultural University, Harbin, China received the 2023 **AGFD Young Scientist Award**. Prof. Sui's research focuses on how food processing parameters impact soy protein conformation and how soy proteins aggregate/self-assemble in multiple dimensions. He developed a cost-efficient and fiber-rich extrusion method to develop soy-protein based meat alternatives. Engineering soy protein-based connective layers (epimysium and perimysium) enabled him to overcome a key challenge in developing whole cut meat alternatives. He has published 144 peer-reviewed papers, has one patent pending, edited one book and authored two books in English. His research has been cited more than 3200 times.



Zhuohong (Kenny) Xie, Ph.D. Principal Scientist, US Pharmacopeia, Rockville, MD is the inaugural recipient of the **AGFD Young Industrial Scientist Award**. This award recognizes and highlights important contributions that early career industrial chemists make in our field. Dr. Xie's work focuses on creating and applying methods and standardized documents that ensure the safety, authenticity and efficacy of foods, ingredients and additives. He played a lead role in Expert Panels that developed non-targeted methods and standards for milk ingredients and dietary protein. He developed >12 standards and 3 sets of reference materials. Dr. Xie developed an in vitro model for carbohydrates; optimizing reagents, apparatus, and conditions to simulate digestion. He developed and validated analytical methods to detect adulterants in food proteins, oils and spices. Kenny is the AGFD Functional Foods & Natural Products subdivision Vice-Chair; he co-organized multiple symposia at national meetings;and he led proposal development and coordinates the AGFD led Food Security/Tackling Hunger Convergent Chemistry Community which includes AGRO, ANYL and ENVR. Dr. Xie holds two patents and has 39 peer-reviewed publications.

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MORE AWARD NEWS

Shiming Li, Ph.D., Huanggang National University, Hubei Province, P.R. China and **Rickey Y. Yada**, Ph.D., University of British Columbia, Traditional Ancestral Unceded xʷməθkʷəy̓əm Musqueam Territory, Vancouver, Canada each received a 2023 **AGFD Fellow Award**.

Kaidi Wang, Dept. of Food Science and Agricultural Chemistry, McGill University (advisor Xiaonan Lu) received the 2023 **AGFD Roy Teranishi Graduate Fellowship in Food Chemistry**. This honor goes to a beginning graduate student with an outstanding graduate GPA who shows promise of an excellent research career.

The following loyal members of AGFD marked **25 Years of Membership in AGFD** in 2023: **Douglas Armstrong, Milda Embuscado, Clayton Ericson, David Gang, Joseph John Karchesy, Veronica M McBurnie, Jeff D McCord, Susan A S Parker, Ronald B Pegg, Alexander G Schauss, Kalidas Shetty, Ronald I Thompson, Deepthi Kumar Weerasinghe, Douglas Williams, Yan Zheng**

The following extremely loyal members of AGFD marked 50 Years of Membership in AGFD in 2023: **Rajindra Aneja, Denis Hruza**

Celina Paoletta with AGFD Chair Jonathan Beauchamp

The winners of the Spring 2023 **Undergraduate Poster Competition** included: 1st place (tie) **Celina Paoletta** of Christopher Newport University for a poster describing hop (Humulus lupulus) phytochemical profiles as a function of growth region and **Christopher Prajogo** of UC Davis for a poster describing the effect of trans vaccenic acid on glucose homeostasis in a mouse model of diet-induced obesity and insulin resistance. The 2nd place award went to **Bret Watson** and **Jordon Scalia** of Shippensburg University for a poster describing maintenance of a kombucha starter preparation. The 3rd place award went to **Kourtney Collier** of Purdue University for a poster describing plasticizing capabilities of 2 plasticizer/initiator combinations. (photo credits M. Tunick)

Christopher Prajogo with AGFD Chair Jonathan Beauchamp

The team of **Shari Dhaene, Amar Van Laar, Marc De Doncker, Emma De Beul, Koen Beerens, Charlotte Grootaert, Jurgen Caroen, Johan Van der Eycken, John Van Camp, and Tom Desmet** won the **Journal of Agricultural and Food Chemistry Research Article of the Year Award (AGFD)** for their publication Sweet Biotechnology: Enzymatic Production and Digestibility Screening of Novel Kojibiose and Nigerose Analogues. https://doi.org/10.1021/acs.jafc.1c07709

The team of **Chongxi Liu, Lu Bai, Peng Cao, Shanshan Li, Sheng-Xiong Huang, Jidong Wang, Lei Li, Ji Zhang, Junwei Zhao, Jia Song, Peng Sun, Yanyan Zhang, Hui Zhang, Xiaowei Guo, Xilang Yang, Xinqiu Tan, Wende Liu, Xiangjing Wang, and Wensheng Xiang** won the **Journal of Agricultural and Food Chemistry Research Article of the Year Award (AGRO)** for their publication Novel Plant Growth Regulator Guvermectin from Plant Growth-Promoting Rhizobacteria Boosts Biomass and Grain Yield in Rice.

AGFD and AGRO members employed by ARS/USDA, assisted in selecting **Gary List**, D.Sc., University of Illinois, Urbana-Champaign to present the prestigious 2023 **Sterling B. Hendricks Memorial Lecture** in recognition of his decades of research on soybean oil. See https://www.ars.usda.gov/research/lectures/2023/sb-hendricks/

Joel Coats, Ph.D., distinguished Professor of Entomology and Toxicology at Iowa State University is the recipient of the 2023 **Kenneth A. Spencer Award**, the most prestigious ACS award recognizing advancements in agricultural and food chemistry. A banquet organized by the Kansas City local ACS section honors him and his decades of work on natural products as insecticides and insect repellants.

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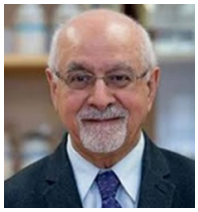
AND MORE AWARD NEWS



Fereidoon Shahidi, Ph.D., FACS, FAGFD-ACS, FAOCS, FCIC, FCIFST, FIAFoST, FIFT, FISNFF, FRSC (UK), University Research Professor and Distinguished Scholar, Dept. of Biochemistry, Memorial University of Newfoundland received the **IFT Chicago Section Nicolas Appert Lifetime Achievement Award**. Dr. Shahidi has authored >1,000 peer-reviewed research papers and book chapters, 78 books, and 10 patents. His research includes nutraceuticals and functional foods with emphasis on lipids, proteins, polyphenols, natural antioxidants and oxidation control in health and disease. He has received awards from ACS, AOCS, IFT CIFST and more. He is past chair of AGFD and the Scientific Council of IUFoST and the President-elect of the International Academy of Food Science and Technology. He is the editor-in-chief of the Journal of Food Bioactives and the Journal of Food Production, Processing and Nutrition. He is the principal founder of the International Society for Nutraceuticals and Functional Foods and founding editor in chief of the Journal of Functional Foods, serving in that capacity for 10 years. He was the principal founder of the Nutraceutical and Functional Food Division of IFT. He has trained ~200 graduate students, visiting professors, scholars and colleagues in >12 countries. See Achievement Awards – IFT.org

Xuetong Fan, Ph.D., USDA Lead Scientist/Research Food Technologist, is now an **IFT Fellow**. Dr. Xuetong Fan works in the fields of postharvest biology and technology, ionizing irradiation and other nonthermal food technologies, food quality, and microbial and chemical safety of foods. His research on the use of 1-methylcyclopropene to extend storage life of fruits and vegetables has led to its commercial application around the world. His studies on food irradiation have helped regulatory agencies make science-based decisions on the approval of irradiation of lettuce, spinach, and other products. He currently leads scientists, technicians and postdoctoral associates in developing and modifying intervention technologies, combining them with other pathogen-reduction treatments to improve microbial safety of fresh produce, while maintaining sensory and nutritional quality, chemical safety and shelf-life. He has >450 publications, including 200 peer-reviewed articles. He has served as chair of AGFD, the IFT Fruit and Vegetable Products Division and several other IFT committees. See Achievement Awards – IFT.org

AGFD congratulates all awardees and looks forward to their continued successes and contributions.

Find information about all AGFD awards at www.agfoodchem.org Scroll down to and click on AGFD Award Details to load a PowerPoint file detailing award eligibility and nomination deadlines as well as lists of past awardees.

AGFD Awards Committee: AAAFC IFF/AGFD Award (Mike Morello), Young Scientist Award (Youngmok Kim), Young Industrial Scientist Awards (Michael Morello & Brian Guthrie), AGFD Fellow Award (Fereidoon Shahidi), AGFD Distinguished Service Award (Mike Tunick), Teranishi Fellowship (Liangli [Lucy] Yu), Graduate & Undergraduate Student Symposia (Kathryn Deibler), Spencer Award (Sarah Leibowitz), ACS Fellow Award (Michael Morello, Michael Appell, Carl Frey)

Special Topics Meeting Minutes

Sunday, 3/26, 2:00-3:00 PM (EDT) Indianapolis, Indiana and via Zoom

Attendees: Alyson Mitchell, Jonathan Beauchamp, Elyse Doria, Michael Appell, Rickey Yada, Nick Flynn, Lucy Yu, Nigel Da Costa, Jun Hu, Fereidoon Shahidi, Robert McGorrin, Michael Morello, Mike Tunick, Jane Leland, Liz Kreger, Jun Hu, Jason Soares, Lucy Yu, Michael Qian, Natasa Poklar, Lingyun Chen, LinShu Liu, Lauren Jackson, Jianping Wu

The meeting started: at 2:04 PM

LinShu and Michael Tunick proposed organizing a Board of Advisors (senate) of mature AGFD members with the objectives of providing advice to the AGFD Ex. Committee and the subdivisions through their combined institutional knowledge and to act as a resource for the Ex. Committee, but not act as formal governance for the Division.

Action Item: Michael Tunick and LinShu will work on clarifying and further establishing the membership, terms and objectives of the Board.

Lucy Yu asked about having the *Exemplary Leadership* award annually as designed. Michael Morello indicated that it is a regular award, but that we need the individual present at the meetings and with COVID-19 this has been difficult.

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Action Item: The committee will have plaques made and restart giving the award on a regular basis.

Neil Da Costa indicated that at the MPGG meeting it was announced that the Spring and Fall meetings of 2025 will change slightly with differentiated formats between the two meetings. The Spring meetings will be more tailored to in-person attendance whereas the Fall meetings will emphasize international and virtual relationships. Furthermore, ACS intends to reduce the overall number of symposia in the Fall meetings and encourage a greater number of inter-divisional symposia (not nominal co-sponsorship, but joint organization and hosting). Mike Morello suggested we push back on these changes, as this will limit AGFD's ability to program independently.

Lauren Jackson gave an update on the Strategic Planning retreat to be held on Oct 7, 2023 in Washington D.C. A critical mass of at least 12 AGFD members needs to convene to make this successful.

Action Item: Lauren Jackson will reach out to Jonathan with recommendations for the attendees.

Jonathan Beauchamp asked about the ACS symposium book series honorarium. Currently the Division gets a $1,000 honorarium per book, however in other Divisions the honorarium goes to the editor(s). Jonathan asserted that providing the honorarium to the editors might incentivize organizing more books for the division. Robert McGorrin also indicated that in the past the revenues helped support travel for international presenters. AGFD has actively published books in the past, thus this income stream was a welcome addition for allocation to said travel support. Challenges with publishing a book were a limited willingness of authors to contribute. Authors need more incentives to write book chapters as they are not considered equivalent to manuscripts in merit/promotion considerations.

Action Item: Michael Morello asked to have Steve Toth involved in the conversation to understand how this will impact the Division finances. *Minutes submitted by Alyson Mitchell*

AGFD TECHNICAL PROGRAM

Abstracts for these papers appear in the section after the Technical Program

SUNDAY MORNING August 13

Moscone Ctr West Rm 3010

Chemistry of Wine - Winemaking Practices and Altering Wine Chemistry E. A. Chang, G. Kreitman, G. L. Sacks, E. Tomasino, *Orgs*, *Pres.*

8:00 Introductory Remarks.

8:05 New insights on the inhibition of potassium bitartrate crystallisation in wine. **K. Bindon**, T. Reilly, A. Schulkin, E. Wilkes

8:30 Advanced monitoring and control of wine fermentations: Redox potential. **R. Runnebaum**

8:55 Winemaking practices to alter thiol and ester production in Chardonnay wines and impact to tropical fruit aroma perception. **E. Tomasino**, C. Lucas, A. Lobbi

9:20 Maillard reaction-associated flavour compounds in base and sparkling wines. **B. Kemp**, H. Charnock, J. Medeiros, G. Pickering

9:45 Intermission.

10:05 Alternative acidification methods of high pH juice and wine. **A. Botezatu**, C. Elizondo, A. Essary, A. Lyne

10:30 Wine matrix impact on smoke marker compound expression in wine. **A. Oberholster**, L.X. Lim, C. Medina Plaza, I. Arias-Perez, Y. Wen, B.P. Neupane

10:55 Sensory significance of aroma carry-over during bottling from aromatized wine-based beverages into regular wine. **U. Fischer**, J. Gottmann, J. Vestner

Moscone Ctr West Rm 3009

Food Security: The Role of Alternative Protein Sources in Addressing World Hunger Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community B. D. Guthrie, *Org.* J. W. Finley, L. Jackson, M. J. Morello, R. Yada, *Orgs*, *Pres.*

8:00 Introductory Remarks.

8:05 Protein valorization from underutilized agriculture by-products. **T. Tanaka**

8:25 Structure, extraction, and function of alternative proteins derived from plants and insects. **X. Sui**

8:45 Algae use as alternative proteins to enhance food security. **M. Hayes**

9:05 Big things come in small packages: prospects of microalgae proteins in addressing global nutrition and health challenges. **C. Udenigwe**

9:25 Intermission.

9:45 Plant-based diets: Addressing human and planetary health and sustainability. **H. Lynch**

10:05 Protein digestion and absorption: Meat analog versus meat. **D. Chen**

10:25 Alternative proteins: A religious perspective. **J.M. Regenstein**

10:50 Inspiring food systems Innovations to improve the health of people and planet. **B. van Lengerich**

11:15 Perfect day's collaborative approach to a kinder, greener future food system. **S. Sukumaran**

Moscone Ctr West Rm 3011

Methods, Data, and their Usage Towards Solving the Food Allergy Problem Y. Zhang, *Org.*, *Pres.*

8:00 Introductory Remarks.

8:05 Seed proteins of common buckwheat: A treasure trove of genetic resources contributing to hypoallergenicity. **T. Katsube-Tanaka**

8:30 Hydrolysed proteins prevent child food allergies in mice: A study on eggs and cow's milk. **B. Zeng**, H. Che

8:55 Effect of two different processing methods on the allergenicity of tropomyosin from Procambarus clarkii and its mechanism. **G. Liu**, H. Che
9:20 Atmospheric cold plasma treatment reduces Ara h 1 antigenicity and stability in roasted peanut. **K. Hsieh**, Y. Ting, J. Wu
9:45 Intermission.
10:00 Allergen cross-contact risk due to the use of shared frying oil. **L. Jackson**
10:25 Modulating the allergic immune response to cow's milk with probiotics. **J. Yang**, J. Song
10:50 Folic acid inhibits food allergic reactions in offspring rats by regulation of allergy-related immune cells. **Q. Wang**, Y. Jiang, H. Che
11:15 New pepper allergen of 2S albumins and its potential impact on nuts allergy. **H. Li**, L. Zhu, R. Wang, L. Zhu, J. Hu, F. Chen, L. Ma, R. Tang, S. Liu, K. Ni, X. Ye, Y. Zhang, J. Sun, T. Jin

SUNDAY AFTERNOON
Moscone Ctr West Rm 3010
Chemistry of Wine - Wine Chemistry Measurements
E. A. Chang, G. Kreitman, G. L. Sacks, E. Tomasino, *Orgs.*, *Pres.*
2:00 Introductory Remarks.
2:05 Oral processing of wine and temporal aroma release and perception. **M. Pozo Bayon**, C. Munoz, M. Perez-Jimenez, C. Criado
2:30 Advancements in rapid and accurate grape quality analysis using A-TEEM and machine learning. **R. Sui**, A. Gilmore, B. Blair, H. Feng, B.S. Pan, L. Chen
2:55 Role of magnetic resonance spectroscopy in the OIV digital transformation plan. **J. H. Pucheta**
3:20 Sorbent sheets coupled to direct analysis in real time mass spectrometry (DART-MS) for rapid volatile phenol analyses in grapes and wine. **G.L. Sacks**, T. Bates, A. Kalenak, B. Bergman
3:45 Intermission.
4:05 Volatile sulfur compounds in wine – from precursor investigation to novel oxathianes. X. Wang, D.L. Capone, A. Roland, **D.W. Jeffery**
4:30 Improved method for analysis of smoke glycoconjugates: a baseline study through phenological development. S.E. Mayfield, J.E. Foster, H. Feng, B.S. Pan, **B. McClure**
4:55 Curse of dimensionality in chromatography: Custom software for four-dimensional LC × LC × IM – MS data analysis. **J. Vestner**, P. Venter, A. de Villiers, U. Fischer

Moscone Ctr West Rm 3011
Methods, Data, and their Usage Towards Solving the Food Allergy Problem Y. Zhang, *Org.* L. Jackson, *Pres.*
2:00 Introductory Remarks.
2:05 Epitope mapping and cross-reactivity analysis of arginine kinases from Crassostrea angulata. F. Huan, S. Gao, L. Ni, M. Wu, M. Liu, **G. Liu**
2:30 Identification of two novel major allergens in white-fleshed and red-fleshed pitaya seeds. **M. Hao**, H. Che
2:55 Screening and characterization of shark-derived VNARs against arginine kinase from Procambarus clarkii. **Y. Yang**, X. He, T. Jin, G. Liu
3:20 Dupilumab for treatment of food-dependent, exercise-induced anaphylaxis. **L. Zhu**, R. Tang, Q. Wang, H. Li
3:45 Intermission.
4:00 IgE epitope mapping: Data, techniques, and needs. **Y. Zhang**
4:25 Mechanism of sulfated oligosaccharide from Gracilaria lemaneiformis on regulating Treg cells differentiation in allergic response. **Q. Liu**, C. Liu, Y. Zhou, W. Liu, **G. Liu**
4:50 Immune consequences of food processing. **S. Maleki**

Moscone Ctr West Rm 3009
Food Security: The Role of Alternative Protein Sources in Addressing World Hunger
Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community B. D. Guthrie, *Org.* J. W. Finley, L. Jackson, M. J. Morello, R. Yada, *Orgs.*, *Pres.*
2:00 Introductory Remarks.
2:05 Genotypes and extraction methods impact pea protein composition, structure and techno- functional properties. **L. Chen**
2:25 Legume seed storage proteins are abundant with amyloid-forming sequences. **D. Dee**
2:45 Structural and functional properties of green lentil protein isolates obtained by pH-shift and membrane ultrafiltration. **R. Aluko**
3:05 Simple post extraction approaches to the improvement of interfacial properties of pulse proteins. **J. Rao**
3:25 Effects of microalgae and mung bean protein combination on 3D printing of seafood analogs. **P. Vijayan**, D. Huang
3:45 From traditional to alternative fish analog: Considerations toward texture development in cell-cased fish. **S. Chuah**, R. Omidvar, B. Zhang, A. Odabasi, C. Sims, R.M. Schneider, A. Porras, R. Farzad
4:15 Intermission.
4:35 Effects of oil content on the structural and textural properties of cottonseed butter products. **Z. He**, S. Rogers, S. Nam, K. Klasson
4:55 Improvement of the solubility of glandless cottonseed protein isolate for fortified beverage applications. **H. Cao**, K. Sethumadhavan, s. Pelitire, Z. He, **K. Klasson**
5:15 Improving legume protein flavor and functionality with exogenous polyphenols. **A. Girard**
5:35 Molecular interactions between pea protein isolate and saccharide with various molecular mass during the course of Maillard reaction. **B. Chen**, J. Rao
5:55 Concluding Remarks.

SUNDAY EVENING
Moscone Ctr South Hall F
General Posters J. Beauchamp, J. W. Soares, *Orgs.*
[note – Monday Evening Sci-Mix includes the first 36 posters listed below (SM01-SM36)]
SM01 Post-storage aroma alteration of vacuum-packaged Virginia hops. **X. Su**, Y. Yin, Y. Xu, L. Rutto, K. Hurley
SM02 Developing chitosan particles as biocompatible carrier. H. Huang, C. Hsieh, M. Chen, H. Huang, **K. Cheng**
SM03 Chemical characterization and quantitative determination of flavonoids and phenolic acids in yerba santa (Eriodictyon spp.) using UHPLC/DAD/Q-ToF. **M. Wang**, J. Zhao, B. Avula, J. Lee, R. Upton, I. Khan
SM04 Encapsulation of anthraquinones extracted from the Aloe-vera plant into casein micelles by ultrasonication. **U. Sadiq**, H. Gill, J. Chandrapala
SM05 Polyphenols improve the biological activity and functional properties of soybean meal hydrolysates. **X. Zhang**, H. Xiao, S. Zhang, Y. Li, H. Du
SM06 Regulated competitive reactions and low carbon footprint in glycerol organosolv pretreatment integrated fast pyrolysis of lignocellulosic biomass. **Y. Zhang**, Z. Guo

SM07 Effect of ultrasound on the level of volatile compounds, total polyphenols, total flavonoids, and isoflavones in soymilk processed with microwave-roasted black soybean (Glycine max (L.) Merr). **Y. Lee**, M. Lee, K.G. Lee

SM08 Exploring the processing technology of a new healthy yogurt with Kombucha and taro. **R. Song**, H. Che

SM09 Analysis of furan and physicochemical properties in various nuts roasted with air fryer and microwave. **J. Oh**, S. Ha, K.G. Lee

SM10 Cellulose nanocrystals recycled from maple leaves as Pickering emulsion stabilizers for shrimp preservation. **C. Ji**, J. Wei, Y. Wang

SM11 Anti-inflammatory activity of extracts and two royleanone-type isomers isolated from Salvia sessei Benth. **A. Gómez-Rivera**, C. Lobato-García, A. Gallegos-García, N. Romero- Ceronio, R. López-Rodríguez, C. Barredo, M. Herrera-Ruiz, M. González-Cortazar

SM12 Citrus pesticides unmasked: A surprising discovery on their effect on heathland ladybird chilocorus bipustulatus. **A. Kaspi-Kaneti**, S. Singh, A. Protasov, R. Kaspi

SM13 Chemical marker's variation in Cecropia sp from Tabasco, Mexico. **C. Lobato Garcia**, J. Alberto-Hernandez, A. Gómez-Rivera, R. López-Rodríguez, E. Medrano-Sanchez, M. González- Cortazar, M.Á. Vilchis Reyes

SM14 Alkaline solubilization and acid precipitation (ASAP) method for green extraction of polyphenolics from fruit peels. **N. Zhan**, D. Huang

SM15 Production, purification and characterization of a local diatom fucoxanthin and polysaccharides by a spinner-flask-based photobioreactor system. **M. Wang**, C. Lin, S. Lai

SM16 Protective effect of quercetin against oxidative stress induced by ochratoxin A in hepatocyte. **H. Kim**, H. Lee, D. Ryu

SM17 Alleviative effect of resveratrol on ochratoxin A (OTA)-induced kidney damage and oxidative stress. **H. Kim**, D. Ryu, H. Lee

SM18 Iron oxide nanocatalyst-based electrochemical sensor for Rapid Detection of E. coli O157:H7. **K. Sangmin**, Y. Kim, H. Adra, D. Kang, L. Dahee

SM19 Hydrogel made from polysaccharide extracted from Antrodia Cinnomomea : characterization and application as carrier for anti-inflammatory agents. **C. Xu**

SM20 Effect of storage conditions on key odorants and quality of southern highbush blueberries (Vaccinium corymbosum). **F. Kulapichitr**, S. Walse, D. Obenland

SM21 Characterization of key aroma compounds in microgreens and mature plants of hydroponic leafy fennel (Foeniculum vulgare Mill.). **J. Liu**, S. Li, S.F. Okeefe, K. Hurley, Y. Yin

SM22 Extraction and characterization of hemp seed (Cannabis sativa) proteins by ESI QTOF LC/MS/MS. **T. Harris**, B. Syed, A. Ahmed

SM23 International bitterness units (IBU) study of bravo hop. **B. Bartholomew**, M.B. Jacobs

SM24 Reactivity and mechanism of glucose oxidoreductase DgpA from human gut bacterium Dorea sp. MRG-IFC3. **H. Kim**, **J. Han**

SM25 Marine phlorotannin from Sargassum pallidum extract attenuates particulate matter- induced skin damage by down-regulating oxidative stress and inflammatory response in HaCaT cells and zebrafish model. **W. Kim**, S. Im, H. Kang, Y. Lee, S. Lee

SM26 Marine phlorotannin extracted from Sargassum pallidum Inhibits α-MSH induced Melanogenesis in B16F10 melanoma cells and zebrafish model via CREB and ERK -associated MITF downregulation. **W. Kim**, S. Im, H. Kang, S. Lee

SM27 Biophysical properties of ampicillin-resistant Escherichia coli. **K. Dungey**, M. Schleining, F. McCoy, P. Kenney, A. Carranza-Parras, L. Sanchez Diaz

SM28 Adverse effects of titanium dioxide nanoparticles on beneficial gut bacteria and host health based on untargeted metabolomics analysis. **Y. Wu**, X. Cao, H. Du, X. Guo, Y. Han, H. Xiao

SM29 Analysis of metabolomic profiles and evaluation of biological activities of six blackberry cultivars. **Y. Wang**, H. Lee

SM30 Organic vs. conventional: A quantitative nutrition/contaminants profiling case study on elderberries. **X. Jones**, N. Bostick, S. Mahdi, M. Uy, N. Navarrete-Tindal, S. Eber, R. Mu, Q. Yang

SM31 Production of soybean protein concentrates with enhanced nutrient profile. **R. Anowar**, L. Gurrala, A. Morais

SM32 Establishment of an analysis method for Trinexapac-ethyl in livestock products. **S. Ka**, K. Hwang, Y. Kim, H. Park, S. Choi, H. Jeong, J. Moon

SM33 Residual characteristics of Sulfoxaflor in Dendranthema zawadskii and changes in the content of flavonoids. **Y. Kim**, K. Hwang, S. Ka, h. park, S. Choi, H. Jeong, J. Moon

SM34 Development of an analytical method for ferimzone and tricyclazole in brown rice: Application in pesticide spraying using a multicopter, and comparison of initial concentration depending on spreader-stickers. **S. Kim**, M. Jeong, W. Ahn, Y. Lee, H. Eun, Y. Lee, S. Kim, Y. Shin

SM35 Basic research on the construction of pesticide library database and suspect analysis using high-resolution mass spectrometry (LC-QTOF). **M. Jeong**, S. Kim, W. Ahn, Y. Lee, H. Eun, Y. Lee, S. Kim, Y. Shin

SM36 Encapsulating peppermint essential oil in chitosan particles to reducing macrophage inflammation. **Y. Tu**, Y. Ting

7:00 Development of eugenol loaded active packaging patch by electrospinning technology. **Y. Chen**, Y. Ting, J. Wu

7:00 Evaluating the effects of Taiwan lemon essential oil on skin health. **Z. Su**, Y. Weng

7:00 Reducing advanced glycation end products in bread through fortification with quercetin nanoparticles. **W. Huang**, C. Ho

7:00 Simple proteolytic enzyme enrichment process for food and cosmetic peptide production. **H. Chung**, J. Lee, H. Bang, Y. Kang, S. Jang

7:00 In situ assessment of macro/micronutrients in soil from the PVA/starch/fertilizer system. **R. Faez**, C. Souza, C. Chiaregato

7:00 Plasma activated water influenced growth and gene expression in mung bean. **Y. Chou**, Y. Ting

7:00 Site-specific carriers of neutraceuticals using pectins with different nanostructural charge distribution and structural characteristics. **Y. Kim**

7:00 New strategy for Omega-3 PUFAs protection and curcumin vectorization via water-in-oil gelled-in-water multiple emulsion. J. Vellido-Perez, E. Brito-de la Fuente, **A. Martinez-Ferez**

7:00 Effect of iota-carrageenan and environmental conditions on the stability of oil-in-water emulsions. **H. Khouryieh**

7:00 Engineering of isoprenoid pathway for production of (–)-α-Bisabolol in metabolically- engineered Saccharomyces cerevisiae. H. Hwangbo, H. Yang, T. Kim, Y. Lee, **Y. Park**

7:00 Production of azelaic acid from nonanoic acid and its esters by whole cell biocatalyst of Candida tropicalis. E. Jeong, J. Hong, J. Kim, M. Jeon, Y. Lee, **Y. Park**

7:00 Microcapsule producted with polymer blend improve the viability of probiotics and oxidation stability. **H. Shan-Ni**, Y. Ting, J. Wu

7:00 Developing water-in-cocoa butter emulsions using cellulose nanofibers hydrogel. **W. Chou**, Y. Ting, J. Wu
7:00 Effect of argon plasma pretreatment on drying rate and qualities of green tea. **Y. Lin**, Y. Ting, J. Wu
7:00 Protective effects of annatto-extracted tocotrienols on brain nerve injury in mice. H. Tsai, Y. Lin, H. Liao, C. Yang, **Y. Chen**
7:00 Using calcium-chelated soy protein isolate as emulsifier to improve the quality of almond milk. **C. Wei**, Y. Ting, J. Wu
7:00 Accurate and Reliable Analysis of Food Samples using ICP-MS. S. Sengupta, B. Surekar, R. Fussell, D. Kutscher, **A. Fornadel**
7:00 Extraction of diatom fucoxanthin with supercritical carbon dioxide optimized by response surface method. S. Lai, Y. Li, C. Lin, Y. Cheng, **M. Wang**, H. Chang
7:00 Acceleration of phytoestrogen accumulation in soy plants (Glycine max L.) by 1- aminocyclopropane-1-carboxylic acid (ACC). **S. Lee**, J. Kim, C. Kim, K. Park
7:00 Strategy for the development of plant-based high-protein foods. **H. Yano**
7:00 Narirutin-rich Celluclast extract from mandarin (Citrus unshiu) peel with anti-obesity potential. **S. Im**, H. Kang, W. Kim, S. Lee
7:00 Fucoidan extracted from Ishige okamurae ameliorates non-alcoholic fatty liver in high- fructose diet-fed mice by modulation of lipid metabolism and gut microbiota. **S. Im**, H. Kang, W. Kim, Y. Lee, S. Lee
7:00 Obtention of antioxidant peptides from pork liver through enzymatic hydrolysis with ultrasounds pretreatment. B. Rubio, L. Mora, F. Toldra, **M. Reig**
7:00 Metabolomic approach of azole fungicides in radish (Raphanus sativus): Perspective of functional metabolites. **J. Yu**, M. Song, Y. Keum, J. Lee
7:00 Using the electronic nose to help guide flavor development in chocolate protein beverages. **G. Milkova**, S. Kokkinidou
7:00 Ameliorative effect of probiotics containing product on gastrointestinal functions in loperamide-induced constipated rats. **T. Lai**, C. YI-PING, C. Wu, J. Wu, S. Shen
7:00 Optimizing the lignan extraction from oat using response surface methodology. **Y. Kim**, J. Kim
7:00 Rapid Screening of 510 Pesticide Residues in Agricultural Product by QuEChERs Method Combined with LC-QTOF and GC-QTOF. **H. Jo**, H. Heo, K. Hwang, J. Sun, J. Moon
7:00 Synthesis of avenanthramides and applications on quantitation as an analytical standard. **M. Song**, J. Yu, L. junghoon, H. Ahn, J. Lee, Y. Keum
7:00 Preparation of nanopesticides by flash nanoprecipitation using Arabic gum as green carrier. J. Yi, E. Ma, L. Li, **X. Guo**
7:00 Residual characteristics and risk assessment of chromafenozide in perilla leaves. **K. Dong Ju**, H. Young Jin, J. Kim, O. Eun Been, L. Chae Yeon, J. Kim, K. Tae Hwa, Y. Keum, K.S. Kyung
7:00 Residual characteristics of boscalid in different parts of welsh onion. **J. Kim**, K. Dong Ju, H. Young Jin, O. Eun Been, L. Chae Yeon, I. Moo-Hyeog, K. Seo Hong, K.S. Kyung
7:00 Residual characteristics of kresoxim-methyl and pyrifluquinazon in Korean goatsbeards. **O. Eun Been**, K. Dong Ju, H. Young Jin, J. Kim, L. Chae Yeon, K.S. Kyung
7:00 Validation of QuEChERS multi-residue methods for 108 pesticides in Litopenaeus vannamei using LC-MS/MS. **H. Young Jin**, K. Dong Ju, J. Kim, O. Eun Been, L. Chae Yeon, P. So Ra, M. Gwi Im, K.S. Kyung
7:00 Enhancement of anti-adipogenic activity of mandarin peel by acid hydrolysis in 3T3-L1 adipocytes. **J. Pyeon**, Y. Kim
7:00 Simultaneous LC–MS/MS quantification of 6 lignans in cereal grain, potatoes and their products. **J. Kim**, J. Pyeon, Y. Kim
7:00 Essential oil composition of Tetrapleura tetraptera (Schum and Thonn) fruit extracted by dichloromethane and hydro-distillation fraction of n-Hexane. **O. Francis**, J. Okello, R. Komakech, E. Kemigisha, S. Kirabo, E. Ssekuubwa, M. Tweheyo
7:00 Pre-processing of near-infrared spectra for multivariate calibrations. **M. Singh**, M. Berhow, S.X. Liu
7:00 Psidial C: Identification of absolute configuration through DFT calculation and its inhibition mechanism on PTP1B via kinetic analysis and molecular docking. **D. Hahn**, T. Cao
7:00 Testing of Per- and Polyfluoroalkyl Substances in the U.S. Domestic Meat and Poultry Supply. **C. Ochoa**, R. Duverna, A. Domesle
7:00 Optimization of a methodology for the extraction and quantification of policosanols by HPLC in Costa Rican sugar cane. **O. Saenz**, J. Castañeda
7:00 Capturing the quality and functional characteristics of the Greek PDO Cheese Anevato through its microbiome. **K. Papadimitriou**, M. Govari, D. Tsoliakou, M.A. Gkerekou, P. Skandamis, M. Papadelli, J. Kapolos
7:00 Implications of the quality of table olive brines in supermarkets assessed by metagenomic analysis. **K. Papadimitriou**, D. Pavlidis, K. Panousopoulos, M. Kafentzi, A. Koliadima, M. Papadelli, J. Kapolos
7:00 Evaluating the effect of mixing corn oil with oils high in antioxidants during deep frying. **T.M. Alanezi**, A. Abu-Ghazaleh, N. Dhahir
7:00 Physicochemical and sensory properties of novel high-intensity sweetener glycosylated neohesperidin dihydrochalcone. **Y. Kim**, S. Chung, J. Hong
7:00 Volatile organic compounds and amino acid composition in the rinds of cantaloupe cultivars during maturity. **G.K. Sah**, K. Crosby, V. Dadwal, B.S. Patil
7:00 Rosé wine quality impacted by storage conditions. **C. Medina Plaza**, A. DuBois, E. Tomasino, A. Oberholster
7:00 Production and analysis of metabolites from solid-state fermentation of Chenopodium formosanum sprouts in a bioreactor. C. Hsieh, S. Yu, Y. Liou, **K. Cheng**
7:00 Structure elucidation of an anthocyanin-based aluminum blue complex and monitoring the changes with pH using electrospray ionization FT-ICR mass spectrometry. **X. Fan**, M. Giusti
7:00 Walnut skin darkening associated with heat extreme is linked to changes in its metabolites and quality. **Z. Afrah**
7:00 Continuous flow high-pressure homogenization is an alternative preservative technique to increase the shelf life of watermelon juice during cold storage. **J. Adhikari**, L. Rahimi Araghi, K. Adhikari, R.K. Singh, B.S. Patil
7:00 Effect of black rice dietary fiber on the metabolism of cyanidin-3-glucoside during in vitro colonic fermentation. **Q. Ma**, S. Zhang
7:00 Chemometric analysis of Mānuka honey meads. **L. Pilkington**, C. Chhouk, R. Deed
7:00 Sensitive and specific electrochemical Nano-biosensor for monitoring of bacterial contamination in wash water of fresh produce. **A. El-Moghazy**, N. Wisuthiphaet, N. Nitin
7:00 Benzenethiols with smoke-derived phenols causing ashy aroma and flavor in red wine. **D.C. Cerrato**, J. Fryer, M. Aragon, P.L. Ashmore, L. Garcia, T.S. Collins, E. Tomasino
7:00 Determination of carbohydrates in peanuts by HPAE-PAD. **Y. Kawahara**, J. Rohrer
7:00 Engineered yeast displaying specific norovirus-binding nanobodies for the concentration

and detection of human norovirus in food matrix. X. Zhao, T. Kasputis, R.C. Wright, **J. Chen**
7:00 Gomphrenin derivatives: alternative anti-inflammatory pigments from fruits of Basella alba L. (Malabar spinach). **S. Wybraniec**, R. Górska, E. Dziedzic, M. Bieniasz, P. Mielczarek, L. Popenda, M. Tyszka-Czochara, K. Sutor-Swiezy
7:00 Chemical profile and antioxidant activity of sweet cherry pulp (Prunus avium L.) from the Apulian region of Italy. P. Crupi, **R. Tardugno**, M. Muraglia, F. Limongelli, M. Clodoveo, F. Corbo
7:00 Physicochemical properties, structural features and biological activities of two fructans obtained from single-clove garlic and multiple-clove garlic: A comparison. **Z. Qiu**, H. Du, Z. Zheng, H. Xiao
7:00 Straightforward synthesis of P-alkylphosphonamidates and bioactivity screening as herbicides or quorum sensing modulators. **S. Backx**, A. Dejaegere, A. Simoens, J. Van de Poel, D. Krasowska, E. De Ridder, a. Willems, K. Audenaert, W. Desmedt, C.V. Stevens, S. Mangelinckx
7:00 Chitosan gel embedded with Nano S as a coating film for Phosphorus fertilizers to enhance use efficiency. **E.A. Davidson**, S. Santra, A. Peresteva, F. Rizzi
7:00 Analysis of volatile phenol interaction with film coatings developed to reduce grape absorption of wildfire smoke compounds. **L. Garcia**, T.T. Tran, J. Jung, D.C. Cerrato, L.R. Lim, M.H. Penner, Y. Zhao, E. Tomasino
7:00 Simultaneous prediction of beta-carotene, anthocyanins, and phenolics in sweet potatoes by near-infrared spectroscopy. **M. Allan**, R. Ibrahem, S.D. Johanningsmeier, K. Pecota, C. Yencho
7:00 Foodborne silica nanoparticles induced adverse effects differentially in obese and non- obese mice. **H. Du**, H. Xiao
7:00 Macroporous adsorbent resin debittering of HLB-affected orange juice and its impacts on consumer sensory acceptance. T. Washington, F. Briceno, C. Sims, R.M. Schneider, J. Brecht, K. Nau, Y. Yagiz, **L. Gu**
7:00 Determination of fatty acid composition, functional group, and compounds found in cocoplum (Chrysobalanus icaco L) seed oil using GC-FID, FTIR, and GC-MS instrument: Extractions, physicochemical and phytochemical parameters. **C.E. Oyeagu**, A.S. Ezeuko, F.B. Lewu
7:00 Sustainable food processing through low-pressure membrane technologies for food quality and safety. **M. Gulied**, F. Zavahir, T. Elmakki, D. Han
7:00 Ice recrystallization inhibition and acceleration by cellulose nanocrystals in the presence of anionic and neutral polymers. **M. Li**, T. Wu

MONDAY MORNING August 14
Moscone Ctr West Rm 3010
Chemistry of Wine - Wine Aging, Sensory, and Health
E. A. Chang, G. Kreitman, G. L. Sacks, E. Tomasino, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:05 What causes red wine headaches?. **A.L. Waterhouse**, A. Devi, M. Levin
8:30 Chemical properties of interspecific red wines bottled with different concentrations of free sulfur dioxide. **A.A. Watrelot**, D. Carter, A.D. Gapinski, Y. Cheng
8:55 Withdrawn
9:20 Evaluation of extraction rates of toasted-oak volatiles in model wines as a function of toast level in oak barrel alternatives. M. Aragon, **T.S. Collins**
9:45 Intermission.
10:05 Impact of micro-oxygenation in combination with barrel aging to shorten maturation time. **C. Medina Plaza**, L.X. Lim, A. Oberholster
10:30 Detection and identification of modified tannins evolved during red wine aging. **A. Devi**, J.F. Harbertson, A.L. Waterhouse
10:55 Modeling wine aroma perception from Key odorant composition and psychophysical measurements: using odor detection probability. **T.E. Acree**, Y. Jiang, T. Hsu
11:20 Concluding Remarks.

Moscone Ctr West Rm 3011
Advances in Food Chemical Informatics, Knowledge Bases and Databases
A.Dunkel, B. D. Guthrie, D. Wild, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:05 Navigating the nexus: AI, data science, and the future of food science and informatics. **D. Wild**, B.D. Guthrie
8:35 Using cheminformatics to speed up the full clarification of the chemobiological space of food compounds. **G. Colmenarejo**, I. Kaya, A. Sánchez-Ruiz
9:00 Exploring the backbone of Nature's chemical space as the primordial source of biological- driven structural diversity. **S. Furrer**, I.M. Ungureanu, C.G. Bologa, J.J. Yang, J. Timm
9:25 Structured Taxonomies for food and flavor databases. **A. Dunkel**, G. Luo
9:50 Intermission.
10:00 Valuable tool for flavor scientists: The Leibniz-LSB@TUM odorant database. **V. Mall**, J. Kreissl, P. Steinhaus, M. Steinhaus
10:20 Food chemicals in epigenetic targets: towards an epi food chemical database. **K. Juárez Mercado**, J. Avellaneda-Tamayo, J.L. Medina-Franco
10:40 Natural products magnetic resonance database (NP-MRD): An essential resource for food chemical informatics. **J.R. Cort**
11:00 Make flavor molecules FAIR (FAIRification). **G. Luo**, V. Somoza, A. Dunkel
11:20 Building food composition and discovery databases in the Periodic table of food initiative (PTFI). **S. Watkins**, C. Chien, T. Shafizadeh, J. Prenni, S. Ahmed
11:40 Discovery framework for natural food chemical activities. **D. Biber**, J. Duerkson, B. Foote, D. Wild, B.D. Guthrie
11:55 Concluding Remarks.

Moscone Ctr West Rm 3009
Biotechnology and Synthetic Biology for Sustainable Foods, Food Ingredients, and Flavor Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community K. R. Cadwallader, M. C. Qian, Y. L. Qian, *Orgs.* X. Du, Y. Jin, *Orgs.*, *Pres.*
8:00 Introductory remarks.
8:05 Flavor sustainability and biotechnology: A review. **X. Du**, M. Davila
8:35 Integrated chemical and biological platform for on-demand food production from minimal resources. **T. Lu**
9:05 Assessing the flavor generation of cultivated beef. **C.R. Luckett**, D. Zhao
9:35 Biotechnological production of dihydromenthofurolactones by basidiomycota. **H. Zorn**
10:05 Intermission .
10:30 Genome-edited yeast strains to modulate the tastes and flavors of fermented foods. C. Kim, Y. Lee, K.R. Cadwallader, **Y. Jin**

11:00 Transforming toxic djenkolic acid in djenkol beans into bioactive and flavorful organopolysulfides by utilizing C-S lyase from stink beans. **M. Zhang**, D. Huang
11:30 Comparison of flavor potentials of yeast extracts produced from acetate versus glucose grown biomass. **K.R. Cadwallader**, N. Hwisa, Y. Jin, C. Kim

Virtual Session
Forever Chemicals in the Environment, Distribution and Risk Cospons. AGRO, ENVR J. W. Finley, *Org.*, *Pres.* Q. X. Li, C. Sayes, *Pres.*
10:00 Introductory Remarks.
10:05 Phthalates: Effect on and transformation promotion of rhizosphere bacterial community. **Q. Cai**, H. Zhao, H. Lü, Y. Li, C. Mo, L. Xiang, Q.X. Li
10:35 Functional endophytic organic fertilizer alleviates the burden of phthalates and promotes vegetable growth. B. Huang, P. Wang, Y. Wang, **J. Ge**, Y. Li, J. Cheng, X. Yu
11:05 Remediation of PFAS from a variety of environmental matrices. **J. Meegoda**
11:35 Phthalate exposure leads to detrimental effects on preimplantation embryo development and viability. **R. Nowak**, L. Parra-Forero
12:05 Introductory Remarks.
12:10 Return of trifluoroacetic acid as an environmental concern. **T.M. Cahill**
12:35 Biostimulating Acidimicrobium sp. Strain A6 in PFAS impacted soils and soil-column experiments to achieve PFAS defluorination. **P.R. Jaffe**, m. sima, J. Park, S. Huang, B.E. Koel, C.E. Shaefer
1:00 Determination of plasticizers in PVC and non-PVC food contact materials. **K. Carlos**, L. Dejager, T. Begley
1:25 Uptake and translocation of perfluorooctanoic acid and perfluorooctane sulfonate in lettuces (lactuca sativa L.). **L. Xiang**, P. Yu, H. Zhao, Y. Li, Q. Cai, C. Mo, Q.X. Li

MONDAY AFTERNOON
Moscone Ctr West Rm 3011
Artificial Intelligence (AI) Applications for Food and Agriculture Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community M. Appell, B. Park, *Orgs.*, *Pres.*
2:00 Introductory Remarks.
2:05 Computer vision and NIR spectroscopy: an intelligent solution to optimize the fresh fruit bunches quality assessment in the Colombian oil palm agroindustry. **C.A. Diaz**, **J.A. Garcia- Nunez**
2:30 Protein language model-based universal deep learning architecture for bioactive peptide discovery. **Z. Du**, X. Ding, Y. Li
2:55 Developing an automated pipeline for the discovery of flower-specific honey markers via non-targeted LC-MS analysis. **S. Chahal**, L. Tian, S. Bilamjian, F. Balogh, T. Anumol, D. Cuthbertson, S. Bayen
3:20 Direct recognition of zearalenone and related metabolites using Raman spectroscopy. **M. Appell**, B. Park
3:45 Intermission.
4:00 AlphaFold 2-based stacking deep learning model for protein solubility prediction and food application. **H. Kwon**, Z. Du, Y. Li
4:25 Rapid quantitative analysis of olive oil fraud using recurrent neural network and Raman spectroscopy. W. Song, **K. Chou**
4:50 Foodborne bacteria classification using imaging spectroscopy with Fusion-nets deep learning. **B. Park**, T. Shin
5:15 Panel Discussion.

Moscone Ctr West Rm 3009
Biotechnology and Synthetic Biology for Sustainable Foods, Food Ingredients, and Flavor Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community X. Du, Y. Jin, M. C. Qian, *Orgs.* K. R. Cadwallader, Y. L. Qian, *Orgs.*, *Pres.*
2:00 Introductory remarks.
2:05 Withdrawn
2:30 Withdrawn
2:55 Chemistry of puerarin metabolism by human gut bacterium. **J. Han**
3:20 Genetic basis of fruit texture in cucumber. **Y. Weng**, X. Du, C.N. Duan, O. Akinpelu, P. Thapaliya, J. Tan, T. Nguyen
3:45 Intermission .
4:10 Identification of compounds contributing to the umami and bitter attributes of pea protein isolates. P. Ongkowijoyo, E. Tello, **D. Peterson**
4:35 Development of a novel, rapid assessment method for pectin structure and functionality. **W. Zhao**, Y. Kim, R.G. Cameron
5:00 Combination of novel extraction methods and natural, deep eutectic solvents as a greener solution for the recovery of anthocyanins and antioxidant activity from blackberry (Rubus spp). **O. Zannou**, I. Koca, S. Ibrahim
5:25 Characterization of aroma-active compounds in raw grains and grain distillate by gas chromatography-olfactometry dilution analysis and odor activity value. **D. Chen**, K. Yang, Z. He, Z. Liu, J. Zheng, M.C. Qian

Moscone Ctr West Rm 3010
Bioproducts from Biomass H. Ngo, B. Sharma, *Orgs.* M. I. Sarker, M. P. Yadav, *Orgs.*, *Pres.*
2:00 Introductory Remarks.
2:05 Synthesis of mixed chitin esters with thermoplasticity. **J. Kadokawa**
2:25 Developing integrated chemical and biological processes to produce 2-Pyrone-4,6- Dicarboxylic Acid (PDC) from lignocellulosic biomass. **C. Sener**, S.D. Karlen, C. Maravelias, J. Ralph, T.J. Donohue, D. Noguera
2:45 Valorization of agricultural byproducts - ultrafiltration and dialysis separation of myrosinase. A. Wade, M. Blakeley, **I.E. Popova**
3:05 Novel cocoa-derived ingredient towards circular economy and sustainability in the chocolate industry. C.P. Guirlanda, I.D. Alvim, M.T. Pereira, **J. Takahashi**
3:25 Producing a portfolio of commodity chemicals from lignin bound p-hydroxybenzoate. **S.D. Karlen**, V. Tymokhin, C. Sener, J.K. Mobley, J. Ralph
3:45 Production, characterization, and applications of functional components of wheat grains processing by-product. **M.P. Yadav**, A. Kaur, B. Singh, B. Sharma, M.I. Sarker
4:05 Intermission.
4:15 Synthesis of Branched triester for Potential Biolubricant. **M.I. Sarker**, H. Ngo, B. Sharma
4:35 Upcycling of sorghum distillers grains towards quality sorghum protein materials. **B. Mu**, X. Yu, L. Xu, Y. Yang
4:55 Nitrate adsorption on biochar pyrolyzed using concentrated solar radiation. **S. Li**, T. Galoustian
5:15 Combinatorial enzyme technology for production of bioactive oligosaccharides from libraries of converted agricultural fibers. **S.B. Batt Throne**, D.W. Wong, W.J. Orts
5:35 Sequential pretreatment of bamboo to maximize the fermentable sugar yield for the production of biofuels and bioproducts. **A. Salifu**, N. Ekwe, M. Tyufekchiev, K. Schmidt-

Rohr, Z. Zheng, A. Maag, G. Tompsett, W. Soboyejo, M.T. Timko
5:55 Concluding Remarks.

Virtual Session
Food Security: The Role of Alternative Protein Sources in Addressing World Hunger
Cospons. Agro, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community B. D. Guthrie, *Org.* J. W. Finley, L. Jackson, M. J. Morello, R. Yada, *Orgs.*, *Pres.*
3:00 Introductory Remarks.
3:05 New approaches to enhancing protein functionality and digestibility in plant-based foods. **H. Singh**
3:30 Micronutrient variation of plant-based milk alternatives: Influence of formulation and processing. **B. Redan**
3:55 Alternative proteins: Food safety risks and their mitigation. **L. Manning**
4:20 Intermission.
4:40 Analysis of insect cross-reactivity with crustacean allergen detection methods. **A. Eischeid**, R. Panda, C. Cho, S. Stadig
5:05 Proteomics in alternative protein research – evaluating protein food safety and quality. **M.L. Colgrave**
5:30 Regulation of protein-based food ingredients in the United States. **J. Dietz**
5:55 Panel Discussion.

Virtual Session
Virtual Graduate Students Symposium in Asia-Pacific Region on Agricultural and Food Chemistry D. Ren, C. Zheng, *Orgs.*, *Pres.* J. Hou, *Pres.*
5:30 Introductory Remarks.
5:35 Impact of ultrasound treatment on structural, emulsifying, and rheological properties on ultrasound treatment of oxidative oat (Avena sativa L.) protein. **X. Yue**, Y. Yang, C. Ma, X. Bian, L. Ren, B. Liu, l. Ai, N. Zhang
5:45 Withdrawn
5:55 Effects of different commercial mixed lactic acid bacteria on physical and chemical properties of soy protein yogurt. **X. Xu**, H. Cui, J. Xu, Z. Yuan, H. Liu
6:05 Intermission.
6:10 Typical emulsions as probiotic food carrier: Effect of cells position on its viability. **M. Li**, F. Van Bockstaele, W. Lou
6:20 White-light crosslinkable milk protein hydrogels with ultrafast gelation for first-aid wound treatment. **Q. Zhu**
6:30 Formation and characterization of oleogels derived from emulsions: Evaluation of polysaccharide ratio and emulsification method. **L. Huang**, Y. Cai, M. Zhao, Q. Zhao, P. Van der Meeren
6:40 Intermission.
6:45 Physical treatment synergized with natural surfactant for improving gas-water interfacial behavior and foam characteristics of α-lactalbumin. **J. Li**
6:55 Food-grade seamless capsules loaded with probiotics: gastrointestinal protection and long- term storage. **K. Zhang**, C. Ma, J. Zhang, Y. Liu, L. Zou
7:05 Exploration of interaction between α-lactalbumin and β-lactoglobulin under dUHT treatment and storage: Experimental and molecular dynamics study. **T. Zhang**, Y. Liu, P. Wang, Y. Li, F. Ren, H. Yi
7:15 Intermission.
7:20 Metabolic diversity in fermented milk of Lactococcus lactis isolated from naturally fermented dairy products. **W. Li**, Z. Sun
7:30 Withdrawn
7:40 Intermission.
7:45 Prevention of loperamide-induced constipation in mice and alteration of 5- hydroxytryotamine signaling by Ligilactobacillus salivarius Li01. **B. Qiu**, M. Yao
7:55 Lonicera caerulea L. polyphenols alleviated oxidative stress induced intestinal environment imbalance and lipopolysaccharide translocation liver injury by regulating pathways of Nrf2/HO-1/NQO1 and MAPK in rats. **Z. Cheng**, B. Li, Y. Wang
8:05 Effects of acute and chronic heat stress on rumen microbiome in dairy goats. **M. Li**, L. Xu, C. Zhang, H. Liu
8:15 Intermission.
8:20 Sleep promoting effect and mechanism of goat milk Casein Hydrolysate on rat and Caenorhabditis elegans. **Z. Li**, Q. Zhu, X. Liu, Y. Zhang, Z. Zeng, G. Liu, Y. Cao, Y. Chen
8:30 Study on the preparation, bacteriostatic mechanism and intestinal microecological regulation function of antimicrobial peptide AMP1043. **Z. Zhang**, P. Li, X. Zheng, Y. Huang
8:40 Effect of the probiotic strain, Lactiplantibacillus plantarum P9, on chronic constipation: a randomized, double-blind, placebo-controlled study. **T. Ma**, Y. Li, H. Zhang
8:50 Ultra-Deep metagenomic sequencing-based high-quality metagenome-assembled genomes reveal novel insights into the microbial genomic dark matter in the human gut. **H. Jin**, Z. Sun
9:00 Concluding Remarks.

MONDAY EVENING
Moscone Ctr South Hall F
AGFD Sci-Mix Live Session *(see first 36 posters listed under Sunday Evening General Posters session)*

AGFD Sci-Mix Virtual Session
8:00 Determination of phytochemical content and antioxidant capacity of dried haskap berries (Lonicera caerulea L.) and its potential value-added products. **Y. He**, **K. Singh**, **X. Lu**
8:00 Protein Extraction from Spent Oil-Cakes. **D. Kumar**, H. Makwana
8:00 Quality evaluation of artificially cultivated Atractylodes lancea (Thunb.) DC. from genuine producing areas. **J. Chen**, L. Li, Y. Liu, M. Huang, C. Wang
8:00 Impact of foliar and shade application on blackberry flavor and phenolics. **T. Xu**, J. Samtani, H. Chen, Y. Yin
8:00 Developing food preference behavior-based method to identify effectors of substance use disorder. **A.T. Kim**, Y. Park
8:00 Molecular assessment of metabolome alterations in Lotus japonicus roots induced by arbuscular mycorrhiza. **J. Ranner**, M. Paries, G. Stabl, C. Gutjahr, T.D. Stark, C. Dawid

TUESDAY MORNING August 15
Moscone Ctr West Rm 3010
JAFC Best Paper and AGFD Young Scientists Awards Symposium J. Beauchamp, T. D. Hoffman, Y. Kim, W. King, M. J. Morello, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:05 Introduction: JAFC Best Paper Award.
8:10 Sweet biotechnology: enzymatic production and digestibility screening of novel kojibiose and nigerose analogues. **S. Dhaene**, A. Van Laar, M. De Doncker, E. De Beul, K. Beerens, C. Grootaert, J. Caroen, J. Van Der Eycken, J. Van Camp, T. Desmet
8:40 Intermission.
9:00 Introduction: AGFD Young Industrial Scientist Award.
9:05 Cracking the code of food quality and health: combating fraud and unlocking nutraceutical potential. **Z. Xie**
9:35 Introduction: AGFD Young Scientist Award.
9:40 Importance influence of gums on promoting the fiber

formation for soy proteins-based meat analogues by high moisture extrusion. **X. Sui**
10:10 Concluding Remarks.

Moscone Ctr West Rm 3009
ACS Microbiome Consortium Kick off Symposium
L. A. Doherty, M. Kobori, L. Liu, *Orgs.* K. Mahalak, T. Wang, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:05 Bidirectional interactions between the small intestinal microbiota and bile acids in health and disease. **G.D. Wu**
8:50 Comprehensive metabolomics analyses of gut microbiome. **C. Zhu**
9:10 Bridging preclinical and clinical gut microbiota research using the ex vivo SIFR® technology. **P. Van den Abbeele**, S. Deyaert, C. Thabuis, C. Perreau, D. Bajic, E. Wintergerst, M. Joossens, J. Firrman, D. Walsh, A. Baudot
9:30 Bioenergy homeostasis: Major node in holobiont's stress response model. **N. Chakraborty**, A.B. Lawrence, A. Hoke, A. Gautam, R. Hammamieh
9:50 Intermission.
10:05 Reference-free and ecology-based discovery of microbiome biomarkers for disease monitoring and therapeutics development. **L. Zhao**
10:50 Quantitative analysis of bile acids in complex biological matrices by UHPLC-MS/MS for the assessment of microbiome alterations. **M. Gigl**, S. Reiter, A. Dunkel, D. Haller, C. Dawid, T. Hofmann
11:10 Bifidogenic effect of tomato seed extract on the gut microbiota demonstrates new potential for valorization of tomato waste. **J. Firrman**, A. Narrowe, L. Liu, K. Mahalak, J.M. Lemons, P. Van den Abbeele, A. Baudot, S. Deyaert, M. Slavin, L. Yu, B. Fanelli
11:30 Analysis of human, soil, and wildlife microbiomes in forensic science. **K.M. Elkins**, **J. Malbrough**, C. Ihearahu
11:50 Concluding Remarks.

Moscone Ctr West Rm 3011
Nutraceutical Lipids, Proteins and Biopeptides
F. Shahidi, J. Wu, R. Yada, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:05 Bioactive lipids and their conjugates. **F. Shahidi**
8:25 Functional lipids from food processing byproducts. **B. Gao**, H. Zhu, Y. Luo, **L. Yu**
8:45 Comparison of nutritional quality of fourteen wild Linum species based on fatty acid composition, lipid health indices, and chemometric approaches revealing their nutraceutical potential. **N. Plaha**, N. Kaushik, S. Awasthi, M. Singh, V. Kaur, S. Langyan, A. Kumar, S. Kalia
9:05 Lipids as a source of flavors. **K.R. Cadwallader**
9:25 Intermission.
9:45 Extraction and measurement of total lipids in fresh royal jelly samples: Comparison of several methods. **W. Zhang**, A. Ray, G. Tundo, P. Lau, Y. Zhu
10:05 Quantification of Chemical compounds of Linseed and their health benefits. **S. Awasthi**, N. Kaushik, N. Plaha
10:25 Sensoproteomics discovery of taste-active and DPP-IV inhibitory peptides in quinoa. **M. Holzer**, V.K. Mittermeier, T. Kröber, R. Kerpes, T. Becker, C. Dawid
10:45 Selection of qPCR reference gene for human colon cancer cells in cottonseed bioactive research. **H. Cao**, K. Sethumadhavan
11:05 Concluding Remarks.

Virtual Session
Bioproducts from Biomass H. Ngo, B. Sharma, *Orgs.* M. I. Sarker, M. P. Yadav, *Orgs.*, *Pres.*
10:00 Introductory Remarks.
10:05 Hydrophobic modification of arabinoxylan for improving emulsifying properties. **B. Sharma**, M.P. Yadav, A. Biswas, H. Cheng
10:25 Evaluation of sugar yields from biomass pretreated with alkaline solution from absorption of recovered CO_2. **V. Garcia-Negron**, M.J. Toht
10:45 Assay-guided isolation, structural elucidation, and action mechanisms of anti- inflammatory compounds in papaya leaves. **Y. Cao**, X. Wang, D. Huang
11:05 Counteracting roles of lipidic aldehydes and isoflavone antioxidants on soy protein oxidation revealed bychemometric survey of solvent and mechanically extracted soybean meals. **J. Zhang**, P.E. Urriola, S.L. Naeve, G.C. Shurson, C. Chen
11:25 Intermission.
11:35 Biochemical analysis of polysaccharides from Indian ginseng, Withania somnifera. **S. Badshah**
11:55 Green synthesized trimetallic (Cu/Ni/Co) oxide nanoparticles used to enhance rice straw and pressmud based vermimanure quality: Growth performance of Abelmoschus esculentus. **S. Yadav**, P.K. Srivastava, A.K. Choubey
12:15 Concluding Remarks.

TUESDAY AFTERNOON
Moscone Ctr West Rm 3010
Award for the Advancement of Application of Agricultural and Food Chemistry in honor of Liangli (Lucy) Yu
J. Beauchamp, M. J. Morello, *Orgs.*, *Pres.*
2:00 Introductory Remarks.
2:05 Decoding chemosensory systems for flavor innovations. **T. Hofmann**
2:35 Factors affecting the formation of process contaminants and transfer of toxic elements to food and beverages. **L. Jackson**
3:05 Nutraceutical properties of soybeans. **M. Slavin**
3:35 Intermission.
3:55 Food, food function and human health. **T. Wang**, Q. Pham
4:25 Bioactive food factors, and their health beneficial and toxic effects. **L. Yu**
5:10 Concluding Remarks.

Moscone Ctr West Rm 3011
Sustainable Agriceuticals Cospons. AGRO, ANYL, ENVR
Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community H. Kim, W. H. Yokoyama, L. Yu, *Orgs.* L. Liu, D. Ren, *Orgs.*, *Pres.*
2:00 Introductory Remarks.
2:03 . Capsinoids enriched extract from Capsicum sp. fruit and its associated pharmacological activities. **C.L. Cantrell**, R.L. Jarret, H. Chae, A. Andersohn, S.P. Marrelli, S. Khan
2:33 . Effects of high hydrostatic pressure pretreatments of orange peel on pectin extraction, structural and functional properties of the extracted pectin. **W. Zhao**, Y. Xu, C. Dorado, H.K. Chau, A.T. Hotchkiss, R.G. Cameron
2:53 . Evaluation of grape marc from different varieties as potential sustainable agriceuticals. **X. Li**, S. Wang
3:13 . Wine grape seed waste improves brain health of mice on high-fat diets. H. Lee, C. Tam, P. Alves, B. Shukitt-Hale, **W.H. Yokoyama**
3:43 . Hesperetin modulates gut microbiota, and attenuates bleomycin-induced pulmonary fibrosis. **P. Li**, X. Meng, Z. Zhang, Y. Huang

3:53 Intermission.
4:13 . Dietary macronutrients determine the pathological process of alcoholic liver disease. **S. Li**, J. Li, R. Guo, Q. Ding, J. Qiu
4:33 . Improved anti-colitis activity of Faecalibactrium prausnitzii by incorprated in a riboflavin conjugated alginate based delivery system. **M. Yao**, B. Qiu, L. Li
4:53 . Extracting bioactive phytochemicals and macronutrients from agriculture waste and food processing side streams: Simple solutions to complex global problems on food security, aging population, and sustainability. **D. Huang**, J.y. Toy, X. Yang, B. Neo, Y. Lin
5:13 . Rapid photocrosslinking α-LAMA hydrogels biomaterial to facilitate wound healing. **Y. Huang**, Q. Zhu, D. Ren
5:53 Concluding Remarks.

Moscone Ctr West Rm 3009
ACS Microbiome Consortium Kick off Symposium
L. A. Doherty, M. Kobori, L. Liu, K. Mahalak, T. Wang, *Orgs.* J. Firrman, J. M. Lemons, *Pres.*
2:00 Introductory Remarks.
2:05 Stress and the gut-brain axis in military health. **R. Hammamieh**, A. Gautam, N. Chakraborty
2:50 SRS-FISH: A high-throughput platform linking microbiome metabolism to identity at the single cell level. **J. Cheng**
3:10 Differential modulatory effects of kale microgreen and mature kale on the gut microbiome. **T. Wang**, A. Narrowe, Q. Pham, J. Wan, L. Yu, Y. Luo, T. Yang, L. Liu
3:30 Microbiome assessment of diet and stress effects in rodent models of brain insults. **A. Gautam**, J. DeMar, N. Chakraborty, M. Rusling, A. Hoke, F. Rossetti, D. Wilder, J. Long, M. Jett, R. Hammamieh
3:50 Intermission.
4:00 Relationship between functional components of agricultural products and the gut microbiome in several human intervention studies. **M. Kobori**
4:20 Taking a closer look: What we can learn by incorporating food type into analyses of fiber- microbe relationships. **M. Kable**
4:40 Impact of three traditional Chinese herbal extracts on the human gut microbiome. **J.M. Lemons**, A. Narrowe, L. Liu, J. Firrman, K. Mahalak, P. Van den Abbeele, A. Baudot, S. Deyaert, M. Slavin, L. Yu
5:00 Broad-spectrum antimicrobial triclosan and the gut microbiome. **K. Mahalak**, L. Liu, J. Firrman, A. Narrowe, L. Chau, E.S. Friedman, L. Herman, G.D. Wu
5:20 Degradation of food-grade λ-carrageenan by human gut microbiota: Potential adverse effect. **X. Guo**, Y. Han, Z. Zhu, P. Thanuphol, H. Xiao
5:40 Identification of a human gut bacterial strain with anti-inflammatory potential in gastrointestinal tract. **Y. Sun**, M. Gu, H. Xiao

Virtual Session
Nutraceutical Lipids, Proteins and Biopeptides
F. Shahidi, J. Wu, R. Yada, *Orgs.*, *Pres.*
3:00 Introductory Remarks.
3:05 Structure-function of the Plant-specific insert: A natural antimicrobial domain. **R. Yada**, L.K. Cheung, B.C. Bryksa, J.H. Dupuis, J.J. Tian, P. Baumik, A. Wlodawer, X. Zhao, R. Qi, X. Ma, S. Wang
3:25 Quantitative structure-activity relationship modelling of penta- and hexapeptide inhibitors of islet amyloid polypeptide fibrillation. **R. Abioye**, J. Oballa, M. Delgado Martinez, R. Aluko, C. Udenigwe
3:45 Structure, assembly and applications of peanut oil body proteins. Y. Pan, **Q. Huang**
4:05 Structure-function properties of peptides with dual inhibitory activity against acetylcholinesterase and butyrylcholinesterase. **R. Aluko**, N. Asen, C. Udenigwe
4:25 Intermission.
4:45 Food proteins in the prevention of osteoporosis. **J. Wu**
5:05 Bioactive peptides with antioxidant and DPP-IV inhibitory activity extracted from bones by-products. G. Carrera-Alvarado, L. Mora, **F. Toldra**
5:25 Valorisation of surimi processing by-products and formulation of value-added product (Ready to cook protein enriched soup mix). **A. Kumari**, K.N. Kaushik, R. Slizyte
5:45 Optimizing gelatin from pink perch skin and bones and its application in development of ready-to-cook chicken meatballs. **K. N. Kaushik**, K. Widell, R. Slizyte, A. Kumari
6:05 Concluding Remarks.

Virtual Session
Virtual Graduate Students Symposium in Asia-Pacific Region on Agricultural and Food Chemistry
D. Ren, C. Zheng, *Orgs.*, *Pres.* C. Li, *Pres.*
5:30 Introductory Remarks.
5:35 Development of method for simultaneously determining 11 triterpene alcohols and analysis of their characteristics in camellia oil. **Y. Li**, Y. Dong, Y. Gao, Q. Li, X. Yu
5:45 Dynamics of composition, structure, and metabolism of three energy substances in flaxseed (Linum usitatissimum L.) during germination. **Y. Dong**, Q. Li, Y. Gao, X. Yu
5:55 SlRBP1 promotes translational efficiency via SleIF4A2 to maintain chloroplast function in tomato. **L. Ma**, H. Zhu
6:05 Intermission.
6:10 Recent advances on the stability of anthocyanins regarding the interaction with food proteins and polysaccharides. **Z. Zang**, B. Li
6:20 Effects of soybean isoflavone aglycone on osteoporosis in ovariectomized rats. **L. Li**, N. Zhang, Y. Yang, C. Ma, X. Li, X. Bian, L. Ren
6:30 Effect and mechanism of thermostable β-glucosidase on aroma enhancement of instant Oolong tea at high temperature. **Q. Lin**
6:40 Intermission.
6:45 Structural characterization and hypoglycemic activity of glycoproteins extracted from Porphyra haitanensis by different extraction methods. **O. Yujia**, B. Zheng
6:55 Effects of non-covalent interactions between pectin and volatile compounds on the flavor release of tomato paste. **X. Li**, J. Li
7:05 Investigation of the anti-aging activity of the R-phycocyanin of Porphyra haitanensis. **Y. Feng**, Y. Zhang
7:15 Intermission.
7:20 Effects of genes required for exopolysaccharides biosynthesis in Lacticaseibacillus paracasei S-NB on cell surface characteristics and probiotic properties. **L. Xiao**, W. Li
7:30 Novel viscous hydrophilic colloidal polysaccharide produced by Lactiplantibacillus plantarum T1: structural characterization, rheological behavior and biological activity. **Z. Xueliang**
7:40 Small molecules interaction-mediated steady system for the construction and mechanism. **X. Chen**, H. Liang
7:50 Intermission.
7:55 Physicochemical stability and in vitro digestibility of goat milk affected by freeze-thaw cycles. **Y. Ma**, J. Hou
8:05 Digestive properties of meat and plant-based meat analogue and their effects on gastrointestinal digestion function

in mice. **Y. Xie**, C. Li
8:15 Surface modifications of Pediococcus pentosaceus Li05 for improved adhesion and function against Citrobacter rodentium infection. **S. Han**
8:25 Intermission.
8:30 Hypoxia impairs lactation in bovine mammary epithelial cells. **Y. Jin**, H. Liu
8:40 Construction of EGCG loaded in the edible complex delivery system: Masking bitterness and control release. **C. Ma**, K. Zhang, Y. Liu, Y. Zhou, X. Ye, L. Zou
8:50 Endogenous enzymes-based fermentation simulation reactions reveal metabolic pathways of key aroma compounds in fermented sea bass (Lateolabrax japonicus). **X. Liu**
9:00 Proteins from different sources in a high-fat food matrix influence lipid hydrolysis through bolus coalescence and interactions with bile salts. **M. Ding**
9:10 Concluding Remarks.

Virtual Session
General Posters J. Beauchamp, J. W. Soares, *Orgs.*
12:00 Insights into effects of simultaneous uptake, controlled release and antioxidant activity of β carotene and curcumin by Octenylsuccinated gastrodia elata starch micelles. **Z. Wu**
12:00 Determination of phytochemical content and antioxidant capacity of dried haskap berries (Lonicera caerulea L.) and its potential value-added products. **Y. He**, **K. Singh**, **X. Lu**
12:00 Protein Extraction from Spent Oil-Cakes. **D. Kumar**, H. Makwana
12:00 Towards the structure elucidation of an antibiotic adjuvant alkaloid Corozine A from corozo palm (Attalea cohune) applying experimental and computational tools. **L. Nitsch Velasquez**
12:00 Nutraceutical potential of industrial hemp (Cannabis sativa L.) extracts: physicochemical stability and bioaccessibility of cannabigerol (CBG) nanoemulsions. **H. Zheng**, B. Chen, J. Rao
12:00 Quality evaluation of artificially cultivated Atractylodes lancea (Thunb.) DC. from genuine producing areas. **J. Chen**, L. Li, Y. Liu, M. Huang, C. Wang
12:00 Exploration of conditions for high-concentration leaching of aromatic components by surface treatment of oak wood using pulsed arc discharge. **M. Iitomi**, M. Sasaki, I. Yamashina
12:00 Impact of foliar and shade application on blackberry flavor and phenolics. **T. Xu**, J. Samtani, H. Chen, Y. Yin
12:00 β-Cyclodextrin encapsulated garlic oil and diallyl disulfide for sclerotium cepivorum sclerotia germination to control allium crop white rot disease. **Y.L. Qian**, G.K. Hua, J.K. Dung, M.C. Qian
12:00 Effect of simulated gastrointestinal digestion on composition of anthocyanins and catechins and antioxidant properties of purple tea. **E.M. Abdelaal**, I. Rabalski, I. Rai
12:00 Computer-aided design and synthesis of novel flavanone derivatives for use as potential inhibitors of the COVID-19 papain-like protease. **A. Sigmon**, N. Yennawar, E. Margulis, J. Fecko, H. Al-Quaid
12:00 Developing food preference behavior-based method to identify effectors of substance use disorder. **A.T. Kim**, Y. Park
12:00 Promoting food and nutritional security through value added products of under-utilized Hibiscus sabdariffa calyces. **S.A. Marak**, N. Kaushik, A. Dikiy, E. Falch, E. Shumilina
12:00 Tuning the amphiphilicity of β-Cyclodextrin and L-Tryptophan nanoparticles in the development of ultrastable and eco-sustainable Pickering emulsions. **J. Wang**, Y. Dadmohammadi, A. Abbaspourrad
12:00 Development of a method to separate toxic compounds from fungal pathogens in hemp. **I.A. Kagan**, N. Gauthier

WEDNESDAY MORNING August 16
Moscone Ctr West Rm 3010
Chemical Intervention Technology to Improve Microbial Stability of Food
Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community X. Fan, T. Jin, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:05 Active polymers containing silver nanoparticles combined with active formulations based on essential oils: Quality effect on cereals and dairy products. **M. Lacroix**
8:30 Development of antimicrobial food packaging materials with electrospinning technology. **T. Jin**, L. Liu
8:55 Fabrication of antimicrobial packaging materials using natural polymers by coaxial- electrospray. **Z. Yi**, **Y. Wu**, R. Mu, T. Jin
9:20 Investigating chemical safety of a new N-halamine rechargeable antimicrobial coating for food processing equipment. **Y. Sapozhnikova**, R. Taylor, B. Demir, M. Qiao
9:45 Intermission.
10:00 Food safety applications of reversible guanylhydrazone antimicrobial agents. **W. Hart-Cooper**, J.H. Kim, J. Wilson-Welder, K. Orcutt, W.J. Orts
10:25 Antimicrobial efficacy of fatty acid amide derivatives for inhibition and reduction of Listeria monocytogenes and other bacterial strain. **O.M. Olanya**, Y. Hailemichael, R. Ashby, B. Niemira, D. Ukuku, S. Mukhopadhyay, J. Msanne, M.I. Sarker, X. Fan
10:50 Novelty of extraction of Rosmarinic acid from balm-mint /lemon balm (Mellissa Officinalis) using alkylation hydrocarbons at retrogression temperature for the use as food preservative and treatment of chronic viral diseases. **S.N. Olatunji**
11:15 Concluding Remarks.

Moscone Ctr West Rm 3009
Renewable Polymer Materials: Preparation, Processing, Application, and Disposal L. Liu, *Org.* J. Zhan, *Org.*, *Pres.* M. L. Robertson, *Pres.*
8:00 Introductory Remarks.
8:05 Lignin-based thermoset and composite polymers for the circular economy. **M.M. Abu-Omar**, M. Sanchez, P.C. Ford
8:35 Design of thermoset polymerization and materials for energy and environmentally efficient applications. **R.D. Allen**
9:00 Trojan horse repeat sequences for triggered chemical recycling of polyesters for films and bottles. **E.W. Cochran**, D. Dileep, T. Lee, M.J. Forrester, T. Wang, B.W. Kuehl, D. Finley, A. Ananin, G.A. Kraus
9:25 Degradable and thermally stable Spiro polycycloacetals from renewable resources. M. Shen, S. Vijjamarri, H. Cao, F. Khakzad, Y. Tang, E. Enebeli, **M.L. Robertson**
9:50 Intermission.
10:05 Developing bio-based covalent adaptable network polymers with designed recyclability. **N. Yan**
10:30 Developing a roadmap for bio-derivable and recyclable composites: Re-design and scale- up considerations. **N. Rorrer**, E. Rognerud, M. Mcgraw, R. Clark, R.D. Allen
10:55 Natural epoxy oil (Euphorbia oil) polymerization in liquid carbon dioxide-green media. **Z. Liu**
11:20 Development of high-performance recyclable structural composites from vegetable oils. **B. Zhao**, Y. Cao, J. Zhang
11:45 Concluding Remarks.

Moscone Ctr West Rm 3011

Sustainable Agriceuticals Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community L. Liu, D. Ren, L. Yu,*Orgs.* H. Kim, W. H. Yokoyama, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:03 . In vitro study of polymethoxyflavones (PMFs) from orange peel for their potential to inhibit trimethylamine (TMA) and trimethylamine-N-oxide (TMAO)-producing enzymes and reduce TMA/TMAO production. **Y. Wang**, H. Lee
8:23 . Elderberry fermentation promotes structural and metabolic changes to the gut microbiota. **L. Liu**, J. Firrman, A. Narrowe, K. Mahalak, J.M. Lemons, P. Van den Abbeele, A. Baudot, S. Deyaert, M. Slavin, L. Yu
8:43 . Interaction between extracts of black cumin, turmeric, and Ceylon cinnamon and the human gut microbiome. **K. Mahalak**, L. Liu, A. Narrowe, J. Firrman, J.M. Lemons, P. Van den Abbeele, A. Baudot, S. Deyaert, M. Slavin, L. Yu
9:03 . Human gut microbiome is rapidly and extensively altered by Senna sp. seed extracts. **A. Narrowe**, L. Liu, J. Firrman, K. Mahalak, J.M. Lemons, P. Van den Abbeele, A. Baudot, S. Deyaert, M. Slavin, L. Yu
9:23 . Monitoring the cellular response to whole food digests. **J.M. Lemons**, E.S. Friedman, D. Curry, F. Hao, A. Patterson, L. Liu, G.D. Wu
9:43 . 2′- Fucosyllactose modulates the function of intestinal microbiota to reduce intestinal permeability in mice colonized by feces from healthy infants. **B. Li**, Q. Chen, Z. Guo, R. Zhang
10:03 Intermission.
10:13 . Lactobacillus plantarum ZJUIDS04 alleviates DSS-induced colitis by regulating the immune response and modulating gut microbiota. C. Yu, Q. Ding, **D. Ren**
10:33 . Potential health benefits of upcycled romaine lettuce powder on metabolic syndrome. **E. Teran-Cabanillas**, K.F. Garcia Rocha, U. Osuna Martinez, W.H. Yokoyama, R. Avena Bustillos
10:53 . Potential of mealworm (Tenebrio molitor larva) protein: Improvement of its techno- and health functional properties via various extraction methods and purification. E. Oh, **Y. Kim**
11:13 . Prebiotic potential of water-soluble yellow mustard mucilage: Microbial evaluation on gut health promotion. **C. Fletcher**, Y. Wu
11:33 . Functionalized nanoclays as sustainable carriers for antimicrobials and festicides. O. Prinz Setter, S. Sharma, H. Abu Hamad, N. Ivanir, **E. Segal**
11:53 Concluding Remarks.

Virtual Session
ACS Microbiome Consortium Kick off Symposium
L. A. Doherty, L. Liu, K. Mahalak, T. Wang, *Orgs.* M. Kobori, *Org.*, *Pres.* W. Chen, *Pres.*
10:00 Introductory Remarks.
10:05 Investigating the molecular mechanism of anthocyanins in ameliorating type 2 diabetes and ulcerative colitis from the perspective of modulating gut microbita composition and metabolites. **W. Chen**
10:50 Modulatory effects of tea consumption on gut microbiota and gut microbiota-related metabolites. **M. Zhu**, J. Huang, Z. Liu
11:10 Systematic evaluation of metabolites composition and antioxidant activity of anthocyanin-rich berry extracts subjected to gut microbiota fermentation. **L. Xie**, W. Chen
11:30 Development and utilization of lactic acid bacteria resources. **Z. Sun**, F. Zhao
11:50 Intermission.
12:05 Impact of gut microbiota on avenanthramide metabotype from whole grain oat intake. **S. Sang**
12:50 Gut microbiota, metabolites and pancreatic diseases. **J. Sun**
1:10 Akkermansia muciniphila-derived outer membrane vesicles alleviate ulcerative colitis by regulating the intestinal barrier. **T. Zheng**, **J. Li**, Y. Yao, Y. Liu, Q. Liu, **H. Yi**
1:30 Health effects of pectin: reshaping gut microbiota and circulating metabolites. **S. Nie**, H. Tan, L. Fan, Q. Wu, Q. Xiao, M. Chen
1:50 Concluding Remarks.

WEDNESDAY AFTERNOON
Moscone Ctr West Rm 3010
Chemical Intervention Technology to Improve Microbial Stability of Food Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community X. Fan, T. Jin, *Orgs.*, *Pres.*
2:00 Introductory Remarks.
2:05 Photo-sensitive vitamin compounds as potential antimicrobial agents for food safety applications. **G. Sun**, Z. Zhang, L. Wang
2:30 Photodynamic inactivation of plant pathogenic fungus on fresh produce using food-grade plant-derived antimicrobials and sunlight. **Y. Kim**, C.H. Nguyen, A. El-Moghazy, H. Zhao, S. Wang, **N. Nitin**
2:55 Chlorine dioxide fumigation of fresh produce and nuts: microbial reduction and quality change. **X. Fan**
3:20 Intermission.
3:35 Combined effects of microencapsulated essential oils and γ-irradiation on microbiological and physicochemical properties of dry fermented sausages during ripening and storage. **M. Lacroix**
4:00 Withdrawn
4:25 NMR-based metabolomic investigation on antimicrobial mechanism of Salmonella on pea sprouts treated with Nanoemulsified basil essential oils and ultrasonic. **L. Zifei**
4:50 Development of bacteriophage added coating material to reduce Escherichia coli O157:H7 contamination in mushroom. **E. Evran**, E.K. Tayyarcan, I.H. Boyaci
5:15 Concluding Remarks.

Moscone Ctr West Rm 3011
Food Toxicants: Occurrence, Detection, Formation Mechanism and Mitigation Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community M. Appell, L. Yu, *Orgs.* X. He, L. Jackson, *Orgs.*, *Pres.* B. Gao, *Pres.*
2:00 Introductory Remarks.
2:05 Detection and occurrence of PFAS in food and food packaging. **Y. Sapozhnikova**, R.B. Taylor, M. Bedi, C. Ng
2:25 Analysis of Alternaria and Fusarium toxins in cereals and cereal-based food products via LC-MS/MS. **F. Dick**, A. Dietz, M. Rychlik
2:45 Analysis of volatile compounds and α-dicarbonyl compounds in Robusta coffee by soaking with various amino acids, organic acids and monosaccharides. **K.G. Lee**
3:05 Differential induction of shiga toxin in environmental Escherichia coli strains. **M.Q. Carter**, X. He
3:25 Intermission.
3:40 Development of tools for mycotoxin analysis in foods. **K. Zhang**
4:00 Geographical discrimination of 94 geographically authentic wheat samples and non- targeted metabolomics of moldy wheat by ultra-performance liquid chromatography-

quadrupole time-of-flight mass spectrometry. **B. Gao**, M. Jin, **Y. Luo**, L. Yu
4:20 Using mass spectrometry and whole genome sequencing to relate shiga toxin production with stx phage induction in shiga toxin-producing Escherichia coli (STEC). **C.J. Silva**, B. Quiñones, B. Lee, B.A. Amézquita-López, M.L. Erickson-Beltran
4:40 Discussion.

Moscone Ctr West Rm 3009
Renewable Polymer Materials: Preparation, Processing, Application, and Disposal
L. Liu, J. Zhan, *Orgs.* M. Nejad, C. Tang, *Pres.*
2:00 Introductory Remarks.
2:05 Additive manufacturing advancing sustainability. **T.E. Long**, C. Barker, C.W. Weyhrich, R. Bean, J. Wen, G. Nayyar
2:35 Plant-based Biofoam to replace Styrofoam for temperature-controlled packaging applications. **X. Zhang**
3:00 Efficient production of aliphatic α,ω-dicarboxylic acids using mild aqueous catalytic oxidation of low-density polyethylene. **O. Davydovich**, D. Martinez, J. Salinas, R.D. Davis, E. Martinez, H. Choudhary, M. Kent
3:25 Biodegradability and antifungal property of nanosilver-imbibed cotton fabric. **S. Nam**, H. Tewolde, Z. He, K. Rajasekaran, J. Cary, G. Thyssen, C. Sickler
3:50 Intermission.
3:55 Lignin-based PU foams. **M. Nejad**, C. Henry, E. Acquah, K. Dunne
4:20 Graphene Quantum Dots Improve the Dispersion of Cellulose Nanocrystals and Thermo- mechanical Properties of High Density Poly(ethylene) based Composites. S. Chanda, **D.S. Bajwa**, S.G. Bajwa, C. Ryan
4:45 Strong and ultrafast healing lignin-based copolymer elastomers via a grafting strategy. **Y. Zhang**, Y. Ou, J. Huang
5:10 Uniform, size controllable, and pH-sensitive protein microgels as efficient aqueous bio- lubricants: a soft ball-bearing mechanism study. **Y. Chu**, L. Chen
5:35 Antimicrobial, catalytic and thermophysical applications of internally synthesized Cu_2O nanoflowers in cotton fibers. **M.B. Hillyer**, S. Nam, J.H. Jordan, M.W. Easson, C. Madison, D. Hinchliffe

THURSDAY MORNING August 17
Moscone Ctr West Rm 3011
Food Toxicants: Occurrence, Detection, Formation Mechanism and Mitigation Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community X. He, L. Jackson, *Orgs.* M. Appell, L. Yu, *Orgs.*, *Pres.*
W. Zhu, *Pres.*
8:00 Introductory Remarks.
8:05 Thermostaility modification of zearelenone lactonase by two different methods. **W. Xu**, B. Ouyang, W. Mu
8:25 Baseline determination of azole-resistant aspergilli in California farms: Correlation between azole resistance and aflatoxin production. **J.H. Kim**, K.L. Chan, D. Ford, S.L. Sarreal, J.D. Palumbo
8:45 Dilute-and-shoot quantification of As, Cd, Pb, Be, Ni, Co, Cu, Mn, Se, Zn, Ba, Ag, and V in fruit juices by ICPMS based on matrix overcompensation calibration. **G. Chen**, B. Lai
9:05 Technologies for the detection of bacterial and plant toxins that impact food safety and security. **C. Tam**, P. Alves, L.H. Stanker, L. Cheng
9:25 Intermission.
9:40 Chlorothalonil induces metabolic syndrome in mice by regulating host gut microbiota and bile acids metabolism via FXR pathways. **W. Zhu**
10:00 Chemopreventive effect of natural dietary compounds on food-borne toxicants induced colon carcinogenesis. **M. Pan**
10:20 Effects of sulfonation on metabolic fate of deoxynivalenol in nursery pigs. **W. Mosher**, D. Yao, R. Faris, M. McGhee, C. Chen
10:40 Discussion.

Moscone Ctr West Rm 3012
Oat Bioactives and their Health Benefits
C. Hu, *Org.* Y. Chu, S. Sang, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:05 Pharmacokinetics of novel biomarkers of oat intake after single and repeated intakes of liquid and solid oat products. M. Armeni, R. Fristedt, N. Jansson, O. Savolainen, **R. Landberg**
8:40 Oats lower biological age in adults at risk for cardiovascular disease. **Y. Chu**
9:05 Oat protein modulates cholesterol levels and improves cardiac systolic function in high- fat, high-sucrose fed rats. **S. Joseph**
9:30 Phytochemical-rich sprouted oats as a novel functional food to attenuate gut inflammation. **P. Lee**, J. Hu, S. Sang
9:55 Intermission.
10:15 Germination and false germination increase the levels of bioactive steroidal saponins in oats. **J. Hu**, C. Hu, Y. Zhao, S. Sang
10:40 Assessing the impact of nitrogen supplementation in oats across multiple growth locations and years with targeted phenotyping and high-resolution metabolite profiling approaches. **W. Allwood**, P. Martinez-Martin, Y. Xu, A. Cowan, S. Pont, I. Griffiths, J. Sungurtas, S. Clarke, R. Goodacre, A. Marshall, D. Stewart, C. Howarth
11:05 Variations in avenanthramide concentration in oats. **L. Malunga**

Moscone Ctr West Rm 3018
Renewable Polymer Materials: Preparation, Processing, Application, and Disposal
J. Zhan, *Org.* L. Liu, *Org.*, *Pres.* L. Jiang, *Pres.*
8:00 Introductory Remarks.
8:05 Bioorthogonal protein engineering. **Y. Ito**
8:35 Development of soy protein-based hydrogels for a wide range of applications. **L. Jiang**, Q. Ma, R.S. Hazra
9:00 Zinc-coordinated chitosan nanocrystal for quercetin delivery. **P. Ma**, Q. Wang, C. Wei
9:25 Utilization of hemp biomass waste: Physicochemical properties of protein isolated from leaves, flowers, and stems of industrial hemp after cannabidiol extraction. **J. Crew**, **Y. Wu**
9:50 Intermisssion.
10:05 Fabrication of Bio-based multiple-functional materials for a beneficial food-energy-water nexus. **Z. Tong**
10:30 Oxidized chitin nanocrystals-enhanced colorimetric sensor array for accurate monitoring of beef freshness combined with deep learning models. **X. Jia**, P. Ma, Q. Wang
10:55 Modified cellulose nanocrystals as functional nanofillers for antibacterial food packaging. **Y. Wang**, S. Huang
11:20 Influence of pH, ethanol content, ionic environment, and casein concentration on electrospinnablility of casein dispersions. **D. Sharma**, G.R. Ziegler, F.M. Harte
11:45 Concluding Remarks.

Moscone Ctr West Rm 3016
Smart Food Safety
Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community X. Lu, R. Yada, *Orgs.*, *Pres.*

8:00 Introductory Remarks.
8:05 Non-targeted analysis using high-resolution mass spectrometry as a smart and innovative tool to assess the safety of food contact materials. **S. Bayen**, B. Hales, C. Goodyer, Z. Xu, L. Tian, L. Liu
8:45 EpCAM : Eco-friendly, Polymer-based nanozyme integrated with colorimetric sensing platform for agricultural biomolecule detection. **D. Lee**, M. Kamruzzaman
9:15 Phage-based nanobots to recognize, separate, and concentrate bacteria for food and water safety. C.M. Carmody, **S.R. Nugen**
9:55 Probiotic biopolymer-based encapsulation enhances limonene oil stability and antimicrobial efficacy. **S. Balyan**, **N. Dhowlaghar**, B.S. Patil
10:25 Point-of-need microfluidic device to safeguard food integrity. **Y. Hu**, X. Lu, Y. Chen
11:05 Panel Discussion.
11:25 Concluding Remarks.

Moscone Ctr West Rm 3009
Sustainable Agriceuticals
Cospons. AGRO, ANYL, ENVR Financially supported by Food Security: Tackling Hunger Convergent Chemistry Community H. Kim, L. Liu, D. Ren, W. H. Yokoyama, *Orgs.* L. Yu, *Org.*, *Pres.* J. Firrman, *Pres.*
8:00 Introductory Remarks.
8:03 . Effect of polyphenol extract-derived postbiotics on microbiota dysbiosis in HF-induced obese mice. **H. Kim**, K. Seo, H. Youn
8:33 . Macro and nanocapsules of essential oil in the protein/pectin system stabilized by ultrasound. S. Alieva, G. Kodirova, J. Bobokalonov, Z. Sherova, **Z. Muhidinov**
8:53 . Multi-crosslinked hydrogels with multi-functions for seawater-immersed wound healing. **X. Shi**, Y. Lv, J. Yang
9:13 . Chemical composition of honeysuckle (Lonicerae Japonicae) extracts and their potential in preventing COVID-19 and scavenging free radical capacities. **B. Gao**, **H. Chen**, L. Yu
9:33 . Associations of diet quality, mediating metabolomics, with frailty and sarcopenia: Findings from the UK biobank. **Z. Chen**
9:53 Intermission.
10:03 . Combination of cinnamon bark and astragalus extracts reduces metabolic dysfunction and improves microbiome composition in mice fed high-fat diets. H. Kim, P. Alves, **W.H. Yokoyama**
10:33 . Milk fat globule membrane regulates the physicochemical properties and surface composition of prepared infant formula powders by improving the stability of the emulsion. Q. Chen, F. Xiang, X. Ma, **B. Li**
10:53 . Identification of exposure biomarkers for apple consumption by targeted metabolomics approach. **J. Yu**, Y. Zhu, W. Wang, S. Sang
11:13 . Changes in functional properties of eggplant during pickling process using fermented rice bran. H. Kamo, **Y. Ogawa**
11:33 . Whey protein hydrolysate alleviated atherosclerosis and hepatic steatosis by regulating lipid metabolism in apoE-/- mice fed a Western diet. K. Wang, **Y. Tan**
11:53 Concluding Remarks.

Moscone Ctr West Rm 3010
ACS Microbiome Consortium Kick off Symposium
L. A. Doherty, M. Kobori, L. Liu, K. Mahalak, T. Wang, *Orgs.* A. Narrowe, I. Pantoja Feliciano, *Pres.*
8:00 Introductory Remarks.
8:05 Algorithms and analysis approaches in microbiome research. **W. Zeng**
8:50 Sudden change in diet acutely affects the gut microbiome response after an in vitro resistant starch supplementation. **I. Pantoja Feliciano**, J. Karl, M. Perisin, L.A. Doherty, H. McClung, N. Armstrong, R. Renberg, K. Racicot, T. Branck, S. Arcidiacono, J.W. Soares
9:10 Deciphering diet-microbiota interactions by integrating metabolomics and metagenomics with topological data analysis. **L. Guthrie**, J. Sonnenburg
9:30 Chemistry in the rhizosphere: Using fabricated ecosystems and exometabolomics to match plants with beneficial microbes. **T. Northen**
9:50 Intermission.
10:00 Microbiome data augmentation using deep learning models. **L. Zhang**
10:20 Applying metagenomic sequencing to decipher the human gut microbiome. **M.R. Olm**, D. Dahan, B. Merrill, M. Carter, J. Sonnenburg
10:40 Interplay between gut microbiota and curcumin. **M. Luo**, H. Xiao
11:00 Identification, distribution and structural diversity of Fusarium molecules with potential to modulate plant-microbiome interactions. **H. Kim**, G. Hao, C. Andorf, R. Proctor
11:20 Towards gut microbiome-based precision dieting: understanding interindividual variations in resveratrol hydrogenation through a gut bacterial pathway. **Y. Wu**, F. Li, H. Xiao
11:40 Impact of antibiotic ivermectin on the gut microbial community. **L. Liu**, K. Mahalak, A. Narrowe, J. Firrman, J.M. Lemons, P. Van den Abbeele, A. Baudot, S. Deyaert

Moscone Ctr West Rm 3020
General Papers
J. Beauchamp, J. W. Soares, *Orgs.*, *Pres.*
8:00 Introductory Remarks.
8:05 Integrative approaches for identifying bitter-tasting compounds. **V. Somoza**
8:25 Structural elucidation, anti-inflammatory activity and intestinal barrier protection of longan pulp polysaccharide. **Y. Bai**
8:45 Predictive Breeding for Wine Quality: From Sensory Traits to Grapevine Genome. **U. Fischer**, J. Vestner, A. Siebert, F. Schwander, F. Röckel, T. Heinekamp, L. Frenzke, S. Wanke, T. Wenke, R. Töpfer
9:05 Replacing shortening with high oleic soybean oil oleogels in bakery products: Impact on dough properties and quality of baked goods. **M. Zhao**, B. Chen
9:25 Chemical composition of pyrolyzed vegetation foliage utilizing a pyro probe coupled to two-dimensional gas chromatography. **R.K. Moore**
9:45 Intermission.
10:00 Conformational Epitope of important peanut allergens Ara h 5 is the dominant epitope triggering allergies. **J. Wang**, M. Hao, Q. Wang, H. Che
10:20 New LC-HRMS method for the simultaneous determination of 67 phenolic compounds in Canadian prairie berries to introduce them as a potential source of bioactive compounds. **C. Kodikara**, S. Sura, N. Bandara, T. Netticadan, C. Wijekoon
10:40 Flavor elucidation and simultaneous quantitation of key tastants and odorants of sourdough bread crumb. **L.S. Eckrich**, O. Frank, C. Dawid, T. Hofmann
11:00 Mechanochemical extraction of protein from moor grass. **O. Olalere**, H. Leese, C. Chuck, B. Castro Dominguez

11:20 Preservation of food by isochoric (Constant volume) freezing. **C. Bilbao-Sainz**, B. Chiou, T. McHugh, B. Rubinsky, V. Wu
11:40 Electrochemical lab-on-kitchen approach towards combinatorial testing for food contaminants. **D. Poudyal**, V. Dhamu, M. Samson, S. Muthukumar, S. Prasad

Virtual Session
General Papers J. Beauchamp, J. W. Soares, *Orgs.*, *Pres.*
10:00 Introductory Remarks.
10:05 Molecular assessment of metabolome alterations in Lotus japonicus roots induced by arbuscular mycorrhiza. **J. Ranner**, M. Paries, G. Stabl, C. Gutjahr, T.D. Stark, C. Dawid
10:25 Nutrients characteristics of the leaf, stem and root of Eclipta prostrata (L) . O.O. Onawumi, **A. Sodamade**, O.A. Onawumi, D.L. Abiona
10:45 Evaluation of the light stability of anthocyanins extracted from blackberry (Rubus spp) using a natural, deep eutectic solvent. **O. Zannou**, I. Koca, S. Ibrahim
11:05 Fatty acids and derivatives inhibit the spore germination of the barley pathogen Drechslera teres : An activity-guided search for natural pathogen resistance. **K.M. Hille**, T.D. Stark, A. Rexhaj, P. Gläser, F. Hohenender, H. Hausladen, A. Vlot, T. Hofmann, R. Hückelhoven, C. Dawid
11:25 Investigation of allergy prevalence and cross-sensitization in China: a survey based on self-reported and clinical testing data. **W. Xiong**, **H. Che**, **M. Zhang**, **T. Meng**, **Y. Liu**
11:45 Intermission.
12:00 Formation of amino acid derivatives during wine fermentation. **C. Yilmaz**, V. Gökmen
12:20 Saltiness enhancement in commercial soups and sauces using pyroglutamyl peptides. **O. Sahni**, J.P. Munafo
12:40 Predicting the baking quality of wheat using protein analytical and functional parameters. C. Schuster, J. Huen, **K. Scherf**
1:00 Characterization of odorants in dried and rehydrated lobster mushrooms. **T. Nguyen**, J.P. Munafo
1:20 Substantial equivalence of tobacco products: are all tobacco products of the same type substantially equivalent? Examples of equivalence and nonequivalence among waterpipe tobaccos. **J.H. Lauterbach**
1:40 Development and validation of a food frequency questionnaire for adults in Fiji to estimate nitrate and nitrite intake. **A.A. Chetty**, J. Lal, S. Prasad

AGFD TECHNICAL PRESENTATION ABSTRACTS

SUNDAY MORNING August 13
Chemistry of Wine - Winemaking Practices and Altering Wine Chemistry
8:05 New insights on the inhibition of potassium bitartrate crystallisation in wine Keren Bindon, keren.bindon@awri.com.au, Timothy Reilly, Alexander Schulkin, Eric Wilkes. Research, The Australian Wine Research Inst. Limited, Glen Osmond, South Australia The management of potassium bitartrate (KHT) instability in wine is critical, since KHT crystals can be perceived as a wine fault, particularly in white wine. KHT generally exists in a supersaturated state in wine systems, which can be minimised by inducing crystallisation through chilling, a process known as cold stabilisation. It has long been recognised that the presence of certain factors in wine can inhibit KHT crystallisation, thereby preserving its supersaturation. The primary compounds thought to confer this protection are macromolecules, including polysaccharides and phenolics, apparently explaining why red wine systems tend to have a greater resistance to KHT crystallisation than white wines. To better characterise the role of wine macromolecules as protective factors against KHT crystallisation reconstitution experiments guided by response surface methodology were performed to understand interactive effects between the key macromolecule categories found in white or red wine. In the white wine response surface models, it was found that protein and monomeric phenolics could inhibit KHT crystal formation, independently or in combination. White wine polysaccharides had no impact on KHT crystal formation, contrary to expectation, and in fact reduced the protective effect of phenolics. The key red wine macromolecule categories, tannin, anthocyanin and polysaccharide and their interactions were assessed at wine-like concentrations. Tannin introduced some protection against KHT crystallisation when applied in the higher concentration range. Red wine polysaccharides, which are present at higher concentrations in red than in white wines, also showed no protective effect against KHT crystallisation. Red wine polysaccharides also reduced the inhibiting effect of tannin on crystal formation when in combination. Surprisingly, anthocyanin was found to bring the model wine close to cold stable, at the lowest applied concentration, and this effect was exerted even when tannin or polysaccharide were present. It was found that the addition of anthocyanin to a bentonite-fined white wine or model wine was able to cold stabilise the wine to the same extent as a commercial dose of the crystallisation inhibitor, potassium polyaspartate. These results will be discussed in terms of the intrinsic differences between red and white wine systems and how this may impact the respective management of cold instability in the winemaking process.

8:30 Advanced monitoring and control of wine fermentations: Redox potential Ron Runnebaum1,2, rcrunnebaum@ucdavis.edu. (1) Viticulture & Enology, U. of California Davis(2) Chemical Engineering, U. of California Davis Redox potential, or Oxidation Reduction Potential (ORP), is a process parameter utilized in various processing environments for biofuels, wastewater, dairy, and fermented foods. While redox potential is understood and employed in a variety of other anaerobic processes, minimal work has been conducted on characterizing wine fermentations. The measurement mechanism of ORP is electrochemical and is influenced by pH, dissolved oxygen (DO), temperature, and chemical half-reactions taking place in solution. In low-oxygen yeast fermentations, changes in redox potential are primarily driven by the physiological and metabolic status of the yeast population: as yeast depletes molecular O2, produces CO2, and excretes reductive metabolites, it causes the ORP to decrease. Monitoring and controlling of redox potential via aeration have the potential to facilitate more robust fermentations including reducing the time for fermentation to complete. By monitoring redox potential during fermentation, an objective is to gain insights into the underlying biological and chemical differences between fermentations, including those from (1) vineyard sites and (2) fermentation replicates. In addition, this work set out to evaluate how the introduction of air during fermentation improves fermentation performance. Redox potential, Brix (density), yeast cell densities were collected and compared against un-aerated

fermentations. Different oxygenation timing and redox set points were explored to assess their impact on the fermentation outcomes of a single juice composition. Lastly, the redox potential of wine fermentations from a single load of grapes were controlled at three volumes: 100 L and 1500 L in a research winery and 10,000 L in a commercial winery by using only pulses of air delivery. The rapid ORP responses observed related to winemaking decisions and yeast activity suggest ORP is a useful process parameter in addition to Brix and temperature for monitoring fermentations. Experimental results to date demonstrate that aerated fermentations with higher redox status have faster fermentation kinetics and reach overall greater cell densities than those that were un-aerated. In addition, the timing of aeration was found to be important for this effect. Experiments up to 10,000 L demonstrates the scalability (i.e., from 1 L to 100 L to 10,000 L) of control of redox potential in wine fermentations and the potential to impact commercially relevant fermentation outcomes.

8:55 Winemaking practices to alter thiol and ester production in Chardonnay wines and impact to tropical fruit aroma perception Elizabeth Tomasino1, elizabeth.tomasino@oregonstate.edu, Chase Lucas1, Angelica Iobbi1,2. (1) Food Sci. & Technology, Oregon State U., Corvallis(2) American Group, Lactalis, Buffalo, New York Wines with tropical fruit aromas have become increasingly more available. With increased availability of different wine styles, it has become important to understand the compounds that cause the fruity aromas in wine. Previous work using micro fermentations showed that fermentation temperature gradients and time on skins resulted in an increase in thiol and ester compounds post fermentation and these compounds are known to cause tropical fruit aroma in wines. This work aimed to scale up these fermentations/operations to determine if the desired aromas could still be achieved and if there is a perceivable difference in tropical fruit aromas, liking, and emotional response in the wines at the consumer level. Four treatments were tested at varying fermentation temperature gradients and skin contact times: control fermentation at 13 °C with no skin contact (SC0FG0), fermentation at 13 °C with 18 hours of skin contact (SC1FG0), fermentation temperature gradient by time (20 °C for 4 days then reduced to 13 °C) with no skin contact (SC0FG1), fermentation temperature gradient by time with 18 hours of skin contact (SC1FG1). A change in winemaking scale did not alter the pH, residual sugar, or alcohol of the wines. Chemical analysis and descriptive sensory analysis were conducted to determine the alterations on the composition and aroma profiles of these wines. Check-all-that-apply (CATA) showed different prominent aromas for each wine treatment, with pome fruit, stone fruit, pineapple, honeysuckle, honey, and passionfruit being the most perceived aromas. Descriptive analysis (DA) showed that SC1FG0 was significantly different from both SC0FG1 and SC1FG1. SC1FG0 presented the most tropical fruit aromas, SC1FG1 presented more stone fruit, and SC0FG1 presented more honey and lemon/lime. Understanding the causes of tropical fruit aromas in wine and processes that alter these compounds is necessary to ensure winemakers can achieved tropical fruit quality consistently.

9:20 Maillard reaction-associated flavour compounds in base and sparkling wines Belinda Kemp1, belinda.kemp@niab.com, Hannah Charnock2, Jacob Medeiros2, Gary Pickering2. (1) NIAB East Malling, Kent, United Kingdom(2) Brock U., Saint Catharines, Ontario, Canada Maillard reaction-associated (MR) products have been identified and quantified in base and sparkling wines, despite the lack of high temperatures during the production stages. Acidic hydrolysis of sucrose can occur rapidly at low pH (pH 3), a similar pH to that of sparkling wine, and is likely the reason MR-associated compounds are prevalent in aged sparkling wine. To investigate factors that influence MR product formation in sparkling wine several studies were undertaken using sugar additions, amino acid additions, metal ion additions, and chitosan addition to base wine using an accelerated aging technique. Firstly, the influence of dosage sugar composition on Maillard reaction-associated products and precursors in traditional method (bottle-fermented) sparkling wines was evaluated over 18-months of storage in climate-controlled cellar conditions (14 °C, 70 % relative humidity). MR-associated products were quantified by headspace solid-phase microextraction coupled to gas-chromatography-mass spectrometry (HS-SPME-GC/MS), and amino acids by proton (1H) nuclear magnetic resonance (NMR) spectroscopy. Alanine and glycine decreased after 18-months, suggesting that MR-associated product formation could be partially related to their depletion. Secondly, mushroom-derived chitosan (Agaricus bisporus) was added to base wine that was stored for 90 days at 15° and 30°C, to investigate its influence on furan-derived compounds (products of MR in wine). Our results contribute to our understanding of MR pathways in the low-temperature and a low pH sparkling wine matrix and establishes the greater effect of aging duration and temperature compared to dosage sugar-type or chitosan treatments on the formation of MR-associated products. Additionally, the combined application of HS-SPME-GC/MS and 1H NMR based metabolomics presents new insights into the chemical composition of sparkling wines during aging.

10:05 Alternative acidification methods of high pH juice and wine Andreea Botezatu1, bia76@gmx.net, Carlos Elizondo1, Aaron Essary2, Andrew Lyne1. (1) Horticultural Sciences, Texas A&M U. System, College Station(2) Horticultural Sciences, Oklahoma State U., Stillwater Grapes grown in warm/hot climates such as Texas are often harvested at high pH and low titratable acidity levels, leading to concerns regarding their microbiological and color stability as well as tannin structure. As such, acidification, usually prior to fermentation, is seen as mandatory and most often achieved by addition of tartaric acid. As an alternative to this practice we investigated two different approaches of managing pH in the winery - an enzymatic approach, using glucose oxidase in conjunction with catalase to convert glucose into gluconic acid and, as a result, raise titratable acidity levels, and a sustainable/natural approach, using verjus - the juice produced from underripe grapes generated during cluster thinning - as an acidifier. Results indicate the suitability of both methods. In red wine (tempranillo) the pH was decreased by 0.84 when using the enzyme mix at a rate of 1.0 g/L with 11g/L of gluconic acid being produced, while a 0.5 g/L addition decreased pH from 4.6 to 3.8 and led to a production of 9 g/L of gluconic acid. Titratable acidities also increased from 3.6 g/L in control wine to 8.5 and 7.9 g/L, in treated wines, respectively. Similarly, in white wine (riesling) at the highest dose (1 g/L), pH was reduced from 3.9 to 3.2, with 20.5 g of gluconic acid produced, leading to a final titratable acidity of 11 g/L while at the lowest dose (0.2 g/L), pH decreased from 4.0 to 3.5 and 8.8 g of gluconic acid was produced, with a final titratable acidity of 9 g/L. Sensory evaluation indicated a positive impact on the color and organoleptic profiles of the wines, both red and white. In the case of verjus, which we produced in-house, we found that a 2% by volume addition was sufficient for a 0.1 decrease in pH in a white wine, while a 10% addition resulted in a 0.3 pH drop.Titratable acidity, tartaric and malic acid all increased in the treated wines, with the highest TA being 7.2 g/L in the 11% verjus addition treatment, up 1.6 g/L from the 5.6 g/L levels in control wine. Preliminary sensory and consumer data indicate no negative impact of verjus addition on the organoleptic profiles of the wines.

10:30 Wine matrix impact on smoke marker compound expression in wine Anita Oberholster, aoberholster@ucdavis.edu, Lik X. Lim, Cristina Medina Plaza, Ignacio Arias-Perez, Yan Wen, Bishnu P.

Neupane. Viticulture and Enology, U. of California Davis The increasing incidences of wildfires in winegrape growing regions pose a significant risk to the grape and wine industry. Exposure to smoke can compromise the quality and value of winegrapes and adversely affect resulting wines. During wildfires, large amounts of volatile phenols (VPs) are released into the air from the pyrolysis of lignin. These compounds can be absorbed through the berry skin, where they are quickly glycosylated, potentially as part of the defense mechanism of the plant. Thus, VP smoke exposure marker compounds can be present in the grapes as various glycoconjugates. Research has shown that both free and bound VPs contribute to smoke taint perception due to slow hydrolysis of glycosides during winemaking, aging, as well as bacterial enzymes in saliva that can release smoke taint aroma in the mouth. To improve risk assessment, the baseline free and bound VP levels of different red winegrapes not exposed to smoke were determined as well as the free and bound VPs composition of their smoke exposed counterparts. Descriptive analysis of the different wines identified the main sensory attributes. The main non-volatile profiles of these wines were also determined to elucidate the relationship between wine matrix composition and smoke taint expression. Additionally, wines with different levels of smoke marker compounds were made by serial dilution of the smoke impacted wines with their respective non-impacted wines. Consumer studies were conducted to determine the change in 'liking' for a wine depending on the percentage inclusion of smoke impacted wine. Using multivariate statistics, "liking" scores were related to specific wine attributes and composition data to determine threshold levels of smoke marker compounds in different red wine matrices. The defined baseline and threshold levels are the first steps in creating clear guidelines to determine wine taint risk from grape berry smoke marker compound analysis.

10:55 Sensory significance of aroma carry-over during bottling from aromatized wine-based beverages into regular wine Ulrich Fischer, ulrich.fischer@dlr.rlp.de, Jörg Gottmann, Jochen Vestner. Inst. for Viticulture and Enology, Dienstleistungszentrum landlicher Raum, Neustadt, Rheinland-Pfalz, Germany When bottling flavoured wine-based beverages aroma compounds are absorbed by sealings and may migrate into subsequently bottled wines. This unintentional carry-over bears the risk to violate the legal ban of any aromatization of wine. Thus we investigated the absorption and desorption process during bottling and cleaning in order to minimize aroma carry-over by improved cleaning efficacy. If cleaning obeys good manufacturing practice (GMP) and traces of aroma compounds in the subsequently filled wine show no sensory significance, this unintended aroma carry-over will be considered as technically unavoidable and has no legal consequences. Sealing polymers were exposed to aromatized wines followed by GMP cleaning in a model system. A novel direct analysis of studied aroma compounds such as γ-decalactone, α-ionon or eugenol revealed that only 11-62% of them was remove by cleaning1. High temperature of 85 °C revealed the largest cleaning efficacy, while chemical additives such as citric acid, caustic soda or ozone exhibited only minor impact. A total removal of absorbed aroma compounds was not achieved, enabling a later release from the sealing into subsequent wines. To study the requested absence of sensory significance, odor detection thresholds of seven aroma compounds commonly used for aromatization were determined in water, model wine and white wine. Applying the odor activity concept allowed to determine unequivocally the sensory impact to traces of aroma compounds detected in the subsequent bottled wines. Monitoring uptake, cleaning and further release in two industry scale bottling lines we could confirm the uptake of aroma compounds into built-in sealing during the filling of mulled or aromatized wines. GMP cleaning removed only small amounts of absorbed aroma compounds from the sealing, allowing migration into the subsequently bottled regular wines. Sensory evaluation of the wine before and after bottling did not yield any significant difference. In fact, concentrations of respective aroma compounds remained either below their analytical limit of detection or way below their respective sensory thresholds. In conclusion, despite of migration of aroma compounds into sealing in a bottling line, execution of GMP cleaning and dilution effects in the subsequently filled wine prevented any aroma carry-over of sensory significance. Thus, a potential analytical determination of aroma traces would not lead to legal prosecution.

Food Security: The Role of Alternative Protein Sources in Addressing World Hunger

8:05 Protein valorization from underutilized agriculture by-products Takuji Tanaka, takuji.tanaka@usask.ca. Food and Bioproduct Sciences, U. of Saskatchewan College of Agriculture and Bioresources, Saskatoon, Canada We are facing the food shortage with the explosive increase of population. We must provide more foods to meet the demands from 9.7 billion, up from 8 billion today, by 2050. Meanwhile the further increase in agriculture production is constrained from the available farmland. Clearing more forest for farmland cannot be employed in the today's pressure for environmental protection. A solution to the issue is utilization of inedible organic materials produced from today's agriculture practice for food production. In my research group, a theme is dedicated for this direction: Utilization of underutilized agriculture by-products for food and feed production. Saskatchewan is a major agriculture province of Canada, and she is a leading producer in the global supply of legume, canola, and wheat. These agriculture crops produce a huge amount of inedible by-products, and only a part of the by-products is utilized as an inexpensive feedstuff for animal rearing. In our study, two concepts are examined to recover proteins as readily-utilizable products from these agriculture byproducts. The first concept is utilization of fermentation on the starch fraction of legume. The legumes are generally commodity products. But in recent years, they are milled and fractionated into protein- and starch-rich flour fractions. The former is utilized as protein ingredients in many processed foods, but the latter is considered as a byproduct of protein fraction as its utilization is limited due to flavour and other reasons. We utilize this fraction (5 to 8% proteins, 60%+ starch) as the fermentation bed, and successfully increased the protein contents to above 60%. This conversion would allow to use this byproduct as protein-rich feedstuff. In the second concept, we utilized insect culture to recover nutrients from another agriculture byproduct, oilseed meals. Oilseed meals are high in protein, but proteins are trapped within their lignocellulosic matrix, allowing less bioavailability. We ferment the meals with GRAS microbes, and then fed it to black soldier fly larvae. As a results, we successfully recovered 90%+ proteins from the meals in the form of larval biomass. Proteins in insect biomass have characteristics of animal proteins, i.e., amino acid profiles show no particular shortage in essential amino acids. We are currently working to increase the efficiency of these concepts and also investigating the methods of utilization of resulting protein-rich products.

8:25 Structure, extraction, and function of alternative proteins derived from plants and insects Xiaonan Sui, xiaonan.sui@neau.edu.cn. College of Food Sci., Northeast Agricultural U., Harbin, China Population growth and environmental degradation have made it unsustainable to rely on conventional proteins. Novel alternative protein sources are being sought for their greater sustainability, including non-animal proteins from plants, insects, algae, bacteria, and fungi. These alternative proteins have high protein content, a balanced amino acid composition, and are considered healthy and nutritious. Additionally, their cultivation can have restorative effects on the

environment by utilizing greenhouse gases or converting industrial waste into useful organic matter. However, further research on the structure, extraction methods, and safety of these alternative proteins is still needed, particularly for insects, algae, bacteria, and fungi. This presentation provides an overview of recent developments in alternative proteins, including their nutrition, sustainability, classification, and structure, as well as methods of extraction and potential safety factors.

8:45 Algae use as alternative proteins to enhance food security Maria Hayes, maria.hayes@teagasc.ie. Food BioSciences, Teagasc Food Research Centre Ashtown, Dublin, Ireland The increasing global population coupled with limited resources of arable land and fresh water requires a new approach to protein generation to feed the population. Algae (micro and macroalgae) are examples of under-exploited "crops" with potential for use as alternative proteins. Algae do not compete with traditional food crops for space and resources, are protein rich and can, in some instances be comparable crops like wheat in terms of their protein content and amino acid composition. Commonly consumed algae have potential for use as protein sources based on their protein quality, amino acid composition, and digestibility. Protein extraction methods applied to algae include enzymatic hydrolysis, physical processes, and chemical extraction and novel methods such as ultrasound-assisted extraction, pulsed electric field, hydrolysis and microwave-assisted extraction. Results vary in terms of quantity of protein recovered and the quality of protein in terms of digestibility and bioavailability. Protein enrichment methods used in the dairy industry, could play a role and assist in enhancing protein quality from algae and assist in making algal proteins high value ingredients. Methods such as hydrolysis and fermentation can be used to generate hydrolysates and fermentates rich in bioactive peptides with functional and health applications. Issues such as the protein digestibility corrected amino acid score (PDCAAS) and Digestible Indispensible Amino Acid Score (DIAAS) are knowledge gaps that must be filled if algal proteins are to be used as alternative proteins in the future.

9:05 Big things come in small packages: prospects of microalgae proteins in addressing global nutrition and health challenges Chibuike Udenigwe, cudenigw@uottawa.ca. U. of Ottawa, Ontario, Canada Microalgae have been increasingly explored as sustainable, alternative food protein sources. Several microalgae species are rich in their quantity and quality of proteins, comparable to conventional food proteins, hence their tremendous potential in combating nutritional deficiencies and health issues globally. Microalgae proteins also have variable techno-functional properties for potential applications in extruded products, additive manufacturing, and functional biomaterials such as edible packaging and delivery systems. However, the digestibility of microalgae proteins is lower than the gold standard animal proteins due to the extremely complex matrix of the microalgae biomass. This presentation provides a roadmap for the adoption of practical food innovations for efficient release and recovery of proteins from microalgae biomass. To promote a circular agri-food system, there is a growing emphasis on efficient processing methods to enhance downstream processing and product recovery. The various mechanical, chemical, enzymatic, and emerging technologies used in microalgae pre-treatment and protein extraction will be discussed in the context of zero-waste processing. Also presented are advances in nutraceutical peptides generated from microalgae proteins and the obstacles impeding application of the proteins with respect to biomass production, downstream processing, safety, and the inherent properties of derived products. Taken together, increased microalgae utilization has the potential to facilitate food and nutrient diversification, novel clean-label food product formulation, human health enhancement, environmental sustainability, and global food security.

9:45 Plant-based diets: Addressing human and planetary health and sustainability Heidi Lynch, hlynch@pointloma.edu. Kinesiology, Point Loma Nazarene U., San Diego, California Anthropogenic greenhouse gas emissions (GHGEs) result from many sectors, including agriculture, which produced about 11.2 percent of total US greenhouse gas emissions in 2020. In addition to GHGEs, agriculture places a toll on natural resources through land, water, and energy use; water acidification and eutrophication, and biodiversity loss. Not all crop and livestock production leads to the same amount of environmental impact, however. Producing protein from animal sources, particularly ruminants, typically demands more environmental resources and emits more GHGEs than producing protein from plant sources. Continuing current agricultural practices is likely incompatible with achieving international climate goals such as those set forth by the United Nations, and as such more sustainable food systems and individual dietary patterns are warranted. Plant-based dietary patterns, including vegetarian and vegan diets, are associated with marked reductions in resource utilization and GHGEs, and are also associated with significant reductions in risk of developing numerous chronic diseases including cardiovascular disease, type 2 diabetes, cancer, and obesity. Thus, it is possible to eat in a way to optimize human and planetary health simultaneously. Entomophagy, or the consumption of insects as a protein source, is another means to reduce diet-related GHGEs. In addition to shifting toward a more plant-based diet (with or without the inclusion of insects), minimizing food waste of any source is a highly effective means by which we may reduce diet-related GHGEs. The U.S. Environmental Protection Agency (EPA) estimated in 2021 that annual food loss and waste in the U.S. results in 170 million metric tons of CO_2 equivalents of GHGEs. The global population is expected to increase by close to two billion people in the next 30 years. In order to maximize food security, minimize hunger, and remain within planetary boundaries, it is imperative that we support food systems and embrace dietary patterns that promote both human and environmental health. This session will present differential environmental impacts of several dietary patterns and specific food items, discuss human physical health associated with various dietary patterns, and conclude with some practical applications for making more sustainable dietary choices.

10:05 Protein digestion and absorption: Meat analog versus meat Da Chen, dchen@uidaho.edu. U. of Idaho, Moscow The shift of diets towards more plant-based foods has raised the concern regarding the protein digestion and nutrition, especially plant-based meat analog (MA). Understanding the protein digestibility in MA is essential for improving its nutrition. Depending on the formulation and the processing condition, protein digestion and subsequent absorption varies significantly. Whether proteins in MAs enable to provide equivalent nutrition as their animal counterpart remains unclear. MAs produced from soy and wheat protein will be used as representatives. They were subjected to in vitro digestion followed by absorption by Caco-2 cell layer. The permeability of the peptides and the amino acid composition of the permeates were measured. Chicken breast was used as comparison throughout the experiment. The study found less essential amino acids were found in the permeate of MA digesta than those of chicken breast, implying its inferior protein nutrition.

10:25 Alternative proteins: A religious perspective Joe M. Regenstein, jmr9@cornell.edu. Food Sci., Cornell U., Ithaca, New York Traditionally, proteins came from both animals and plants and society used these multiple sources. The world population is

increasing and with it the need for food, particularly protein, increases. At the same time there is concern for other issues such as climate change and sustainability. Possible solutions are to increase the pool of materials available either by using new sources including using new technologies, and/or by optimizing and expanding currently available proteins. Of course, the new systems and materials must be acceptable to consumers. Among the consumer constraints are the needs of the religious communities, particularly the Jewish and Muslim communities that have comprehensive food laws — kosher and halal respectively— that are nominally required of its adherents and are observed by a significant number of people in each community. Given that almost a quarter of the world's population is Muslim or lives in countries that operate with halal regulations, these new systems must fulfill these laws if they hope to be accepted widely. Focusing on halal foods, the following issues impacting alternative proteins need to be discussed: (a) The use of alcohol in processing and fermentation systems. (b) The use of ingredients derived from animals that were not religiously slaughtered. (c) The use of animals or the derivatives of animals (including their DNA) that are not halal (which includes how they were fed), e.g., especially from the pig. (d) The determination of which new animals, e.g., among the insects, are halal and which are najis (filth). (e) The use of plants that may have toxic components (not tayyab or wholesome). (f) The need to segregate halal and haram (prohibited materials). (g) And how to convert a food processing plant to halal if needed. The Jewish (kosher) laws would be accommodated by some of these processes; others would have to be addressed more specifically for this considerably smaller population.

10:50 Inspiring food systems Innovations to improve the health of people and planet Bernhard van Lengerich1,2, bvl01@comcast.net. (1) Former Chief Science Officer and VP Technology Strategy, General Mills Inc, Minneapolis, Minnesota(2) Founder, Seeding The Future Foundation, Minneapolis, Minnesota Providing a growing global population with access to affordable, safe, and nutritious food for a healthy diet while maintaining the health of our planet will require transformational changes in the food system. Advances and discoveries in science and Tech., as well as creative new approaches and, as importantly trusted collaborations across disciplines and cultures can lead to an abundance of innovations with the potential for significant food system changes. Most impactful food system innovations need to aim to improve planetary as well as personal health and lead to food solutions that are accessible, affordable, appealing, and trusted by consumers. The annual Seeding the Future Global Food System Challenge, funded by the Seeding The Future foundation and operated by the Inst. of Food Technologists (IFT) since 2021, has the goal to inspire and support passionate, diverse and multidisciplinary teams to create game changing innovations that will help transform the food system to be more sustainable, make healthier diets more accessible, and empower consumers to make choices benefitting both, personal and planetary health. The Challenge is rewarding several grants and prizes between $25,000 and $250,000, totaling $1 Mio annually and aims to inspire impactful innovations leading to benefits of one or more of the following intersecting domains: safe and nutritious food for a healthy diet, sustainable practices, and accessible, appealing, affordable, and trusted by consumers. Innovations within this 'white space' are critical for a successful food system transformation. Prominent examples from prior Challenge Winners are alternate protein solutions, eliminating post-harvest losses, or eliminating harmful substances such as arsenic or aflatoxin.

11:15 Perfect day's collaborative approach to a kinder, greener future food system Sunil Sukumaran, sunil.sukumaran@perfectday.com. R&D, Perfect Day, Inc., Berkeley, California Perfect Day has created the world's first nature-identical animal protein, without any animal inputs, using precision fermentation. Precision fermentation uses glucose (sugar) from plant sources and GRAS microflora that have been designed to produce beta-lactoglobulin. The microflora is cultivated to produce whey protein, the protein is purified to over 95% purity, and spray dried for shipment to customers. Analytical methods are used at every step, in line with regulatory requirements, to ensure that it is identical to the beta-lactoglobulin in traditional milk, and verify the quality, safety, and consistency of the product. Food Sci. analytical and sensory methods similarly validate that the product behaves identically to bovine beta-lactoglobulin for use in non-animal dairy products and new product development. This innovation is creating a new category of foods which offer a sustainable, nutritious, delicious way to feed our growing population. According to an ISO-conformant lifecycle assessment, this production process reduces greenhouse gas emissions up to 97% compared to traditional production methods. And because it's identical to the milk protein (whey) that we all love, it offers a way to leverage that planet-positive impact in a way that doesn't compromise on taste, texture, or nutrition. In this session, Perfect Day's Chief Technology Officer, Sunil Sukumaran, will share how the company uses an established technology in a new way to create high-value ingredients, and how collaboration is at the core of scaling the impact of what the company has unlocked. The company is bringing others along on this journey by partnering with the largest CPGs and most mission-driven startups who want to use its animal-free protein as an ingredient as a tool in their own kinder, greener mission. It also offers the expertise its built going from an idea to global scale to others, via its enterprise biology business nth Bio, helping extend what's possible through precision fermentation in our food system—and even beyond.

Methods, Data, and their Usage Towards Solving the Food Allergy Problem

8:05 Seed proteins of common buckwheat: A treasure trove of genetic resources contributing to hypoallergenicity Tomoyuki Katsube-Tanaka, tanakato@kais.kyoto-u.ac.jp. Kyoto Daigaku, Kyoto, Japan Common buckwheat (Fagopyrum esculentum Moench) has excellent palatability, nutritional and health-promoting properties, and labor-saving and environmentally harmonious cultivation characteristics. However, since it sometimes causes severe allergic reactions, hypoallergenicity is necessary. Major allergens identified are 13S globulin (Fag e 1) and 2S albumin (Fag e 2). The 13S globulin is composed of Met-rich subunit and Met-poor subunits with or without 1-6 repeats of an insert consisting of 15 residues in its α-chain. Since the inserted sequences are hydrophilic with many arginine residues, the α-chains of the 1-6 repeat subunits are trypsin-digestible, while that of the 0-repeat subunit is trypsin-resistant. Genetic diversity analyses of the 0-repeat subunit revealed that some alleles have a 10 amino acid residue-long insertion or a miniature-inverted repeat transposable element (MITE)-like sequence, which were expected to change their digestibility or expression, respectively. Among them, GlbNB2 did not express the 0-repeat subunit and was anticipated to contribute to hypoallergenicity. Meanwhile, 2S albumin, the causative protein of anaphylaxis, has five types of genes, g03, g11, g13, g14, and g28. We found that g03 is a pseudogene and that g13 has a null allele with a transposable element (TE)-like insertion. Furthermore, we found a novel g11 allele that lacks one of the disulfide bonds important for steric structure formation and is easily digestible with trypsin, and the possible null allele for g28, which has another TE-like insertion. Therefore, common buckwheat, which is allogamous and has many TEs in its genomic DNA, is considered to have high genetic diversity and to contain many genetic resources useful for reducing allergens. For g14, for which no genetic resources useful

for hypoallergenicity have been found, we are trying to mutagenize g14 using a heavy ion beam. By combining abundant natural variations and artificial mutations, it is considered possible to reduce allergens in common buckwheat.

8:30 Hydrolysed proteins prevent child food allergies in mice: A study on eggs and cow's milk Binghui Zeng, zengbinghui0831@sina.com, Huilian Che. China Agricultural U., Beijing Food allergy has become a serious public health concern in recent years, while the prevalence of it in children is higher than in adults. To prevent food allergies in infants, a new and functional strategy should be developed. In this study, we evaluated the properties of hydrolysed egg proteins and hydrolysed milk proteins in preventing egg allergy and milk allergy, respectively. We observed the structure of the jejuna of young mice and calculated the thymus index and the spleen index. Two antibodies and three cytokines as indicators of T helper 2 cells (Th2) responses, while Immunoglobulin G2a (IgG2a) and Interferon-γ (IFN-γ) as characterisation of Th1 reactions. Papain-hydrolysed egg proteins were found to increase the immune organ indexes, suppress Th2 responses, and significantly suppress the allergy-induced drop in rectal temperature of young mice. Milk proteins hydrolysed by trypsin and flavourzyme have been shown to activate both the Th1 and Th2 reactions but prevent the allergy-induced drop in rectal temperature as well. Enzymatic hydrolysis has emerged as a popular mechanism for processing proteins and a typical way to lessen allergen sensitisation. Therefore, focusing on the mechanisms of food allergy, we revealed that the related food allergies may be prevented in different ways by the hydrolysed proteins of egg and milk, respectively. This page will help to guide the early diets for babies and the development of anti-allergic infant formula.

8:55 Effect of two different processing methods on the allergenicity of tropomyosin from Procambarus clarkii and its mechanism Guirong Liu, liuguirong1998@cau.edu.cn, Huilian Che. Food Sci. and Nutrition Engineering, China Agricultural U., Beijing Background: The rapid rise in Procambarus clarkii has increased the related food allergy (FA) rate, impeding the development of associated food products. Although high hydrostatic pressure (HHP) treatment and polyphenols, such as chlorogenic acid (CA), have shown potential for alleviating seafood allergies, their effect on Procambarus clarkii remains unclear. Methods: The main Procambarus clarkii-tropomyosin (PC-TM) allergen was treated using HHP and CA. The PC-TM structure was analyzed via fluorescence chromatography, circular dichroism, and Fourier-transform infrared spectroscopy. The PC-TM allergenicity was compared via serological experiments and an FA mouse model. QPCR, Western blotting, and a mouse model treated with inhibitors and antagonists were used to explore the regulatory role of the TLR8 signaling pathway in PC-TM allergy. Results: Although both HHP and CA changed the secondary tropomyosin structure, CA was more significantly. Furthermore, the animal experimental results showed that CA significantly reduced the PC-TM allergenicity compared with untreated tropomyosin, mainly manifesting as lower specific IgE/IgG_1, mast cell protease 1, histamine, and Th2 cytokine levels, as well as spleen and intestinal histopathological scores. Contrarily, HHP may aggravate PC-TM allergenicity. The WB and PCR results indicated significant variation in the Toll-like receptor-8 (TLR-8)-MyD88-NF-κB signaling pathway expression in PC-TM-sensitized mice exposed to different treatments. Moreover, TLR-8 agonist treatment alleviated the allergic symptoms of both HHP- and CA-treated PC-TM sensitized mice to a certain extent, while antagonist treatment further aggravated the allergic symptoms. Conclusion: CA significantly reduces PC-TM allergenicity, while HHP may induce an increase. Therefore, polyphenol treatment may be vital for reducing Procambarus clarkii allergenicity in the future. Additionally, the TLR-8 signaling pathway plays a crucial regulatory role in shrimp allergy and may be a critical therapeutic target for future treatment.

9:20 Atmospheric cold plasma treatment reduces Ara h 1 antigenicity and stability in roasted peanut Kuan-chen Hsieh, a10035750@gmail.com, Yuwen Ting, James Wu. National Taiwan U. Inst. of Food Sci. and Tech., Taipei Peanut is a popular crop for its edible seeds. To bring out the unique flavor, peanut is usually roasted at high temperature. However, peanut is one of the most common food allergies, and Maillard reaction is owing to glycation on allergens, resulting in badly allergenic potential. The allergenicity and glycation degree both depend on protein structure. Atmospheric cold plasma is a non-thermal processing technology that generates reactive species allowing protein structural changes. We aim to investigate the relationship between protein structure, allergenicity and Maillard reaction in peanut, and clarify mechanisms in mitigating allergenicity through cold plasma treatment. The nitrogen and air cold plasma treated-peanut protein was added glucose, freeze-dried, and roasted. The advanced glycation end products content in samples was measured. The allergenicity was evaluated by IgG antibody-binding activity and in vitro digestion assays. The protein structural was assessed via electrophoresis, amino acid profile, secondary and tertiary structure. The antigenicity of Ara h 1 decreased by 91% and 76% respectively after 30 minutes of air and nitrogen plasma treatment, and the allergen stability and glycation degree were also reduced. These results correlated with protein structural changes, denaturation and aggregation. Therefore, cold plasma could have good potential for reducing peanut allergen.

10:00 Allergen cross-contact risk due to the use of shared frying oil Lauren Jackson, Lauren.Jackson@fda.hhs.gov. Division of Food Processing Sci. & Technol., U.S. FDA, Bedford Park, Illinois Approximately 3-4% of people in the U.S. suffer from food allergies. Strict avoidance of the offending food allergen is the only recourse for consumers with food allergies. However, allergens can be inadvertently introduced into food through cross-contact during processing or cooking operations. One mechanism by which cross-contact can occur is when foods are fried in oil previously used to cook or process allergen-containing foods. Several lab-scale experiments investigated transfer of allergens to frying oil and to other foods fried in reused oil. Separate experiments evaluated the effectiveness of filtering treatments for removing allergens from frying oil. Concentrations of allergens in frying oil were measured with allergen-specific ELISA kits and total protein methods, while ELISA was used to quantify allergens in fried foods. In general, the allergen content of frying oil increased with the number of batches of allergenic food fried. However, the concentration of allergens detected in oil, particularly by ELISA, did not increase linearly, suggesting that they become less detectable during the frying process. Use of allergen-specific ELISA kits verified that allergens present in frying oil transferred to other foods. Use of filtering treatments reduced allergen levels in frying oil. These studies indicate that allergen cross-contact from shared frying oil can occur, and that oil filtration treatments can be effective at reducing the risk of cross-contact. New analytical methods such as mass spectrometry are currently being developed to accurately quantify the presence of allergens in frying oil and in fried food. These methods will provide a better understanding on the levels of allergens transferred to foods prepared in shared frying oil.

10:25 Modulating the allergic immune response to cow’s milk with probiotics Jing Yang1, jyang@ctbu.edu.cn, Jiajia Song2. (1) Chongqing Technology and Business U., China(2) Southwest U., Chongqing, China Milk serves as a crucial protein source for

infants and young children. Nonetheless, it should be noted that milk protein is one of the most frequent food allergens. Cow's milk allergy (CMA) is mainly caused by immune dysregulation characterized by the Th1/Th2 imbalance. Modulating the host's immune response to allergens is a promising approach for the prevention and treatment of CMA. Various studies show that supplementation with probiotics protects against the development of CMA by regulating the host immune response. However, the underlying mechanisms are not fully understood. Our study investigated the protective effects of Bifidobacterium longum BBMN68 on allergic immune response in mice with CMA. The BBMN68 consumption reduced allergic sensitization to cow's milk allergen and reversed the abnormal balance of Th1/Th2 responses in mice. Additionally, BBMN68 administration increased the population of T regulatory cells (CD4+CD25+Foxp3+Treg cells) in lymph nodes in the gut. Furthermore, BBMN68 induced the expression of CD103 in dendritic cells (DCs) and the semi-mature status of DCs in mice. CD11c+DCs isolated from BBMN68-treated mice promoted Foxp3 expression in CD4+T cells and shifted the imbalanced Th1/Th2 responses to cow's milk allergen in vitro. These data suggest that BBMN68 might be a potential therapeutic approach to alleviating CMA, and BBMN68-specific induction of CD11c+CD103+DCs and semi-mature DCs are closely associated with this protection. Recently, increasing evidence suggests that probiotic-derived polysaccharide capsules (PSs) play a central role in controlling the immune response to food allergies. Probiotic-derived PSs can stimulate DCs by engaging pattern recognition receptors, which regulate cytokine production and activation in murine DCs. The effects of BBMN68-derived PSs on DCs-mediated immune regulation in CMA need to be further investigated in the future.

10:50 Folic acid inhibits food allergic reactions in offspring rats by regulation of allergy-related immune cells Qianwei Wang, wqw202106@163.com, Yuchi Jiang, Huilian Che. China Agricultural U., Beijing In recent years, the incidence of food allergy has continued to rise, especially in infants and young children. Food allergy, associated with mild redness, pruritus, diarrhea, breathing difficulties and even death, seriously affects the normal life of patients. However, there is no effective way of prevention except for avoidance of allergens. Therefore, the use of anti-allergy ingredients in food may be an appropriate strategy. The development of food allergy is closely related to nutrients, and vitamins are one of the research focuses. Folic acid (FA), a water-soluble vitamin that is widely found in leafy greens, has been found to have an effect on the body's immune system. However, the relationship between FA supplementation and food allergy is controversial. In the present work, the anti-allergic activity of FA and its possible mechanism were investigated by animal model, cellular model and transcriptomic analysis. Studies based on a Brown Norway (BN) rat food allergy model showed that FA downregulated IgE and IgG1 expression and was able to regulate T cell subpopulation differentiation levels and affected Th1/Th2 balance. Also, FA was able to reduce the release of particulate matter such as histamine and mast cell proteinase. Transcriptomic evidence suggested that FA intervention can reverse food allergy-induced gene expression changes from the clustering level. Among 208 differential genes, the gene hsp90, which expresses heat shock proteins, is a potential key gene for FA intervention in food allergy. RBL-2H3 cell-based immunological assay in vitro suggested that FA may affect HSP90 expression through the glucocorticoid receptor (GR) while inhibiting the degranulation level of effector cells. All these results suggested that FA has a relieving effect on food allergy, and the effect is more pronounced with high doses of FA. And it may affect HSP90 expression through GR, further inducing a decrease in degranulation levels during the allergic effect phase. This study provides new evidence on the relationship between FA and food allergy.

11:15 New pepper allergen of 2S albumins and its potential impact on nuts allergy Hong Li1, lihong@pumch.cn, Lixia Zhu2, Rui-qu Wang1, Liping Zhu1, Jing Hu2, Feng Chen2,3, Li Ma4, Rui Tang1, Siyu Liu2, Kang Ni5, Xiaodong Ye5, Yuzhu Zhang6, Jing-Lyu Sun1, Tengchuan Jin2,7. (1) Allergy Department, Peking Union Medical College Hospital, Beijing, China(2) Division of Life Sciences and Medicine, U. of Science and Tech. of China, Hefei, Anhui, China(3) Anhui U. of Chinese Medicine, Hefei(4) Morehouse School of Medicine Cardiovascular Research Inst., Atlanta, Georgia(5) Dept. of Chemical Physics, U. of Science and Tech. of China, Hefei, Anhui(6) ARS-PWA-WRRC, USDA, Albany, California(7) Inst. of Health and Medicine, Hefei Comprehensive National Science Center, Anhui, China Zanthoxylum bungeanum (Sichuan pepper; Hua jiao in Chinese) is used as a spice worldwide and is a potentially life-threatening allergenic food source, as first reported by our team in 2005. However, its allergen components are unknown. Thus, we aimed to identify and characterize its major allergens and determine its cross-reactivities with citrus seeds, pistachios, and cashew seeds. For these purposes, the protein components from Sichuan pepper seeds were isolated using ion exchange and size exclusion chromatography. An allergen was characterized by SDS-PAGE, analytical ultracentrifugation, mass spectrometry, and circular dichroism spectroscopy, confirming that it is a 2S albumin allergen of approximately 14 kDa, similar to an α-amylase inhibitor domain-containing protein of citrus sinensis. It has thermal stability, possibly due to its disulfide bridges. Its coding region, a 303 bp DNA sequence of the AAI domain, was amplified from the genome. ELISA and competitive ELISA assays demonstrated positive cross-reactivities between Zan b 1 and citrus, pistachios, and cashew seeds. This allergen might play an active role in precise, individual diagnosis and better prevention of food allergies.

SUNDAY AFTERNOON

Chemistry of Wine - Wine Chemistry Measurements

2:05 Oral processing of wine and temporal aroma release and perception Maria Pozo Bayon, m.delpozo@csic.es, Carolina Munoz, Maria Perez-Jimenez, Celia Criado. Instituto de Investigacion en Ciencias de la Alimentacion, Madrid, Spain Wine aroma is one of the most important sensory attributes driving consumers' liking. It is formed by hundreds of volatile organic compounds (VOCs) produced in different steps during winemaking mostly related to viticultural (e.g. grape variety, soil type or hydrological regime) and oenological (e.g. grape processing, fermentation and ageing) practices. Although most wine aroma research has focused on the characterization of wine VOCs trying to elucidate their sensory impact, the chemical and biochemical reactions taking place during the oral processing of wine (OPW) are key factors in understanding wine aroma perception. In fact, aroma compounds can be submitted to the action of oral physiology (interaction with saliva proteins, saliva enzyme metabolism), which are also affected by the physico-chemical characteristics and structure of the aroma molecule, but also by the chemical composition of the wine matrix (e.g. ethanol, polyphenols), and even by biological factors such as sex or age. The reactions that these compounds might experience in the mouth will affect the amount and rate of release of aroma molecules reaching the olfactive sensory receptors, which is related to the immediate but also to the prolonged aroma perception, also known as aroma persistence. The use of ex-vivo (assays of retention and or metabolism of aroma compounds by human saliva), in-vivo analytical (in-mouth SPME, intra-oral SBSE, in-nose PTRMS, Spit-Off-Odor measurements-GCMS) and dynamic sensory approaches (Time intensity,

Progressive profiling) has been shown to be useful tools in order to establish the importance of OPW for understanding inter-individual differences in aroma perception and aroma persistence. The most recent results in this topic performed in our research team will be presented during this talk.

2:30 Advancements in rapid and accurate grape quality analysis using A-TEEM and machine learning Robert Qiang Sui[1], qiang.sui@ejgallo.com, Adam Gilmore[2], Bryant Blair[1], Hui Feng[1], Bruce S. Pan[1], Lyufei Chen[2]. (1) Winegrowing Research, E & J Gallo Winery, Modesto, California(2) 2. HORIBA Instruments Incorporated, Piscataway, New Jersey Grape quality, significantly influenced by factors such as color, phenolics, and basic chemistries, is essential for producing wines with desirable characteristics. On the other hand, monitoring and controlling smoketaint compounds is crucial as they can negatively impact the final wine with undesirable sensory traits, such as smoky, burnt, or ashy flavors and aromas. Traditional methods for measuring grape color and phenolics involve multiple analytical platforms, including UV-Vis, HPLC, HPLC-MS, and FTIR. Smoketaint analysis typically requires costly GC-MS and HPLC-MS to measure both free and glycoconjugate-bound compounds. These techniques necessitate different matrix processing steps for grapes, adding complexity, increasing time requirements, and potentially burdening small wineries with high costs. There is a growing need for the wine industry to develop rapid, accurate, and cost-effective analytical methods for assessing key quality marker compounds and smoketaints to enhance winegrowing and winemaking decisions and optimize wine production. Absorbance-Transmission and Fluorescence Excitation Emission Matrix (A-TEEM) has been recently developed for the quantitation of phenolics and anthocyanins in wine, utilizing machine learning (ML). Specifically, Extreme Gradient Boosting (XGB) has shown to be highly effective for A-TEEM data and is employed in this study. This presentation reports rapid and accurate quantification of grape phenolics, anthocyanins, and tannins using A-TEEM with automated sample preparation by a Hamilton Liquid handling robot and automated A-TEEM acquisition by an autosampler. Promising results for basic chemistries, such as YAN and malic acid, are also demonstrated. Preliminary findings on the measurement of smoke taint compounds in grapes for screening purposes are shown. The work presented here suggests that the A-TEEM method is a promising technology for rapidly measuring essential grape quality compounds using a single analytical platform.

2:55 Role of magnetic resonance spectroscopy in the OIV digital transformation plan Jose Enrique Herbert Pucheta, jherbertp@ipn.mx. Organic Chemistry, Instituto Politecnico Nacional Escuela Nacional de Ciencias Biologicas, Mexico City, Mexico Central goals of the International Organization of Vine and Wine (OIV) are focused in promoting harmonized international practices, develop vine and wine standards, assist further International Organizations in the procurement and vigilance of said practices and standards, as well as informing to their 49 Member States, the consequences of implementing these actions. The 2020-2024 OIV Strategic Plan comprises specific action fields in order to attend the priorities of the sector such as promoting an eco-friendly vitiviniculture, implement harmonized regulatory environments, consolidate the scientific, technical and cultural role of the OIV and the development of the digital transition of the vine and wine sector, throughout a Digital Transformation Plan. Currently, the OIV Digital Observatory Hub reports that the vine and wine sectors that have advanced towards an integrative digitalization ecosystem are the vineyards (38%), wineries (49%) and chain supply (50%), with the implementation of outstanding technologies such as the use of combined advanced analytical methods with artificial intelligence for obtaining genomics, transcriptomics, proteomics and metabolomics fingerprints in diverse vine and wine products, in turn feeding E-Labels for notably increasing the traceability of products with a digital identity. To the best of our knowledge, the combination of nuclear magnetic resonance spectroscopy (NMR) with diverse artificial intelligence algorithms (NMR-AI) affords digital identities of diverse oenological products with the highest resolution so far reported within the Digital Transformation Plan, as a foodomics tool for retrieving discriminant features related to geographical origins, grape varieties, oenological standard and degradation parameters, fermentation products, polyphenols, amino acids, appellations d'origine contrôlée and type of monovarietal strains in wines. Said omics methods have gained such attention that Intergovernmental Organizations and Control Agencies are currently recommending their massive use amongst Member States as quality and authenticity compliances. Recent innovations presented at the OIV Digital Transformation Plan include the use of NMR-AI methodologies for obtaining highly discriminant data matrixes for metabolomics studies, ideal for complex polyphenolic profiles, as well as for discriminate between wine samples produced from the same grape variety and geographical origin but fermented with different yeast strains.

3:20 Sorbent sheets coupled to direct analysis in real time mass spectrometry (DART-MS) for rapid volatile phenol analyses in grapes and wine Gavin L. Sacks1, gls9@cornell.edu, Terry Bates1,2, Andre Kalenak1, Brett Bergman1. (1) Food Sci., Cornell U., Ithaca, New York(2) Bruker Corporation, Billerica, Massachusetts Quantitative analysis of volatile phenols (VPs; e.g. (4-ethylphenol, 4-ethylguiacol, guaiacol, 4-methylguaiacol, and cresol) are of interest to the wine industry as markers of microbial spoilage or "smoke taint" contamination. Current approaches to VP analysis by chromatography-based approaches (e.g., SPME-GCMS) require 20 min or more per analysis, and are poorly suited to accommodating large sample influxes as occur following smoke taint events. We demonstrate that etched poly(dimethylsiloxane) (PDMS) thin film sorbent sheets (SPMESH) can be used for parallel headspace extraction of derivatized VPs, and that extracted analytes can be then be rapidly quantitated by direct analysis in real time mass spectrometry (DART-MS). VPs were acetylated with isotopically labelled acetic anhydride to increase SPMESH extractability and resolve isobaric MS/MS interferences. Measurement of free vs. total VPs could be distinguished by adjusting the pH during derivatization. The validated HS-SPMESH-DART-MS method could quantitate VPs in 24 samples in ~60 min, including derivatization and extraction time. The method achieved limits of detection below sensory threshold for targeted VPs (< 1 µg/L) in juice and wine with good accuracy (92-98%) and repeatability (3-6% RSD).

4:05 Volatile sulfur compounds in wine – from precursor investigation to novel oxathianes Xingchen Wang[1], Dimitra L. Capone[1,2], Aurélie Roland[3], David W. Jeffery[1,2], david.jeffery@adelaide.edu.au. (1) School of Agriculture, Food and Wine, The U. of Adelaide, Adelaide, South Australia, Australia(2) ARC Training Centre for Innovative Wine Production, The U. of Adelaide, South Australia(3) SPO, INRAE, Institut Agro, U. de Montpellier, Languedoc-Roussillon, France Decades of research have been devoted to polyfunctional thiols in wine, but there are still questions that remain unanswered. One intriguing aspect is the formation of precursors to 4-methyl-4-sulfanylpentan-2-one (4-MSP) in grape berry and another is the fate of thiols during winemaking and beyond. In contrast to non-volatile precursors of 3-sulfanylhexan-1-ol (3-SH), which incorporate (E)-2-hexenal formed in grape berry, the alkenal skeleton necessary for analogous formation of 4-MSP precursors, namely mesityl oxide (MO), has

been scarcely reported in grape juice or wine. Indeed, the pathway to MO formation has not been determined, in contrast to the LOX/HPL route to (E)-2-hexenal from linolenic acid. When it comes to chemical fate of thiols such as 3-SH after its release from precursors during fermentation, disulfide formation or reaction with quinones have been considered, but the role of other wine electrophiles such as acetaldehyde had escaped attention. Considering the research gaps, we undertook isotope tracer studies with d_{10}-MO applied to grape berries and leaves of potted grapevines, analysing these tissues using HPLC-MS/MS to investigate the formation of glutathione conjugates of labelled 4-MSP. The experiments involved three grape varieties and treatment with d_{10}-MO for different durations. After solid-phase extraction of berry and leaf extracts, HPLC analyses with triple quadrupole and high resolution MS led to the tentative identification of deuterated isotopologues of the glutathione conjugate of 4-MSP, which were matched against an authentic standard, in the two grape varieties that experienced a longer application of d_{10}-MO. The presence of deuterated cysteine conjugates of 4-MSP was also observed by high resolution MS. Separately, we investigated the formation of 1,3-oxathianes arising from reaction of 3-SH and 4-MSP with acetaldehyde, which constitute a novel type of volatile sulfur compound in wine. After rigorous compound identification, deuterated standards were prepared and stable isotope dilution analysis methods were validated, including for chiral analysis of these oxathianes. A number of studies were undertaken to explore the significance of the new oxathianes, and the relationship between thiol and oxathiane chirality was assessed.

4:30 Improved method for analysis of smoke glycoconjugates: a baseline study through phenological development Sarah E. Mayfield, James E. Foster, Hui Feng, Bruce S. Pan, Beth Anne McClure, bethanne.mcclure@ejgallo.com. E & J Gallo Winery, Modesto, California The growing incidence of wildfires in California subjects wine grapes to increasing risk of smoke exposure and potential sensory defects, which can be estimated through characterization of volatile phenol and non-volatile phenol glycoconjugate markers. While volatile phenol compounds are routinely measured among laboratories, phenol glycoconjugates require advanced instrumentation, limiting broader implementation of testing. We report significant adaptations to the literature method (Hayasaka, 2013), including changing from negative mode MRM to positive MRM, modifications to the mobile phase, and optimization of MRM transitions, ultimately yielding a ~10-fold improved reporting limit of 0.5 µg/L on the same HPLC-MS/MS instrument in negative mode. Additionally, sample preparation was streamlined for throughput by automation of solid phase extraction. Phenol glycoconjugate compounds are naturally occurring in grapes at relatively low levels in non-smoke impacted grapes and can change significantly after smoke exposure. In this study we demonstrate how phenol glycoconjugates develop during the course of grape maturation in Cabernet Sauvignon (n=19), Pinot noir (n=23), and Syrah grapes (n=17), as well as their extraction during small-scale fermentation. Total glycoconjugates rose throughout maturation and ranged from 4 µg/L to 9.8 µg/L for Cabernet Sauvignon, 4.2 µg/L to 14.4 µg/L for Pinot noir, and 7.8 µg/L to 31.2 µg/L for Syrah, as grapes progressed from 18 to 28 brix, corresponding to mid-berry ripening to commercial harvest. Our results demonstrate that baseline levels of total glycoconjugates increase in the absence of smoke exposure and provide context on the relevance of assessing risk prior to commercial fruit maturity.

4:55 Curse of dimensionality in chromatography: Custom software for four-dimensional LC × LC × IM – MS data analysis Jochen Vestner1, jochen.vestner@dlr.rlp.de, Pieter Venter2, André de Villiers2, Ulrich Fischer1. (1) Institut for Viticulture and Enology, DLR Rheinpfalz, Neustadt an der Weinstraße, Rheinland Pfalz, Germany(2) Chemistry and Polymer Sciences, Stellenbosch U., Stellenbosch, Western Cape, South Africa Comprehensive two-dimensional liquid chromatography (LC×LC) and ion mobility spectrometry-mass spectrometry (IMS-MS) are increasingly used to address the challenges associated with the analysis of highly complex samples. The complexity of natural products such as structurally diverse proanthocyanidins in grapes and wine emphasizes the necessity of improved chromatographic systems including intelligent coupling to sensitive and selective mass spectrometry technology. Hyphenation of comprehensive two-dimensional LC with IMS in form of a comprehensive three-dimensional LC×LC×IMS separation system coupled to high resolution – mass spectrometry significantly increases separation power for proanthocyanidins in grapes and wine. The gain of separation power results in very opulent and complex four-dimensional data structure. One of the main challenges of such a system is the lack of commercial software to accommodate the resulting four-dimensional data. We therefore developed a Python protocol using Jupyter notebooks for the extraction, visualization and interpretation of such data. Jupyter notebooks allow all methods of signal and data processing and even interactive visualizations. The user, however, needs programming skills to employ the notebooks. To make the data analysis approach available to analytical chemists without programming skills, we developed an interactive analytical browser application based on the Python package Plotly's Dash. The visualization of an extracted ion chromatogram (EIC) of the LC×LC×IMS-MS data is achieved by a 3-dimensional scatter plot representing the first and second dimension retention times and the IMS drift time on the x-, y- and z-axis of the scatter plot, respectively. Peaks appear as clouds of data points in this three-dimensional space. A mouse click on a data point shows the high-resolution mass spectrum in a separate bar plot. An example of the usage of the browser app includes separations of the procyanidin trimers (865 m/z) found in grape seed extract.

Methods, Data, and their Usage Towards Solving the Food Allergy Problem

2:05 Epitope mapping and cross-reactivity analysis of arginine kinases from Crassostrea angulate Fei Huan, Shuai Gao, Ling-Na Ni, Ming-Xuan Wu, Meng Liu, Guang-Ming Liu, gmliu@jmu.edu.cn. College of Ocean Food and Biological Engineering, Jimei U., Xiamen, Fujian, China Oyster has high nutritional value and is an important economic aquatic product in China. Arginine kinase is reported to be a major allergen in Crassostrea angulata (Cra a 2). However, little information is available about its antigenic epitopes and cross-reactivity. This study identified the linear and conformational mimotopes of Cra a 2 by using bioinformatics prediction combined with the phage panning method. Eleven linear epitopes of Cra a 2 (AA56~73, AA77~92, AA93~107, AA105~118, AA121~133, AA134~146, AA165~176, AA185~200, AA227~238, AA236~247, AA306~323) were verified by synthetic peptide technique. IgE-binding activity of four mutants (L7A, M187A, Q227A, and H277A) was significantly reduced by site-directed mutation of key amino acids in conformational mimotopes, indicating that four conformational epitopes of Cra a 2 were identified. Moreover, The cross-reactivity of Cra a 2 among oysters, shrimp, and crab was confirmed. The IgE epitope AA121~133 and AA134~146 were found to be the most conserved, suggesting that these two epitopes may be one of the main reasons for the cross-reactivity of Cra a 2 between crustacean and mollusks. In conclusion, eleven IgE linear epitopes and four IgE conformational epitopes of Cra a 2 were identified. The cross-reactivity of arginine kinase between crustaceans and mollusks was confirmed, and the conserved epitopes AA121~133 and AA134~146 were found. Based on these findings, the antigen epitopes of Cra a 2

can be subsequently modified by processing or deleting epitopes to obtain hypoallergenic products.

2:30 Identification of two novel major allergens in white-fleshed and red-fleshed pitaya seeds Mengzhen Hao, mengzhen.hao@hotmail.com, Huilian Che. College of Food Sci. and Nutritional Engineering, China Agricultural U., Beijing, China White-fleshed pitaya (Selenicereus undatus) and red-fleshed pitaya (Selenicereus costaricensis) are becoming increasingly popular because of their nutritional benefits and taste. Consumption on pitaya increases at the same time pitaya allergy happens in daily life. Although clinical cases of pitaya allergy have been reported, the biochemical identities of allergens haven't been determined, which hinders molecular allergy diagnostic tests of pitaya allergy. Therefore, the study aims to explore what molecule in pitaya seeds is associated with pitaya allergy. Profiles of patients' IgE reactivity to pitaya seeds were analyzed in immunoblots, and purified natural proteins with capacity to bind specific IgE were subjected to peptide mass fingerprinting by LC-MS/MS based on chymotrypsin proteolysis. Biomolecular technologies were used to determine CDS region sequence. The glycosylation modification on natural allergens was tested by PAS staining. Allergens were produced in E. coli with recombinant pColdI vectors. The natural and recombinant allergens' IgE reactivity were analyzed in immunoblot. Fold characteristic and thermal stability were evaluated by CD and fluorescence spectra analysis. The activity of allergens inhibiting trypsin was detected by using substrate BAEE. At protein and nucleic levels, the two novel allergens are identified into Kunitz type protease inhibitors. These two natural allergens in pitaya seeds are glycoproteins with practical molecular weight of 21570.5 Da. The two natural allergens have thermal stability and refolding capacity. Recombinant allergens represent proper folded, predominantly β-sheet proteins, display ability to bind IgE and inhibit trypsin activity in vitro comparable to that of natural counterparts. IgE reactivity analysis in 10 patients who are suspectedly allergic to pitaya reveals that Kunitz type protease inhibitors are major allergens for patients sensitized to pitaya. This study firstly finds there exist allergens in edible seeds of pitaya. Meanwhile, Kunitz type protease inhibitors are found for the first time in the two species at the protein level. These findings expand the understanding of the allergen source species and enrich the protein database of these two species.

2:55 Screening and characterization of shark-derived VNARs against arginine kinase from Procambarus clarkia Yang Yang1,2, yangy@hxxy.edu.cn, Xinrong He2, Tengchuan Jin3, Guang-Ming Liu2. (1) College of Environment and Public Health, Xiamen Huaxia U., Xiamen, Fujian, China(2) College of Ocean Food and Biological Engineering, Jimei U., Xiamen, Fujian, China(3) U. of Science and Tech. of China, Hefei, Anhui, China Arginine kinase (AK) is reported to be a major allergen in crayfish (Procambarus clarkii). However, little information is available about its allergic epitopes. Shark-derived variable domains of new antigen receptors (VNARs) are the smallest antibody fragments with flexible paratopes that can recognize protein motifs inaccessible to classical antibodies. The present study reported three VNARs binders (VNAR-11, VNAR-56, and VNAR-95) isolated from Chiloscyllium plagiosum immunized with AK from P. clarkii. Biolayer interferometry showed that the VNARs with their Fc fusions bound to AK with an affinity KD ranging from 0.2131 to 465.3 M. The bio-panning of phage display random peptide library using VNARs as target proteins identified the amino acid component of antigen-antibody interaction sites. With the help of bioinformatic analysis, the interaction sites were mapped on a 1.5 Å crystal structure of P. clarki AK determined by X ray in the present study. The binding sites of VNAR-65 and VNAR-95 were in the structural similar regions among AK from invertebrate. Besides, they are distributed in thermal-resistant and digestion-stable epitopes, suggests the good potential applications of VNAR-65 and VNAR-95 in allergen detection of shellfish and its processed products. The achievements above may lay the foundation for the development of hypoallergic foods and the establishment of detection methods of shellfish allergen.

3:20 Dupilumab for treatment of food-dependent, exercise-induced anaphylaxis Liping Zhu1,2, pumc_zhulp@student.pumc.edu.cn, Rui Tang1,2, Qing Wang1,2, Hong Li1,2. (1) Allergy Department, Peking Union Medical College Hospital, Dongcheng-qu, Beijing, China(2) Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing Food-dependent, exercise-induced anaphylaxis (FDEIA) is a potentially life-threatening disorder that often occurs with exercise, and with a history of eating relevant foods within a few hours before onset. This disease is exceedingly rare with a prevalence was approximately 0.02%. No known therapies can prevent anaphylaxis. We present an 11-year-old boy with a history of recurrent anaphylaxis more than 10 times within 2 years. The patient was given the subcutaneous injection of dupilumab 7 times for a period of 33 weeks. During dupilumab treatments, the patient was exposed to culprit mushrooms plus exercises at least twice a month, surprisingly, no anaphylaxis occurred within this time. No published report has clarified the clinical implication of dupilumab treatment for food-induced IgE-mediated anaphylaxis, especially for FDEIA, a rare disorder. This case might provide a new clue about treatment with dupilumab which improves the severity of allergic reactions in a child with FDEIA. Meanwhile, wheat and shellfish are the most common foods associated with FDEIA in Asian populations, and wheat, other grains, and nuts are in Western populations. Now we report the FDEIA caused by mushrooms. Vigilance should be maintained in patient education, diagnosis, and care for this new allergen. And further research might be needed for mushroom allergens.

4:00 IgE epitope mapping: Data, techniques, and needs Yuzhu Zhang, yuzhu.zhang@ars.usda.gov. ARS-PWA-WRRC, USDA Agricultural Research Service, Albany, California Both linear and confirmational IgE binding epitopes may play crucial roles in food allergy. Although some information about the importance of conformational epitopes of food allergens is available, systematic mapping of confirmational IgE epitopes has yet to be reported. IgE epitope studies were mostly on linear epitopes. However, the vast majority of linear IgE epitope data obtained with various methods need to be improved. Widely used and recently developed techniques are reviewed, and their advantages, disadvantages, shortcomings, and the need for perfection are discussed.

4:25 Mechanism of sulfated oligosaccharide from Gracilaria lemaneiformis on regulating Treg cells differentiation in allergic response Qingmei Liu1, 435782572@qq.com, Chenfeng Liu2, Yu Zhou3, Wen-Hisen Liu3, Guang-Ming Liu1, gmliu@jmu.edu.cn. (1) College of Ocean Food and Biological Engineering, Jimei U., Xiamen, Fujian, China(2) Dept. of Cell Biology, School of Life Science, Anhui Medical U., Hefei, Anhui, China(3) State Key Laboratory of Cellular Stress Biology, Innovation Center for Cell Signaling Network, School of Life Sciences, Xiamen U., Fujian, China Allergic diseases have become a global health problem. Dietary intake with anti-allergic nutritional components to improve allergic constitution can provide accurate guidance for allergy patients' daily diet and moderate the immune imbalance of allergic patients. Marine-derived sulfated oligosaccharide from Gracilaria lemaneiformis (GLSO) was used as a research object in the present study. The effects of GLSO on food allergy and allergic asthma mice are explored. In the present study, the biological activity of GLSO on inhibiting allergic reactions is shown in not only

effectively relief diarrhea and intestinal inflammation in mice with food allergies, but also significantly inhibit lung inflammation in mice with allergic asthma. GLSO can inhibit the polarization of Th2 cells, significantly upregulate the differentiation and function of Treg cells, and playing a strong protective role in allergic organisms. Additionally, under the stimulation of T-cell receptors and cytokines, GLSO can directly up-regulate the formation of Treg cells, enhance the continuous proliferation of Treg cells, and effectively maintain the stability of Treg cells. Furtherly, the FoxO signal transduction pathway is up-regulated by GLSO, while the HIF-1 and mTOR signal pathways are inhibited in Treg cells. In conclusion, GLSO can promote the formation of Treg cells, and regulate the formation, proliferation, and stability of Treg cells, so as to exert the biological activity of inhibiting allergic reactions.

4:50 Immune consequences of food processing Soheila Maleki, soheila.maleki@ars.usda.gov. ARS-SEA-SRRC, USDA, New Orleans, Louisiana The prevalence of peanut allergy has more than tripled in the U.S. in the last 20 years with an estimated annual cost of $4-$7000 per child. Meanwhile, it is not known why certain proteins in foods are allergenic and others are not. Also, while progress some has been made, the specific contribution of food processing to allergenicity is not known at the molecular level. Roasted peanut proteins can form higher order structures (oligomers), are less soluble, more resistant to digestive enzymes, and bind higher levels of IgE than raw peanut proteins. We also show that in the majority of patients, roasted peanuts resulted in a higher skin prick test (SPT) reactivity. To determine if processing-induced structural changes in allergens contribute to an increase in IgE binding by roasted peanuts, the major allergens were purified from raw and roasted peanuts and while the secondary structures did not show significant changes, the IgE binding and SPT to the roasted samples were higher. However, deliberate unfolding of Ara h 1, a major allergen, resulted in a significant reduction in the IgE binding. Therefore, it is highly likely that structural components of an allergen and processing induced chemical modifications contribute to enhanced IgE binding in roasted peanuts. The specific modifications that contribute to enhanced IgE binding by sera from allergic individuals and uptake by immune cells were identified by LCMSMS. Understanding the effects of processing at the molecular level and determining the differences in structure, function, and IgE binding to various processed foods will contribute to the development of more specific and improved detection, diagnostic, therapeutic tools for food allergy.

Food Security: The Role of Alternative Protein Sources in Addressing World Hunger

2:05 Genotypes and extraction methods impact pea protein composition, structure and techno-functional properties Lingyun Chen, lingyun.chen@ualberta.ca. Agricultural, Food and Nutritional Science, U. of Alberta, Edmonton, Canada Plant-based food products have taken a center stage in product innovation in food industry. This trend has spurred academic and industrial communities to explored towards diversified plant protein sources. Legumes, consisted of 18–30% protein, are important and affordable protein sources around the world. Pea proteins have attracted more attention due to their sustainability, balanced amino acid profile and low allergenicity. This study revealed that both genotypes and extraction methods significantly impact pea protein compositions and subsequently the protein ingredient techno-functional properties. Breeding of pea genotype has long been driven by the yield, disease resistance and protein content without considering the functionality of protein. This research analyzed proteins from different pea genotypes. Although the protein samples shared similar secondary structures, they had significantly different 11S/7S ratios. The functionality study suggested correlation between 11S/7S ratio and protein functionalities. The pea protein samples with higher 11S/7S ratios showed relatively lower solubility, but higher emulsifying and foaming capacities. The higher surface hydrophobicity of 11S may facilitate the reduction of oil/water or air/water interface tension. The protein recovery methods also directly determine the protein composition. Those obtained by ultrafiltration contained albumins, whereas the alkaline-isoelectric precipitation and micellar precipitation methods specifically retained globulins. Pea proteins prepared by alkaline solution had higher 11S/7S ratio. Pea proteins extracted by micellar precipitation or ultrafiltration formed superior gels with a compressive strength of 60–80 kPa, comparable to soy protein gels. The appropriate level of 7S allowed unfolded proteins to aggregate in a more organized manner through intra-floc links during heating. In summary, these studies demonstrate potential to use breeding technology to select pea genotype for specific functionality as food ingredients. In addition, by modulating the protein composition through extraction methods, stronger gels can be achieved for wider applications of pea protein.

2:25 Legume seed storage proteins are abundant with amyloid-forming sequences Derek Dee, ddee@mail.ubc.ca. Faculty of Land and Food Systems, The U. of British Columbia, Vancouver, Canada Fibrillation of food proteins is widely studied as a way to enhance protein functionality to form gels, films, coatings, and other materials. Legume proteins can be induced to self-assemble into amyloid-like fibrils (protein aggregates that are ~10 nm wide and ~1000 long). Fibril assembly can be induced by heating at low pH that causes hydrolysis, and a subset of the protein fragments assemble into fibrils. The core region of the fibrils is composed of β-sheets aligned perpendicular to the long fibril axis, with flanking surface-exposed regions of poorly-defined structure. Fibrillation of crude protein concentrates or isolates results in a heterogeneous mix of fibril morphologies, yet the exact identities of these amyloid-forming protein fragments is largely unknown. Here, LC-MS/MS was used to identify the fibril core regions of seed storage proteins from pea and soy, along with a bioinformatics analysis of lupin, pea, peanut and soy. The experimental and prediction results were generally in agreement, revealing dozens of fibril core peptides from each of the 7S and 11S proteins. Pea 7S globulins were found to be particularly rich in amyloid regions (108 unique peptides), while soy 11S had the least (43). The core regions were, on average, 11-13 aa in length. While each 7S and 11S variant had some unique amyloid regions, many were also mapped to conserved regions (across variants from the same plant and different plant sources). The abundance of amyloid-forming regions (average of 1 region/45 aa across 70 proteins), including in conserved domains, may indicate a biological role. Indeed, there is recent evidence that seed storage proteins form amyloid in vivo. Insight into the amyloid-core forming regions will be key to the rational design of novel food/materials using nanofibrils derived from legume proteins, and to understanding their biological roles.

2:45 Structural and functional properties of green lentil protein isolates obtained by pH-shift and membrane ultrafiltration Rotimi Aluko, rotimi.aluko@umanitoba.ca. Food and Human Nutritional Sciences, U. of Manitoba, Winnipeg, Canada Green lentils are an important group of cultivated legumes but utilization of the seed proteins as food ingredients is scanty due to limited information on their structural and functional properties. Protein isolation using wet fractionation protocols, especially the pH-shift method is widely used to produce novel food ingredients but the use of green lentils for this purpose is not common. Therefore, the aim of this work was to produce green lentil protein extracts using the traditional isoelectric pH precipitation and compare with membrane-based methods. For the membrane isolation, green lentil was extracted with 0.1 M NaCl or an alkaline solution, followed by membrane

ultrafiltration to remove salts and non-protein materials. Results showed significantly ($P<0.05$) higher protein yield of 48.81% for the isoelectric isolate when compared to 35.05% and 13.35% for the alkaline and NaCl isolates, respectively obtained through ultrafiltration. Protein content was significantly ($P<0.05$) higher for the NaCl extract (90.28%) than the 86.13% and 82.55% for the isoelectric and alkaline isolates, respectively. At pH 3-5, the NaCl and alkaline protein isolates had 27.78-40.98% and 25.74-27.22% protein solubility, respectively when compared to 2.26-11.84% for the isoelectric isolate. However, the isoelectric isolate had significantly ($P<0.05$) higher protein digestibility of 89.82% when compared to 77.87% and 77.61% for the alkaline and NaCl isolates, respectively. The alkaline and NaCl isolates had significantly ($P<0.05$) higher sulfur containing amino acids than the isoelectric isolate. Surface hydrophobicity was significantly ($P<0.05$) higher for the isoelectric pH and NaCl extracted proteins when compared to the alkaline extracted protein. Near-UV circular dichroism spectra showed that the alkaline extracted protein had loose tertiary conformation in comparison to the more compact structures of the isoelectric pH and NaCl extracted proteins. At pH 3 and 5, the NaCl extracted proteins were better emulsifiers with smaller oil droplet size of the emulsions when compared to the isoelectric and alkaline extracted proteins. In contrast, at pH 7 and 9, the NaCl extracted proteins had poorer emulsification (bigger oil droplet sizes) than the isoelectric and alkaline extracted proteins. However, foaming capacity was significantly ($P<0.05$) higher for the isoelectric extracted proteins than the NaCl and alkaline extracted proteins.

3:05 Simple post extraction approaches to the improvement of interfacial properties of pulse proteins Jiajia Rao, jiajia.rao@ndsu.edu. North Dakota State U., Fargo Recently, the utilization of pulse protein has been raised a remarkable interest because of its nutritional benefits, and it offers a lower environmental impact. However, the application of plant proteins is still underutilization due to its poor functional properties. For instance, the abilities of pulse proteins to adsorb at oil/water or air/water interfaces are limited due to their compact structure with multiple subunits largely linked through hydrophobic patches. To overcome the above limitation on pulse proteins, a number of techniques have been developed to modify the structure properties of pulse proteins for improving their foaming and emulsifying properties. These include ultrasound, heat treatment and pH shift. In this presentation, pea protein isolate (PPI) will be selected as a pulse protein representative. This talk begins with a brief introduction of hierarchical structure of PPI material to better understand the structure characteristics. It will comprehensive discussed the impact of ultrasound, heat treatment, pH shift and their combination on protein secondary structure, kinetic adsorption and rheological interfacial properties of pea fraction (e.g., vicilin) at interface, and then to research its relationship with foaming and/or emulsifying properties. In general, foaming properties could be greatly enhanced by means of pH-shift, controlled heating and their combination methods because these processing aid irreversibly disrupted the original large micron-sized aggregates in untreated protein samples and change their secondary structure of PPI. For instance, the secondary structure of the pea vicilin was changed (e.g., decreased β-sheet content, increased α-helix and β-turn contents), the ability of the protein to increase the interfacial pressure ($D\pi$), and the rates of protein diffusion (Kdiff) was increased. Consequently, the foaming capacity was increased. Our results suggested that protein structure function researches are valuable in tailoring proteins for specific functional outcomes and expanding the availability of pulse proteins as foaming agent in variety of food application.

3:25 Effects of microalgae and mung bean protein combination on 3D printing of seafood analogs Poornima Vijayan, e0383697@u.nus.edu, Dejian Huang. Food Sci. and Tech., National U. of Singapore The employment of 3D printing technology using sustainable alternative protein sources can potentially aid in resolving global food challenges by offering customizable and nutritious food products. Recently, seafood mimics using alternative proteins are gaining traction due to the growing concerns associated with unsustainable practices such as overfishing, heavy metal contamination, and so on. Mung bean protein is an undervalued by-product of the mung bean starch noodle industry, which can be utilized for the development of high-protein seafood mimics. Another such sustainable protein source is microalgae, which is gaining interest due to its high protein content and technologically functional properties. We incorporated them into an ink-based formulation and applied them to a 3D food printer to obtain layer-by-layer deposition to simulate seafood products. The printing performance and characteristics were studied regarding rheology, microstructure, and post-processing stability of 3D-printed seafood analogs. The effects of gellan gum and calcium chloride solution (5 mM) in varying proportions were evaluated to obtain a printable, self-supporting three-dimensional structure. The ink exhibited shear-thinning behavior, and it was observed that adding microalgae protein up to 5% further improved the viscosity, printability, and self-supporting characteristics of the printed structure. The research contributes to the development of plant-based seafood analogs using natural and sustainable alternative protein sources via 3D printing technology.

3:45 From traditional to alternative fish analog: Considerations toward texture development in cell-cased fish **S. Chuah**, R. Omidvar, B. Zhang, A. Odabasi, C. Sims, R.M. Schneider, A. Porras, R. Farzad NO ABSTRACT

4:35 Effects of oil content on the structural and textural properties of cottonseed butter products Zhongqi He, zhongqi.he@usda.gov, Stephen Rogers, Sunghyun Nam, K. Thomas Klasson. USDA-ARS Southern Regional Research Center, New Orleans, Louisiana Plant-based (nut and seed) butters have steadily increased in consumer popularity due to their unique flavors and healthy nutritional properties. Oil content is a critical parameter to create plant butter products with the proper consistency and stability. Pervious work has shown that glandless cottonseed can be used to formulate cottonseed butter products to increase the values of cottonseed. As part of the effort on valorization of cottonseed, this work evaluated the effects of the oil content on the microstructural and textural properties of cottonseed butter. While the oil content in the raw cottonseed kernels is 35% of the kernel biomass, additional cottonseed oil was added to make the cottonseed butter products with six oil content levels (i. e., 36, 43, 47, 50, 53 and 57%). The water activity of these products were between 0.445 and 0.310. The values of three textural parameters, firmness, spreadability, and adhesiveness, decreased rapidly in an exponential mode with the increasing oil content. The oxidation stability with a rapid oxygen measurement was gradually reduced from 250 min with 36% oil to 65 min with 57% oil. The particle size population in these butter samples was characterized the similar trimodal distribution with the majority in the middle mode region of particle size around 4.5-10 micrometers as shown by B50 (Fig. 1). Higher oil content decreased the butter particle size slightly. The results of this work provided information for further optimization of formulating parameters of cottonseed butter products.

4:55 Improvement of the solubility of glandless cottonseed protein isolate for fortified beverage applications Heping Cao, heping.cao@usda.gov, Kandan Sethumadhavan, Scott Pelitire, Zhongqi He, K. Thomas Klasson, thomas.klasson@usda.gov. Southern Regional Research Center, USDA Agricultural Research

Service, New Orleans, Louisiana Cottonseed is classified as glanded or glandless depending on gossypol glands. The presence of toxic gossypol in glanded seed limits this vast protein resource to use primarily for feeding ruminants. Glandless cottonseed present only trace levels of gossypol. may be useful as human food and non-ruminant animalsfeed sources. However, low solubility of seed protein is a major factor affecting its beverage applications. The objective of this study was to improve the aqueous solubility of glandless cottonseed protein isolate (CSPI) by pH adjustment and active additives. CSPI was purified from glandless cottonseed by NaOH solubilization and HCl neutralization. The CSPI (91.71 ± 0.13% of protein) was treated with various buffers with pH 2-10.6, a range of NaOH concentrations and different types of detergents. CSPI showed the highest solubility at pH 2.0 and pH 10-10.6, and the lowest solubility at pH 6. Temperature change from 25 to 37°C significantly increased cottonseed protein solubility. Protein solubility was maximal under 0.1 N NaOH and reduced to half by 1N NaOH. Most of the detergents increased the solubility of the protein isolate but anionic detergents decreased the solubility. The order of solubility was CTAB > BRIJ 35 > Triton X-100 > NP40 > Chaps > Tween-20 > Tween-80 > Water = DMSO > deoxycholic acid > SDS. The protein solubility was only significantly increased by size reduction of protein particles under Brij 35 treatment. UV absorbance at 280 nm and Lowry methods gave higher concentration of the protein than those of BCA and Bradford methods. Cottonseed peptides after trypsin digestion significantly inhibited the viability of mouse macrophages after treatment with 40-80 µg/mL for 24 h. The results provided useful information for increasing the solubility of glandless cottonseed protein for developing protein-fortified acidic juices and drinks.

5:15 Improving legume protein flavor and functionality with exogenous polyphenols Audrey Girard, algirard@wisc.edu. Food Sci., U. of Wisconsin-Madison As a broadly used food ingredient, legume-derived proteins would benefit from bland or minimal flavor profiles. Yet, processing legumes yields unintended flavors, namely significant lipid-derived off-flavors, with few technological solutions available. Further, because legume proteins are often used in meat mimetics and bakery goods, they would also benefit from contributing desirable rheological properties. Our work seeks to modify legume proteins with plant polyphenols known to display important reactivities. Flavonoids are a prominent dietary polyphenol group and are comprised of two phenolic rings with a base carbon structure of C6-C3-C6. Studies from our lab demonstrate that flavonoids reduce the presence of lipid oxidation products in legume ingredients and react with key protein systems to alter their structure-forming properties. For instance, adding catechin, tannic acid (TA), grape seed extract (GSE), and green tea extract (GTE) to model pea and soy protein solutions reduced lipid oxidation products known to contribute to off-flavors. Specifically, TA, GSE, and GTE reduced the secondary lipid oxidation products in pea and soy proteins by an average of 75% and 50%, respectively, compared to the control, versus catechin's 61% and 13%, respectively. TA, GSE, and GTE galloylation and polymerization likely allowed these polyphenols to interact more effectively than catechin with proteins, especially lipoxygenase. However, no significant differences between the samples' antioxidant capacities were observed, measured with FRAP and ABTS methods. Thus, polyphenols predominantly reduced lipid oxidation via interactions with proteins, rather than through polyphenol electron transfer or radical quenching. In complement, research on flavonoid contributions to legume protein-based structure formation is ongoing. Current results concur with previous studies that flavonoid interactions with proteins yield beneficial structure and rheological properties. Highly polymerized flavonoids from sorghum (DP ~19) interacted with pea, fava bean, and lentil proteins through covalent and non-covalent interactions, thus effectively increased protein MW. Further, proteins extruded with sorghum flavonoids (0.1% w/w) to form puffs had 15% greater expansion than non-treated proteins. Altogether, our work indicates that the inclusion of selected flavonoids is a novel solution to improve legume protein flavor and function, which will improve their quality and consumer acceptance.

5:35 Molecular interactions between pea protein isolate and saccharide with various molecular mass during the course of Maillard reaction Bingcan Chen, bingcan.chen@ndsu.edu, Jiajia Rao. North Dakota State U. College of Agriculture Food Systems and Natural Resources, Fargo Pea protein isolate (PPI) has earned a reputable status as natural and substantial plant protein in numerous sectors such as food, agriculture, packaging, and biomedical fields. As functional food ingredients, its inferior solubility and prominent off-odors lower consumer acceptability in food system. In this study, diverse saccharides are effectively grafted to PPI through Maillard-driven chemistry. The development of conjugates (glyco-PPI) was validated by ultraviolet–visible spectroscopy, sodium dodecyl sulfate-polyacrylamide gel electrophoresis, and size exclusion chromatography–high performance liquid chromatography. The impact of covalent conjugation on color development, structural modification, solubility, thermal stability, and volatiles of glycoprotein was examined. The protein solubility was improved, while its thermal stability seemed to be negatively influenced. The principle proposed involves Maillard-driven generation of the conjugates, which enhanced the surface hydrophilicity and unfolding of protein architecture of glyco-PPI. Additionally, both molecular mass and the grafted number of saccharides played a vital role in determining the solubility and thermal stability of glyco-PPI. The findings from this study could furnish valuable in-depth information for dictating functionalities of plant-based protein for food application.

SUNDAY EVENING

General Posters [note – Monday Evening Sci-Mix includes the first 36 posters listed below (SM01-SM36)]

SM01 Post-storage aroma alteration of vacuum-packaged Virginia hops Xueqian Su[1], xueqians@vt.edu, Yun Yin[1], Yixiang Xu[3], Laban Rutto[2], Ken Hurley[1]. (1) Food Sci. and Tech., Virginia Polytechnic Inst. and State U., Blacksburg(2) Agriculture Research Station, Virginia State U., Petersburg(3) Western Regional Research Center, USDA-ARS Healthy Processed Foods Research, Albany, California Hop (Humulus lupulus L.) is known as an essential ingredient in beer brewing that can impart unique flavor to the beer products. With the everlasting consumer passion for locally sourced ingredients and rapid growth of craft breweries, hop has become an emerging specialty crop in Mid-Atlantic. Due to the high perishability of fresh hops, majority of local craft brewers utilize large amount of dried and packaged hops. Vacuum packaging holds potential advantages in oxygen and light protection. This study is the first to evaluate the effectiveness of three popular packaging materials, polyamide/polyethylene (PA/PE), oriented polypropylene/foil/polyethylene (OPP/Foil/PE) and ethylene vinyl alcohol (EVOH), on hop aroma and color over 8 months of refrigerated storage. Cascade hops harvested from Randolph Farm (Petersburg, Virginia) at their optimal ripeness (25% dry matter) were kiln-dried at 52°C until the final moisture content of 8~10% was reached. Hop cones with no apparent defects were selected visually for vacuum packaging and refrigerated storage using PA/PE, OPP/Foil/PE and EVOH, respectively. Solvent-assisted flavor evaporation-gas chromatography-mass spectrometry (SAFE-GC-MS) was performed to analyze the aroma alteration of vacuum-packaged hops. Color attributes were also monitored. SAFE-GC-MS analysis identified 30 aroma compounds in dried hops over storage.

No significant change was observed in concentrations of most aroma compounds during refrigerated storage, except significantly increased contents of p-cymene and trans-α-bergamotene. The most-interesting finding was that packaging material was not a significant factor altering the concentrations for most aromas during refrigerated storage. EVOH-packaged hops, however, showed markedly higher contents of methyl (4E)-4-nonenoate and β-myrcene. Meanwhile, post-storage color degradation was remarkable in all dried hops regardless of the packaging materials while the color distinction among PA/PE, OPP/Foil/PE and EVOH-packaged hops was not significant over 8-month of storage. The minimal material influence on the hop aroma and color offered the possibility of utilizing PA/PE as an affordable packaging strategy to replace standard foil packaging for small and median scale growers.

SM02 Developing chitosan particles as biocompatible carrier Hong-Yi Huang[1], Chenche Hsieh[2], Ming-Hsu Chen[1], Hsiao-Chu Huang[1], Kuan-Chen Cheng[1,2], kccheng@ntu.edu.tw. (1) Institude of Food Sci. and Tech., National Taiwan U., Taipei(2) Inst. of Biotechnology, National Taiwan U., Taipei $PM_{2.5}$ can induced the inflammation via elevate intracellular ROS in alveolar macrophage. Previous study found the fermented Chenopodium formosanum extract could elevate MH-S cell's intracellular ROS and viability when MH-S cell is cultured with $PM_{2.5}$. We want to deliver the fermented Chenopodium formosanum extract to alveolar macrophage more efficiently via pulmonary route. Therefore, we want to investigate biocompatible carrier for making extract more easily be inhaled. The experimental results show that chitosan particle size is 400 nm or less. The surface shape is irregular and the charge is -0.355 mV, which is close to electroneutrality. These factors are far from the characteristics that macrophages tend to engulf(smooth surface, round shape, size 1 - 6 mm, positive charge). Blank chitosan particle take up to 1,000 ppm for showing around 80% cell viability and no significant difference in intracellular ROS on MH-S cell. And it take only half concentration of extract compared with positive control. It shows a potential for further investigating chitosan particle into pulmonary drug carrier.

SM03 Chemical characterization and quantitative determination of flavonoids and phenolic acids in yerba santa (Eriodictyon spp.) using UHPLC/DAD/Q-ToF Mei Wang[1], meiwang@olemiss.edu, Jianping Zhao[2], Bharathi Avula[2], Joseph Lee[2], Roy Upton[3], Ikhlas Khan[2]. (1) Natural Products Utilization Research Unit, Agricultural Research Service, USDA, U., Mississippi(2) National Center for Natural Products Research, U. of Mississippi(3) American Herbal Pharmacopoeia, Scotts Valley, California Eriodictyon species, commonly known as yerba santa, are plants native to the Southwestern US and Northern Mexico. The plants are known for their medicinal properties and have been used by indigenous people for centuries to treat various ailments, in particular, respiratory conditions. Despite a long history of traditional use, many of the species have never been fully chemically characterized and the constituent range of the species has not been comprehensively reported. In an effort to establish a quality control and chemical characterization method, an extensive set of Eriodictyon species samples including E. californicum (n = 85), E. angustifolium (n = 8), E. trichocalyx (n = 5), E. crassifolium (n = 9), E. tomentosum (n = 2), E. traskiae (n = 1), and E. capitatum (n = 1) were investigated. Fourteen compounds from flavonoids and phenolic acids were quantified utilizing an UHPLC/DAD/Q-ToF method. The results from the method validation demonstrated excellent linearity (R^2 >0.99) and sensitivity as evident by LOD (0.01-0.1 μg/mL) and LOQ (0.05-0.11 μg/mL). Likewise, the method was found to be precise (RSD < 2.78%) with recoveries between 88.9-103.2%. Furthermore, the method using UHPLC/ESI/Q-ToF data and protonated, deprotonated, and adduct and fragment ions in positive and negative ion modes were able to identify 53 compounds in yerba santa plant samples. To the best of our knowledge, this work encapsulates the most comprehensive data set currently available for the chemical characterization and quantification of the primary constituents in Eriodictyon species. Additionally, results of this study also demonstrated the applicability of the developed method for quality assessment of raw material and commercial herbal products containing different Eriodictyon species.

SM04 Encapsulation of anthraquinones extracted from the Aloe-vera plant into casein micelles by ultrasonication Uzma Sadiq, uzma.sadiq113@gmail.com, Harsharn Gill, Jayani Chandrapala. School of Science, RMIT U., Melbourne, Victoria, Australia Aloe vera is an excellent source of anthraquinones (Aloin, aloe-emodin, rhein) contains almost 30% of it. Although , aloe vera is being used in health and laxative drinks since decades, However, the available information concerning the effect of food processing on the degradation of anthraquinones during preparation of these drinks is limited. The degradation of those anthraquinones begins right after harvesting the Aloe vera. So, encapsulating these anthraquinones seems an efficient approach for food formulators. Casein micelles (CM) own specific structural and physicochemical properties that might be able to encapsulate these anthraquinones ; as CM possess hydrophilic and hydrophobic domains to interact with these bioactives. Although much work has been executed concerning casein micelles as an encapsulating device for drugs and nutraceuticals, there is hardly any work on the encapsulation of anthraquinones extracted from Aloe vera through ultrasonication. Therefore, this study aimed to encapsulate anthraquinones (aloin, aloe-emodin, rhein) extracted from the Aloe vera plant; (anthraquinone extracted powder (AQ), Spray dried powder (SDP), freeze-dried powder(FDP) and whole leaf gel (WLAG) of Aloe vera within CM. The results showed that he AQ powder had the maximum encapsulation efficiency (EE%) (aloin 99%, aloe-emodin 98%, and rhein 100%) and encapsulation yield while WLAG had the least EE%. A significant increase in size and zeta potential were related to superficial coating instead of encapsulation in SDP and FDP. The considerable variability in size, zeta potential, and EE% were related to anthraquinone type, its binding affinity, and its ratio to CM. FTIR spectra confirmed that the structure of the casein micelle remained unchanged with the binding of AQ powder except in CM loaded with whole-leaf aloe vera gel (CMWLAG), where the system was deformed. More studies are required to determine the steadiness of casein micelles-loaded nanocapsules and their impact on human physiological functions such as digestion and bioavailability.

SM05 Polyphenols improve the biological activity and functional properties of soybean meal hydrolysates Xiaoying Zhang1,2, xiaoyingz@umass.edu, Hang Xiao2, Shuang Zhang1, Yang Li1, Hengjun Du2. (1) Northeast Agricultural U., Harbin, China(2) U. of Massachusetts Amherst Soybean meal, a widely applied animal feed, will result in the waste of resources and restriction of economic benefit. Enzyme hydrolyzation is reported as an effective way to produce soybean meal hydrolysates (SMHs, polypeptides) from the by-product, which shows various biological activities and health-promoting effects. Therefore, the preparation of polypeptides from soybean meal by protease is an alternative to utilize this by-product. However, the poor emulsification of SMHs limits their application in the food industry. In this study, we investigate the effect of polyphenols on the biological and functional properties of SMHs. In this work, the structure, biological activity, and functional characteristics of SMHs with different polyphenols via non-covalent interactions or covalent interactions were investigated. The result showed that interaction with polyphenols significantly altered the structural and functional characteristics of proteins, and polyphenols

were supposed to enhance the biological activity and emulsification of SMHs. We found that epigallocatechin (EGCG), gallic acid (GA), caffeic acid (CA), and, especially, proanthocyanidins (PC) could improve the functional properties of SMHs via covalent interactions. The complexes herein are potential candidates for functional food supplements, providing guidance for exploring the application of polyphenols with soybean meal hydrolysates. Furthermore, improve the by-product utilization of soybean meal.

SM06 Regulated competitive reactions and low carbon footprint in glycerol organosolv pretreatment integrated fast pyrolysis of lignocellulosic biomass Yingchuan Zhang1, yczhangh@connect.hku.hk, Zhengxiao Guo1,2. (1) Dept. of Chemistry, The U. of Hong Kong(2) Dept. of Mechanical Engineering, The U. of Hong Kong Glycerol organosolv (GO) pretreatment integrated fast pyrolysis is an efficient approach to obtaining fermentable sugars from lignocellulosic biomass. However, how the pyrolysis process consisting of numerous reactions was selectively enhanced remains unclear. Here, the compositional and structural amelioration in GO pretreated biomass was associated with the cellulose depolymerization kinetics. Py-GC/MS first suggested that levoglucosan producing reactions (LPRs), mainly glycosidic bond cleavage, were promoted. In contrast, sugar degradation reactions (SDRs) like glucosyl ring scission and rearrangement to light oxygenates were impeded. Thermogravimetric analysis and kinetic study further confirmed the regulated competitive reactions led to a kinetically controlled pyrolysis with activation energy increased from 18.3 to 33.4 kJ/mol. Owing to upgrading use of crude glycerol, life cycle assessment suggested that the environmental impacts of the integrated process were less than those of the typical acid pretreatment and petroleum-based processes, indicating the eco-friendless of organosolv pretreatment for levoglucosan and biofuel production from biomass.

SM07 Effect of ultrasound on the level of volatile compounds, total polyphenols, total flavonoids, and isoflavones in soymilk processed with microwave-roasted black soybean (Glycine max (L.) Merr) Yoojeong Lee, ashley4534@naver.com, Minju Lee, Kwang G. Lee. Dongguk U., Jung-gu, Seoul, Korea (the Rep. of) In this study, the volatile compounds, total polyphenols, total flavonoids, and isoflavones (daidzein, genestein, daidzin, genistin, glycitin) were analyzed after ultrasonic treatment in soymilk processed with microwave-roasted black soybean (Glycine max (L.) Merr). The microwave roasting conditions were 700W and 270s, and black soymilk was treated with ultrasound in three types of amplitude (30, 60, 90%) for 3, 5, 7 and 9 minutes. A total of 23 volatile components were analyzed, and soymilk processed with microwave-roasted soybeans did not contained off-flavors including (E)-2-Heptenal, (E)-2-Octenal, (E,E)-2,4-Decadienal, and 2-Pentyl furan. In soymilk treated with ultrasound, 1-Hexanol and 1-Octen-3-ol, which are unpleasant soybean flavors, were reduced by up to 96.13% and 93.04%, respectively, compared to the control. The highest OIR value in soymilk with microwave-roasted soybean was 2,3-Diethyl-5-methylpyrazine, a baked flavor, which significantly increased during ultrasonic treatment ($p<0.05$). The content of total isoflavones, polyphenols, and flavonoids was significantly increased in ultrasonically treated samples ($p<0.05$). However, the total polyphenol and flavonoid content of the samples treated with ultrasound for 9 minutes decreased. This study discusses the applicability of microwave-roasted soybeans to soymilk and provides information on the effects of volatile compounds, total polyphenols, flavonoids and isoflavones in soymilk during ultrasonic treatment.

SM08 Exploring the processing technology of a new healthy yogurt with Kombucha and taro Ruolin Song, songruolin419@163.com, Huilian Che. China Agricultural U., Beijing Kombucha is a kind of sweet and sour pure natural health drink, which is composed of three kinds of microorganisms that are beneficial to human health -- yeast, acetic acid bacteria and lactic acid bacteria. After fermentation, Kombucha liquid not only retains tea polyphenols, but also contains some fermentation metabolites such as gluconic acid, lactic acid, D-glucaric acid-1, 4-lactone, etc. These active substances can be absorbed into the body and play a series of nutritional and health care functions, such as anti-cardiovascular diseases, improving digestive ability, stimulating the immune system, and reducing inflammation. Taro contains a kind of mucus protein, which can promote the production of immunoglobulin or antibody globulin which can enhance the body's resistance. This project aims to obtain a new healthy yogurt with good color and taste, explore the best processing technology of yogurt with Kombucha and taro, in order to get a new yogurt that could stimulate the immune system and provide other nutritional and health care functions. At present, we have finished single factor experiment and orthogonal test with fermentation time, fermentation temperature, sugar addition, taro addition and Kombucha addition as the influencing factors. In order to obtain the addition formula with the best flavor, the above experiments were evaluated by sensory scoring in terms of taste, acidity and sweetness, color, organization, delicacy, taste and odor. The optimal fermentation conditions of yogurt with Kombucha and taro were determined as follows: sugar 5%, taro 5%, Kombucha liquid 3%, fermentation time was 7h and fermentation temperature was 42°C. In future studies, we will explore the efficacy of taro yogurt with Kombucha by measuring DPPH free radical and hydroxyl free radical scavenging ability to determine the antioxidant capacity of taro yogurt with Kombucha, etc.

SM09 Analysis of furan and physicochemical properties in various nuts roasted with air fryer and microwave Jeong Eun Oh, ohrucy99@naver.com, Seungwoo Ha, Kwang G. Lee. Dongguk U., Jung-gu, Seoul, Korea (the Rep. of) A study was conducted to monitor the levels of furan and changes in physicochemical properties in various nuts roasted with air fryer and microwave. A total 70 samples of 5 different nuts (almonds, peanut, cashew nut, hazelnut, sacha inchi) were analyzed for furan levels using GC-MS combined automated headspace SPME. For the five nuts, furan concentrations were 1.11 – 2.39 ng/g before roasting. As air fryer and microwave roasting were progressed, furan levels were detected 6.39 – 165.52 ng/g and 11.47 – 183.87 ng/g, respectively. The results showed that the amount of furan increased drastically with increasing of roasting power and time. To investigate changes in physicochemical properties, the fatty acid compositions were analyzed by GC-FID. The content of polyunsaturated fatty acids (linoleic acid and linolenic acid) significantly decreased, whereas the content of saturated fatty acids (palmitic acid and stearic acid) increased during roasting. Color index of all nuts indicated a decrease in the L* value and an increase in the a* and b* value, resulting in a rise of browning index. The results of total phenolic contents and antioxidant activity increased up to 337 % and 218 %, respectively, as roasting progressed, but slightly decreased when roasting at 180 °C for 20 minutes in air fryer and at 700, 1000W for 5 min in a microwave oven. These findings can be used to determine the optimal conditions of air-fryer and microwave roasting.

SM10 Cellulose nanocrystals recycled from maple leaves as Pickering emulsion stabilizers for shrimp preservation Chuye Ji, jichuye@qq.com, Jiachen Wei, Yixiang Wang. Food Sci. and Agricultural Chemistry, McGill U., Montreal, Quebec, Canada Canada is known as the land of maple leaf, but the utilization of dead leaves is limited. Considering the promising applications of nanocellulose as sustainable emulsifiers/stabilizers of Pickering emulsions, in this study, cellulose nanocrystals with different

crystalline allomorph were obtained from maple leaves and modified by octenyl succinic anhydride (OSA) to stabilize oil-in-water Pickering emulsions. Both CNC I (length: 220.5 nm, diameter: 13.0 nm) and CNC II (length: 66.7 nm, diameter: 6.5 nm) nanocrystals exhibited rod-like shapes, and CNC I nanocrystals modified with OSA at a mass ratio of 1.0/0.5 (CNC/OSA) exhibited the excellent emulsifying capacity and stability as demonstrated by the analysis of emulsion appearance, microstructure, droplet size distribution and ζ-potential. Cinnamaldehyde was loaded in the optimized Pickering emulsion, which showed the enhanced storage stability of cinnamaldehyde and the long-term antibacterial efficacy against Gram-positive and Gram-negative bacteria. The spray coating of cinnamaldehyde-loaded emulsions improved the inhibitory effect against the growth of bacteria and potentially inactivated psychrophilic bacteria responsible for shrimp spoilage during refrigerated storage to extend the shelf life of shrimp. Therefore, this work demonstrates the feasibility to recycle the abundant biomass waste - maple leaves as a new source of nanocellulose and the potential applications in seafood preservation.

SM11 Anti-inflammatory activity of extracts and two royleanone-type isomers isolated from Salvia sessei Benth Abraham Gómez-Rivera1, abraham.gomez@ujat.mx, Carlos Ernesto Lobato-García1, Ammy Joana Gallegos-García1, Nancy Romero-Ceronio1, Ricardo López-Rodríguez1, Cristian Barredo1, Maribel Herrera-Ruiz2, Manáses González-Cortazar2. (1) Division Academica de Ciencias Basicas, U. Juarez Autonoma de Tabasco, Cunduacan, Mexico(2) Centro de Investigación Biomédica del Sur, Instituto Mexicano del Seguro Social, Xochitepec, Morelos Introduction: Salvia sessei Benth is a species commonly known as "pipiloxochiltl" or "sabanito" in the state of Morelos, Mexico. It is used by cooking the aerial parts and later for washing affected areas with erysipelas. Only two reports have been found on this species, one in which a royleanone-type diterpene was isolated from its aerial parts, but without carrying out studies on its pharmacological activity, and the present one, which aimed to evaluate the anti-inflammatory activity of the organic extracts of the aerial parts of Salvia sessei Benth and of two isomers isolated from the species. Materials and Methods: The extracts of the aerial parts of S. sessei were obtained by maceration with solvents of increasing polarity (n-hexane, dichloromethane and methanol). The compounds sessein (1) and isossesein (2) were isolated from the dichloromethane extract by chromatographic techniques. The anti-inflammatory activity was evaluated in the mouse ear edema model at 1 mg/ear of the extracts and compounds (1 and 2). A dose-response curve was performed on the latter and the mean effective dose (ED50) was determined. Results: The hexanic (40.55 ± 0.5%), dichloromethane (56.01 ± 1.1%) and methanolic (66.0.5 ± 0.3%) extracts, as well as the isolated compounds 1 (79.85 ± 3.5%), and 2 (54.36 ± 1.7%) showed anti-inflammatory activity; the methanolic extract presented the highest percentage of inhibition, while the isolated compounds 1 and 2 did not present differences in their ED50, in addition, 1 had an effect similar to that of indomethacin, the reference drug evaluated at the same dose (75.24 ± 2.4%). Cpnclusions: The results show that the three extracts evaluated presented anti-inflammatory activity and the chromatographic separation of the dichloromethane extract allowed the isolation of isomers 1 and 2 of the royleanone-type, which also presented significant anti-inflammatory activities, thus validating the use in traditional medicine that has been given to the species.

SM12 Citrus pesticides unmasked: A surprising discovery on their effect on heathland ladybird chilocorus bipustulatus Ariela Kaspi-Kaneti1, ariela.w.kaspi@gmail.com, Shashwat Singh2, Alexs Protasov2, Roy Kaspi2. (1) Chemistry, U. of La Verne, California(2) Entomology, Agricultural Research Organization Volcani Center, Bet-Dagan, Israel The study focuses on assessing the chemical impact of commonly used citrus pesticides on Chilocorus bipustulatus, a beneficial predator of armored scale in citrus orchards. Laboratory bioassays were conducted using commercially available pesticide formulations, prepared at concentrations suggested by the manufacturer with and without mineral oil. Pesticides from various chemical families and with different mechanisms of action were tested for their toxicity. Our findings are surprising and highlight the importance of considering the chemical impact of pesticides on beneficial insects in citrus orchards.

SM13 Chemical marker's variation in Cecropia sp from Tabasco, Mexico Carlos Ernesto Lobato Garcia1, carlos.lobato@ujat.mx, Juan Antonio Alberto-Hernandez1, Abraham Gómez-Rivera1, Ricardo López-Rodríguez1, Eric Jaziel Medrano-Sanchez1, Manáses González-Cortazar2, Miguel Á. Vilchis Reyes1. (1) Division Academica de Ciencias Basicas, U. Juarez Autonoma de Tabasco, Cunduacan, Mexico(2) Centro de Investigación Biomedica del Sur, Instituto Mexicano del Seguro Social, Xochitepec, Morelos, Mexico Cecropia is a genus of plant that has been traditionally used to treat various ailments. Regarding the use of this plant for the treatment of diabetes, it has been stated that Chlorogenic Acid (CA) and Isoorientin (ISO) are chemical markers associated with this biological activity. An investigation was carried out to show the presence of these compounds in two species of Cecropia (C. peltata and C. obtusifolia) collected in the five regions of the state of Tabasco, Mexico. The samples were run on a HPLC/PDA (Waters 2695 separation module with a PDA Waters 2996 detector): a reverse-phase column (Supelcosil LC-F) was employed with a gradient elution system (solvent A: TFA 0.5% in water; solvent B: acetonitrile). The respective peaks for CA and ISO were identified in the chromatograms obtained. The areas under the curve of the peaks of interest were extrapolated in the corresponding calibration curves constructed from standards of both metabolites. This procedure made possible the identification of CA and ISO both qualitatively and quantitatively in the five hydroalcoholic extracts analyzed. These compounds presented variations related to their concentration, species and place of collection. In the case of CA, the C. peltata samples from Chontalpa and Pantanos regions showed concentrations above 20%, while in Centro and Ríos regions, the concentrations of this compound were below 10%. In the particular case of C. obtusifolia from the Sierra region, the CA concentration was below 5%. For ISO, the highest concentrations (above 10%) were found in the C. peltata samples from Ríos and Pantanos regions, whereas Chontalpa and Centro regions presented concentrations below 10% for this metabolite. In the case of C. obtusifolia from the Sierra region, the ISO concentration was just above 5%. In addition, the proportion between the concentrations of both compounds (CA/ISO) was also different in the five samples analyzed. In the case of C. peltata, the proportion of AC was higher than ISO in Chontalpa, Pantanos and Centro regions. For C. obtusifolia, from the Sierra region, AC was found in a lower proportion compared to ISO. These phytochemical variabilities may be associated with the plasticity of the plant, which derives from the conditions to which it may be exposed in its environment.

SM14 Alkaline solubilization and acid precipitation (ASAP) method for green extraction of polyphenolics from fruit peels Ningping Zhan, e0427573@u.nus.edu, Dejian Huang. Food Sci. and Tech., National U. of Singapore Fruit peels and seeds are considered as wastes but the contain good amounts of polyphenolic compounds that are valuable for nutraceutical/functional food ingredients. Yet, the current industrial extraction process of polyphenolic compounds utilizes large amount of organic solvents and depend on column chromatography and thus are not cost effective and environmentally

benign. We report here in a water based alkaline-solubilization and acid-precipitation (ASAP) method for selective extracting phytochemicals from fruit peels, particularly from mangosteen pericarp (MP) at room temperature. The ASAP extracts of MP revealed that it mainly contains α-mangostin with 38.56 ± 0.79 % while organic solvent extract (MP-A) and water extract (MP-D) contain 16.54 ± 0.18 % and 1.27 ± 0.04 % α-mangostin respectively. Compared with MP-A and MP-D, ASAP extract (MP-P) has higher α-amylase inhibition activity and anti-inflammatory activity (RAW 264.7 cell model). This ASAP green extraction method is a promising method for exaction of plant xanthones and could be applied on extracting other polyphenolics that have poor water solubility but higher solubility in alkaline water.

SM15 Production, purification and characterization of a local diatom fucoxanthin and polysaccharides by a spinner-flask-based photobioreactor system Min-Ying Wang1, mywang@dragon.nchu.edu.tw, Chen-Hao Lin1, Su-yuan Lai2. (1) Graduate Inst. of Biotechnology, National Chung Hsing U. College of Agriculture and Natural Resources, Taichung, Taiwan(2) Dept. of Food Sci. and Tech., Central Taiwan U. of Science and Tech., Taichung Diatoms are considered to be one of the most diverse photosynthetic phytoplankton species and hold an important place in ecology as they contribute approximately 20% of global primary productivity. Fucoxanthin in diatoms not only helps diatoms capture light energy to promote photosynthesis, but also achieves photoprotection, and therefore it plays an important role in establishing a high-efficiency light energy utilization system for diatoms. It has been believed that diatoms are promising sources for the production of novel biomolecules like fucoxanthin with potential novel bioactivities, i.e., anti-oxidant, anti-cancer and anti-inflammatory. In order to analyze the structure and function of fucoxanthin for the diatoms isolated from the coast of Taiwan for developing high-value products and expanding the prospective research of local diatoms, a local strain of diatom AQ9 has been cultured in the newly developed photobioreactors. These diatoms will be cultured in the photobioreactors with different media (f/2, 2.5f, 5f and 10f), with different culture methods (batch, fed batch and semi-continuous). Two types of photobioreactors with a working volume of 500 mL and 8L will be employed to study the scale-up process for diatom growth and fucoxanthin production. The active substances of diatoms can be divided into two parts, one is a small molecule compound - fucoxanthin; the other is a large molecule - sulfate polysaccharides. Finally, we also design three activity evaluation platforms - anti-inflammation, anti-tumor and anti-oxidant, hoping to evaluate the biological activities of diatom extracts from AQ9 and use the result as a basis for further animal experiments.

SM16 Protective effect of quercetin against oxidative stress induced by ochratoxin A in hepatocyte Haedun Kim, haedun91@gmail.com, Hyun Jung Lee, Dojin Ryu. AVFS, U. of Idaho, Moscow Ochratoxin A (OTA) is a significant food safety concern due to its high occurrence in a wide range of agricultural crops and their derived food products including those foods and snacks destined for infants and young children. Moreover, eliminating OTA in food products is virtually impossible due to the heat stability of OTA during food processing while infants and children are vulnerable to xenobiotics. Therefore, the aim of this study was to evaluate the antagonistic effect of quercetin which is one of the most effective antioxidants that may counteract OTA induced oxidative stress in the liver using human hepatocellular carcinoma cells (HepG2). OTA showed dose-dependent increase of cytotoxicity (IC50 = 1.66 μM, $p<0.05$) at 48 h, while treatments up to 250 μM quercetin did not change cell viability. Whereas level of the reduced form of glutathione (GSH) was significantly increased by treatment of OTA, GSH concentrations were decreased by treatment of quercetin dose-dependently. Among several genes associated with oxidative stress, expression of superoxide dismutase 1 (SOD1), glutathione peroxidase 1 (GPX1), glutathione reductase (GSR), heme oxygenase-1 (HO-1), and nuclear factor erythroid 2–related factor 2 (Nrf2) were significantly up-regulated by OTA treatment, while catalase (CAT) were significantly down-regulated by OTA treatment. In addition, SOD, GPX, GSR, HO-1, and Nrf2 showed decreased expression at 50 – 250 μM quercetin and OTA at IC50 value. These results suggest that quercetin may alleviate potential OTA-induced liver damage and oxidative stress through reducing cytotoxicity and enhancing the cellular antioxidant defense systems.

SM17 Alleviative effect of resveratrol on ochratoxin A (OTA)-induced kidney damage and oxidative stress Haedun Kim, haedun91@gmail.com, Dojin Ryu, Hyun Jung Lee. AVFS, U. of Idaho, Moscow Ochratoxin A (OTA) has become an emerging issue because of its high incidence and wide range of occurrences in various agricultural crops and their derived food products. In addition, its heat stability during food processing resulted in failure of eliminating OTA in final food products. Therefore, the purpose of this study was to demonstrate resveratrol's potential to alleviate OTA toxicity, i.e., reducing oxidative stress in the kidney using human proximal tubule epithelial cells (HK-2). OTA showed dose-dependent increase in cytotoxicity (IC50 = 161 nM, $p<0.05$) at 48 h, while treatment up to 50 μM resveratrol did not change cell viability and this dose was used for further studies. Among several genes associated with oxidative stress, expression of kidney injury molecule-1 (KIM-1) was significantly up-regulated by OTA treatment while its expression decreased dose-dependently when the cells were treated simultaneously with resveratrol in the range of 6.25 – 50 μM with OTA at IC50. To confirm the effect of resveratrol, 7-week-old ICR male mice were treated with OTA, resveratrol, and in combination of both for 8 weeks. The result showed that OTA caused significant increase in oxidative stress and injury of the kidney as well as reversal of the toxicity by resveratrol in dose-dependent defensive and restorative effects. Hence, addition of resveratrol alleviates OTA-induced kidney damage and oxidative stress through reducing cytotoxicity and enhancing the antioxidant defense systems.

SM18 Iron oxide nanocatalyst-based electrochemical sensor for Rapid Detection of E. coli O157:H7 Kim Sangmin, kmn5222@khu.ac.kr, Young-Rok Kim, Hazzel Joy Adra, DongGook Kang, Lim Dahee. Food Sci. and Biotechnology, Kyung Hee U., Yongin-si, Gyeonggi-do, Korea (the Rep. of) Escherichia coli O157:H7 (E. coli) is a highly virulent pathogenic bacteria that causes a range of foodborne illness. Rapid detection of the pathogenic bacteria is crucial to prevent its spread at an early stage. In this study, we present a sensitive and rapid electrochemical immunoassay for the detection of E. coli through magnetophoresis and the intrinsic catalytic activity of iron oxide nanoparticles (IONPs). The surface of IONPs was functionalized with dextrin to enhance their colloidal stability in aqueous environment and make the surface suitable for the immobilization of antibodies through bifunctional linker protein, maltose binding protein-Streptococcal protein G (MBP-SPG), having a specific affinity to the dextrin coating of IONPs and Fc portion of antibody, respectively. The immuno-Dex@IONPs were shown to be effective in binding to the target bacteria. We utilized the different magnetophoretic mobility of the immuno-Dex@IONPs complexed with target bacteria under external magnetic field, which is relatively faster than that of free immuno-Dex@IONPs. The mobility-based separation of the immuno-Dex@IONP complexed with target bacteria was further enhanced by employing viscous hyaluronic acid in separation

medium. Under magnetic field, the bacteria-IONPs complex was directed to the working electrode (WE) placed at one end of the detection chamber. The IONPs that reached to the WE acted as a nanocatalyst, reducing the persulfate (S2O82-) and taking electrons from the electrode. The redox reaction on the surface of WE was found to be proportional to the concentration of target bacteria and readily monitored by electrical measurement. The detection limit of this system was shown to be 104 CFU/mL. The rapid highly sensitive electrical sensing system implemented with the IONP-based nanocatalyst and magnetophoresis would expand its application to on-site detection of pathogenic bacteria in food.

SM19 Hydrogel made from polysaccharide extracted from Antrodia Cinnomomea : characterization and application as carrier for anti-inflammatory agents Chunyuhang Xu, e0669581@u.nus.edu. Food Sci. and Tech., National U. of Singapore Antrodia cinnamomea, a rare medicinal fungus exclusive to Taiwan, possesses potent therapeutic effects, including anti-cancerous, anti-inflammatory, immunomodulatory, anti-hepatitis B virus replication, and antioxidant activities. Conventionally, only the soluble ingredients of A. cinnamomea are extracted and developed as commercial products, while the insoluble part, mainly composed of polysaccharides and protein, is often discarded as waste during industrial processes. In this study, we characterized a novel hydrogel based on the polysaccharides extracted from A. cinnamomea residues. Our goal was to investigate the potential utilization of these polysaccharides as a hemostatic material. We reviewed the current hydrogel systems available, their extraction and characterization. We then discussed the potential of adhesive A. cinnamomea-derived hydrogels with multifunctionality as a promising material for wound dressing applications. Our findings suggest that by utilizing the insoluble part of A. cinnamomea, we can produce sustainable and cost-effective materials for biomedical applications.

SM20 Effect of storage conditions on key odorants and quality of southern highbush blueberries (Vaccinium corymbosum) Fareeya Kulapichitr, fareya2001@hotmail.com, Spencer Walse, David Obenland. San Joaquin Agricultural Science Center, USDA Agricultural Research Service, Parlier, California To preserve quality and extend shelf-life, blueberries need to be maintained at low refrigerated temperatures and high relative humidity during cold storage and transportation. However, within the supply chain system of blueberry storage, temperatures may be much higher during transportation and retail display which could lead to deterioration of blueberry quality based on acidity, sugar, texture and change of aroma-active components. This could potentially affect consumer acceptance and flavor perception of blueberry. It is also possible that even when storing under optimal conditions that this could occur. Therefore, the aim of this study was to investigate the quality changes of highbush blueberry in terms of physicochemical and flavor characteristics during the different storage conditions. Four storage treatments were evaluated: 1) 1°C, at 3 weeks 2) 1°C at 3 weeks and 10°C at 1 week 3) 1°C at 3 weeks, 10°C at 1 week and 20°C for 2 days. Storage conditions did not impact soluble solids but caused a loss of firmness and decrease of total acidity when temperature and length of storage were increased. Sensory directed-flavor analysis by solvent-assisted flavor evaporation and aroma extract dilution analysis revealed that key odorants affected by storage conditions of 'Snowchaser' blueberries with OAV > 64 were ethyl 3-methylbutanoate, (Z)-3-hexenal, (E)-2-hexenal, (Z)-3-hexen-1-ol, linalool, 3-methylbutanoic acid, α-terpineol, eugenol, and vanillin which varied in FD factors and OAVs. Results of this study should aid in the understanding of how storage conditions affect blueberry flavor and may be useful in understanding means to better maintain blueberry flavor in long term storage.

SM21 Characterization of key aroma compounds in microgreens and mature plants of hydroponic leafy fennel (Foeniculum vulgare Mill.) Jingsi Liu1, jingsi@vt.edu, Song Li2, Sean F. Okeefe1, Ken Hurley1, Yun Yin1. (1) Food Sci. and Tech., Virginia Polytechnic Inst. and State U., Blacksburg(2) School of Plant and Environmental Sciences, Virginia Polytechnic Inst. and State U., Blacksburg In recent years, microgreens have gained popularity as novel culinary ingredients with various health benefits. Microgreens are young leafy plants harvested between 7 to 21 days after seed germination. Compared with their mature counterparts, microgreens are believed to have a higher level of bioactive phytochemicals. However, the aroma compounds differences between microgreens and mature plants are species-specific and so far, no information is found for fennel. Fennel is a popular culinary herb native to the Mediterranean region and known for its unique flavor profile. In this study, we identified key aroma-active compounds in fresh fennel (Foeniculum vulgare Mill. cv. Grosfruchtiger) and its microgreens. Fennel was cultivated hydroponically with soilless substrates in a nutrient film technology hydroponic (NFT) system. Samples were ground with liquid nitrogen, and headspace solid phase microextraction (SPME) gas chromatography-mass-spectrometry-olfactometry (GC-MS-O) was used for aroma analysis. A total of 33 and 24 key aroma-active compounds including esters, ketones, aldehydes, alcohols, monoterpenes, sesquiterpenes, terpenoids, and phenylpropenes were identified in fennel microgreens and mature leaf, respectively. Trans-anethole was the predominant aroma compound in all samples. α-pinene, linalool, trans-β-ocimene, and caryophyllene were only identified by olfactometry in fennel microgreens, while hexanal, trans-β-ionone, and methyl eugenol were only identified in mature leaf. Quantitation of aroma-active compounds was performed with standard addition methods. γ-Terpinene was higher in microgreens compared to their mature plants ($p<0.05$) while some other compounds such as α-phellandrene and estragole were not significantly different. The changes in aroma contents over different growth stages revealed the underlying volatile biosynthesis discrepancy. Principal component analysis (PCA) was used to indicate the overall aroma profile between fennel microgreens and mature leaf. This study provided baseline information for understanding the aroma evolution from microgreen to mature herbs.

SM22 Extraction and characterization of hemp seed (Cannabis sativa) proteins by ESI QTOF LC/MS/MS Taran Harris, taraharris@chapman.edu, Basir Syed, Aftab Ahmed. School Of Pharmacy, Chapman U., Orange, California Hemp (Cannabis sativa) has been a versatile plant for thousands of years. Recreational and medicinal use of cannabis surged in the US but was outlawed in 1937. Cannabis was filed as a schedule 1 controlled substance. The war on drugs made quality research extremely difficult. Hemp itself is not psychoactive; however, the flowers containing THC are. The present poster is focused on analyzing cannabis seeds proteome employing top-down proteomics in union with; size exclusion chromatography, high-resolution ESI QTOF LC/MS/MS, and De Novo protein sequencing bioinformatics tools. Cannabis sativa seeds were ground and defatted in hexane, and proteins were extracted in PBS buffer for two days at 4C. The extracted proteins were precipitated in 80% ammonium sulfate, dialyzed using MWCO 3500 dialysis tube in water, and lyophilized. Protein fractions were carried out using gel filtration chromatography with a HiLoad 16/600 Superdex-200 pg column and an automated FPLC system. Fractions were analyzed using 10% Tris/glycine SDS-PAGE electrophoresis. Protein modification was performed using performic acid oxidation succeeded by tryptic digestion at room temperature and 37C. The tryptic digest of hemp seeds was reviewed using high-resolution Q-TOF LC/MS/MS. De

Novo protein sequences and database search were established using PeakStudio-X. Bioinformatic analysis was conducted using the SwissProt Viridiplantae database, with a false discovery rate >1% and a minimum match of 2 unique peptides. No significant differences were observed in the tryptic digest at room temperature and 37C, which revealed 317 and 336 peptides, respectively. The top proteins identified by PeakStudio-X in the digest prepared at room temperature and 37C were 89 and 92. Further work is underway to conduct a comparative proteomic analysis of individual pooled peaks of gel filtration chromatography and cell culture-based cytotoxic activity using MCF-7 breast cancer AsPC1 cell lines.

SM23 International bitterness units (IBU) study of bravo hop Brian Bartholomew, bbartho2@msudenver.edu, Michael B. Jacobs. Chemistry and Biochemistry, Metropolitan State U. of Denver, Colorado Over the centuries, much thought and research have gone towards developing beer, wine, and other alcohol-containing beverages. These drinks have played an essential role in human survival, exemplified by the plethora of historical records, recipes, and other memorabilia dedicated to alcoholic beverages. From those records, beer comprises four essential ingredients: water, yeast, malted grains, and hops. The last two ingredients responsible for the many flavors of beer transform it into a nutritional and disease-fighting drink. Hops are responsible for providing beer flavoring and acting as a preservative. Hops are full of terpenoid-based chemicals, which allow them to impart many different flavors to beer, the most popular being described as a floral, fruity, or citrus flavor. Besides providing the flavor profile, hops contain iso-a-acids that give beer its characteristic bitterness and anti-microbial properties, which help prevent spoilage. Iso-a-acids can be measured based on the International Bitterness Units (IBU) scale by UV-Vis spectroscopy. There are current studies regarding what happens to the IBU level during the production and storage of beer. These studies have compelled more experiments to understand how to preserve this beneficial chemical. It is reported that multiple factors: chemical composition, the pH level of the wort, amount and time of hop addition, and length of the boiling stage, can influence the IBU level. Herein, we present a study examining Bravo Hops in different solutions based on brewing mediums. We will present the bitterness profile of Bravo Hops concerning surrounding factors such as alcohol concentration, pH, and temperature.

SM24 Reactivity and mechanism of glucose oxidoreductase DgpA from human gut bacterium Dorea sp. MRG-IFC3 Heji Kim, miweltneg73@gmail.com, Jaehong Han, jaehongh@cau.ac.kr. Metalloenzyme Research Group and Dept. of Plant Science and Tech., Chung-Ang U., Anseong, Korea (the Rep. of) Biotechnological application of carbohydrate metabolizing enzyme is of a great importance. During the investigation of C-glycoside natural products gut metabolism, an anaerobic gut bacterium, Dorea sp. MRG-IFC3, was isolated and whole genomic sequence was obtained. From the genes responsible for puerarin metabolism, the key enzyme DgpA, initiating the first reaction of glycosidic C-C bond cleavage, was overexpressed and purified. It exhibited a characteristic property of glucose oxidoreductase by utilizing NAD+. The reactivity for various substrates and the reaction mechanism were also studied. It was found that DgpA was able to produce various 3”-oxo-C-glycosides, and β-methyl-3-oxo-glucose was an efficient abiological oxidant.

SM25 Marine phlorotannin from Sargassum pallidum extract attenuates particulate matter-induced skin damage by down-regulating oxidative stress and inflammatory response in HaCaT cells and zebrafish model Wook Chul Kim1, wookchul0828@naver.com, Seung Tae Im1, Hyeon Kang1, Yun Su Lee2, Seung-Hong Lee1,2. (1) Dept. of medical science, Soonchunhyang U., Asan, Chungcheongnam-do, Korea (the Rep. of)(2) Dept. of pharmaceutical engineering, Soonchunhyang U., Asan, Chungcheongnam-do, Korea (the Rep. of) Particulate matter (PM) is well-known for causing harmful effects on human health. Recently, studies have demonstrated that PM induces reactive oxygen species (ROS) generation and inflammatory response resulting in skin damage. A previous study suggested that phlorotannin of Sargassum pallidum extract(PSPE) possesses strong anti-oxidant activities in vitro. However, no studies have investigated the protective effect of PSPE against PM-induced oxidative stress and inflammation in vitro and in vivo. Therefore, this study evaluated the protective effect of PSPE, which is a natural antioxidant against PM-induced oxidative stress and inflammation, in keratinocytes (HaCaT) and a zebrafish model. Our results indicated that PSPE significantly reduced the production of intracellular ROS, nitric oxide, and prostaglandins-E2 in PM-induced damage in HaCaT cells. Furthermore, PSPE significantly suppressed the expression of pro-inflammatory cytokines and inhibited the levels of iNOS, COX-2, and NF-κB expression. In addition, PSPE showed significant protection ability against PM-induced oxidative stress and inflammation n by inhibiting ROS generation, NO production, and lipid peroxidation in a zebrafish model in vivo. These results suggest that PSPE is a potential candidate in the development of pharmaceutical and cosmeceutical products for the treatment of PM-induced skin damage.

SM26 Marine phlorotannin extracted from Sargassum pallidum Inhibits α-MSH induced Melanogenesis in B16F10 melanoma cells and zebrafish model via CREB and ERK -associated MITF downregulation Wook Chul Kim1, wookchul0828@naver.com, Seung Tae Im1, Hyeon Kang1, Seung-Hong Lee1,2. (1) Dept. of medical science, Soonchunhyang U., Asan, Chungcheongnam-do, Korea (the Rep. of)(2) Dept. of pharmaceutical engineering, Soonchunhyang U., Asan, Chungcheongnam-do, Korea (the Rep. of) Melanin overproduction causes various skin diseases such as spots, freckles, and wrinkles. Thus, melanin synthesis inhibitors such as PTU and kojic acid have been generally used in the pharmaceutical industry. However, it contains side effects such as skin irritation and allergy, thus, it is necessary to develop a melanin inhibitor from natural resources. The purpose of this study was to investigate a whitening agent from natural substances using B16F10 melanoma cells and zebrafish model. Therefore, we investigate the melanogenesis inhibiting activities of phlorotannin extracted from Sargassum pallidum (SPP). SPP significantly decreased α-MSH-induced intracellular tyrosinase activity and melanin contents in a dose-dependent manner. SPP also inhibited the expression levels of key melanogenic proteins such as tyrosinase, TRP-1, and TRP-2 in α-MSH-stimulated B16F10 melanoma cells. In addition, SPP effectively decreased the expression levels of MITF by downregulating the phosphorylation levels of CREB and ERK. Furthermore, in zebrafish model, the toxicity and anti-melanogenesis activities of SPP were simultaneously evaluated. SPP provoked no toxicity in generation process and significantly suppressed melanin synthesis in zebrafish model. These results altogether shows that SPP can effectively suppress melanogenesis in B16F10 melanoma cells and zebrafish, and has a potential for using in pharmaceutical and cosmeceuticals.

SM27 Biophysical properties of ampicillin-resistant Escherichia coli Keenan Dungey1, keenan-dungey@utc.edu, Makyah Schleining2, Funtino McCoy1, Patrick Kenney3, Amy Carranza-Parras1, Luis Sanchez Diaz1. (1) Chemistry and Physics, The U. of Tennessee at Chattanooga(2) Ooltewah High School, Ooltewah, Tennessee(3) Graduate Medical Sciences, Boston U., Massachusetts The prevalence of multidrug-resistant bacteria is increasing the risk of infections worldwide. One mechanism of resistance is physical

changes to the cells. Prior studies have measured the instantaneous response of Escherichia coli (E. Coli) cells to an antibiotic: they immediately lost modulus when exposed to ampicillin. In this study we tracked the long-term effects of exposure to ampicillin on the biophysical properties of E. Coli. The question addressed by this study was: are antibiotic-resistant bacterial cells more rigid than cells that are susceptible to the antibiotic? Our hypothesis was that E. coli cells that are more rigid (higher elastic modulus) would be more resistant to ampicillin since this chemical attacks the cell membrane. We tested this hypothesis by analyzing the physical properties of E. coli cells using atomic force microscopy (AFM), comparing native E. coli to an enriched population upon culturing in the presence of ampicillin. E. coli was initially grown in nutrient rich broth to which ampicillin was added in increasing concentrations. This process was followed for four cycles. We used the AFM to measure the cell size (length and diameter) for each cycle. Force-distance curves were measured for individual cells in order to determine any changes in adhesion or elasticity. There was a decreasing trend in cell diameter from Cycle 2 through 4 that could indicate resistant cells are more dense and hence more rigid. An increase in rigidity was measured directly for cells from Cycle 4, with steeper force-distance curves compared with native cells. In future, more replicate measurements are needed in order to increase the statistical significance of these results. Our study demonstrated the effectiveness of the AFM in measuring the biophysical properties of gram-negative cells and indicated a trend that could support our hypothesis.

SM28 Adverse effects of titanium dioxide nanoparticles on beneficial gut bacteria and host health based on untargeted metabolomics analysis Yanyan wu, yanyanwu@umass.edu, Xiaoqiong Cao, Hengjun Du, Xiaojing Guo, Yanhui Han, Hang Xiao. Food Sci., U. of Massachusetts Amherst Titanium dioxide (TiO2) is a common additive in foods, medicines, and personal care products. In recent years, nano-scale particles in TiO2 additives have been an increasing concern due to their potential adverse effects on human health, especially gut health. The objective of this study was to determine the impact of titanium dioxide nanoparticles (TiO2 NPs, 30 nm) on beneficial gut bacteria and host response from a metabolomics perspective. In the in vitro study, four bacterial strains, including Lactobacillus reuteri, Lactobacillus gasseri, Bifidobacterium animalis, and Bifidobacterium longum were subjected to the treatment of TiO2 NPs. The growth kinetics, cell viability, cell membrane permeability, and metabolomics response were determined. TiO2 NPs at the concentration of 200 μg/mL showed inhibitory effects on the growth of all four strains. The confocal microscope results indicated that the growth inhibitory effects could be associated with cell membrane damage caused by TiO2 NPs to the bacterial strains. Metabolomics analysis showed that TiO2 NPs caused alterations in multiple metabolic pathways of gut bacteria, such as tryptophan and arginine metabolism, which were demonstrated to play crucial roles in regulating gut and host health. In the in vivo study, mice were fed with TiO2 NPs (0.1 wt% in diet) for 8 weeks. Mouse urine was collected for metabolomics analysis and the tryptophan metabolism pathway was also significantly affected in TiO2 NPs-fed mice. Moreover, four neuroprotective metabolites were significantly reduced in both in vitro bacteria and in vivo urine samples. Overall, this study provides insights into the potential adverse effects of TiO2 NPs on gut bacteria and the metabolic responses of both bacteria and host. Further research is needed to understand the causality between gut bacteria composition and the metabolism pathway, which is critical to monitor the gut-microbiome mediated metabolome changes in toxicological assessment of food components.

SM29 Analysis of metabolomic profiles and evaluation of biological activities of six blackberry cultivars Yu Wang, yu.wang@ufl.edu, Hana Lee. Food Sci. and Human Nutrition, U. of Florida, Lake Alfred Blackberries are popular fruits that are consumed worldwide and are used in various processing products. They are known to have high antioxidant activity and prevent different diseases due to their bioactive compounds, including flavonoids and phenolic acids. One of the predominant anthocyanins found in blackberries is cyanidin 3-O-glucoside, which contributes to its dark color and has been reported to have numerous health benefits, such as anti-inflammatory, antioxidant, anti-cancer, and anti-neurodegenerative activities. To better understand their nutritional and therapeutic potential, this study aimed to compare the metabolomic profiles and biological activities of six different blackberry cultivars. The targeted and untargeted analysis were conducted using liquid chromatography-mass spectrometry to identify and quantify the metabolites present in the blackberries. The results showed that each blackberry cultivar had a distinct clustering pattern of metabolites, indicating that the metabolite composition of each cultivar through different biosynthetic pathways may affect nutritional and functional benefits. The BL cultivars had high amounts of sugar, organic acid, and amino acid, while the F cultivars showed high amounts of anthocyanin. The antioxidant contents and activities and the anti-inflammatory properties of the six blackberry cultivars were also measured. The F6 cultivar showed the highest antioxidant content and activities, and it protected the lipopolysaccharide-induced macrophages by reducing the generation of nitric oxide, tumor necrosis factor-α, and reactive oxygen species. These cytoprotective effects of F6 cultivar in RAW 264.7 cells may be due to its high antioxidant content and activities by anthocyanin, thus exerting anti-inflammatory properties. In conclusion, this study provides valuable information on the metabolomic profiles and biological activities of six blackberry cultivars. These findings suggest that blackberries have great potential as functional foods or processed products due to their nutritional and therapeutic benefits.

SM30 Organic vs. conventional: A quantitative nutrition/contaminants profiling case study on elderberries Xavier Jones1, xavier.jones346@my.lincolnu.edu, Nadia Bostick2, Samira Mahdi1, Micaela Uy2, Nadia Navarrete-Tindal1, Sarah Eber1, Ray Mu2, Qingbo Yang1. (1) Lincoln U. of Missouri, Jefferson City(2) U. of Health Sciences and Pharmacy in St Louis, Missouri Organic farming is an agricultural method that prioritizes natural processes over synthetic inputs, avoiding the use of chemical fertilizers, synthetic pesticides, or other artificial substances. Instead, it emphasizes sustainable farming practices by utilizing natural fertilizers, biological pest control made from plant or animal waste, and organic manure. Organic farming is associated with healthier and safer produce, as it avoids the harmful effects of synthetic chemicals on both the environment and human health. However, the effectiveness of organic farming may be limited if Good Agricultural Practices (GAPs) are not followed. Therefore, promoting GAPs alongside organic techniques and providing producers with measurable data may be crucial for ensuring food safety, particularly in underserved communities. This pilot project aimed to investigate the significance of GAPs in organic farming by comparing the nutrient levels and contaminant residues in elderberries (Sambucus canadensis) grown with or without GAPs, both in organic and non-organic (conventional) farming. The samples were analyzed using ultra-high performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS) to screen for various nutrients and contaminants. The data obtained was processed using industry-standard software packages with advanced features for peak detection, compound identification, quantification, and statistical analysis. Preliminary findings suggest that implementing GAPs is crucial for achieving expected nutrient

quality and concentration in both organic and conventionally grown elderberries. The detailed results will be presented at the upcoming ACS Meeting. This study highlights the potential benefits of promoting GAPs in conjunction with organic farming practices to improve food safety and address health disparities.

SM31 Production of soybean protein concentrates with enhanced nutrient profile Rafi Anowar, rafi.anowar@ku.edu, Lakshmiprasad Gurrala, Ana Morais. U. of Kansas School of Engineering, Lawrence Defatted soymeal (DSM) is composed of approximately 30 to 35% carbohydrates which can be used as a sustainable source of monomeric sugars. DSM carbohydrates are mostly present as complex oligosaccharides that monogastric pets are unable to digest. This work aims to develop an enzymatic hydrolysis and concomitant fermentation process for converting anti-nutrient oligosaccharides present in DSM into monosaccharides that will be further used as a carbon source for the production of single cell protein (SCP). SCP has enhanced amino acid profile relative to plant-based protein with low-to-no content of antinutrient compounds. After measuring the chemical composition of the feedstock and obtaining an average carbohydrate content of 33.30 ± 3.45 wt%, an in-depth optimization of the enzymatic hydrolysis of DSM, including the type of enzymes, ratios, residence times, and temperature, was performed. A total sugar yield of approximately 55 wt% was obtained using an enzymatic cocktail composed of a-amylase, amyloglucosidase, pectinase, and xylanase at 50 °C for 12h of residence time. The obtained sugars were used as a carbon source to produce single cell protein by aerobic fermentation using Candida utilis and Pichia pastoris as microorganisms. The outputs from this work can be an effective resource for the soybean and pet food industries to develop a high-quality plant-based protein, which is a sweeping alternative to conventional plant and animal-based protein used in animal feed.

SM32 Establishment of an analysis method for Trinexapac-ethyl in livestock products Seung-Jun Ka, rktmdwns@naver.com, Kyu-Won Hwang, Yong-deok Kim, hyunji park, Su-Eon Choi, Hyeon-Kyu Jeong, Joon Kwan Moon. Dept. of Plant Resources and Landscape Architecture, Hankyong National U., Anseong, Korea (the Rep. of) Trinexapac-ethyl is a cyclohenadione-based plant growth regulator that is used to control biological growth to reduce costs in agricultural production. These chemicals are likely to harm livestock or humans through agriculture, the food chain, and the cycle of pesticides, so continuous monitoring is being implemented to ensure the safe supply of livestock products in Korea. Trinexapac-ethyl is rapidly hydrolyzed to acid in the environment or in the living body after which is known as an actual active ingredient. In CODEX and the US, the residue definition and residue tolerance are regulated by the sum of the parent compound and Trinexapac (acid), but in Korea, there are no residue definition and tolerance for livestock products. This study aims establish an analysis method for trinexapac-ethyl in livestock products and to secure the reliability of the analysis by establishing highly reproducible instrumental analysis method. Analysis was performed by LC-MS/MS. Representative samples were beef, pork, chicken, milk, and eggs, and were converted to free acid form to analyze all components. After hydrolysis was performed using NaOH and an analysis method was established using a modified QuEChERS method. The quantification limit of the analysis was 0.01 mg/kg, and the minimum detection amount was 0.1 ng. As a result of validation at the LOQ, 10 LOQ, and 50 LOQ levels with the established analytical method, beef was 88.3~110.6% at the LOQ level, 103.4~108.4% at the 10 LOQ level and 91.4~105.3% at the 50 LOQ level. Chicken was 94.6~110.5% at the LOQ level, 101.8~106.8% at the 10 LOQ level and 101.7~106.4% at the 50 LOQ level. Pork was 89.7~100.9% at the LOQ level, 105.0~111.4% at the 10 LOQ level and 101.2~108.3% at the 50 LOQ level. Milk was 97.7~113.5% at the LOQ level, 94.3~103.4% at the 10 LOQ level and 100.1~103.3% at the 50 LOQ. Egg was 91.9~103.9% at the LOQ level, 102.5~109.5% at the 10 LOQ level and 98.2 ~107.6% at the 50 LOQ level.

SM33 Residual characteristics of Sulfoxaflor in Dendranthema zawadskii and changes in the content of flavonoids Yong-deok Kim, kyd2333@naver.com, Kyu-Won Hwang, Seung-Jun Ka, Hyunji Park, Su-Eon Choi, Hyeon-Kyu Jeong, Joon-Kwan Moon. Dept. of Plant Resources and Landscape Architecture, Hankyong National U., Anseong, Korea (the Rep. of) Sulfoxaflor is a sulfoximine-based insecticide derived from the neonicotinoid-based that acts on the nicotinic acetylcholine receptor (nAChR) in the central nervous system of insects, inducing the accumulation of acetylcholine, and is used to control sucking insects such as aphids. It is highly toxic to bees and is metabolized into X11721061 and X11719474. This study aimed to determine the residual level of sulfoxaflor in Dendranthema zawadskii after treatment and to compare changes in the content of the representative flavonoids, linarin and acacetin, by pesticide treatment. The experiment was conducted in an open field in Jeongeup, Jeonbuk, South Korea. The sulfoxaflor was applied twice at a 7-day interval by 2000 times diluted sulfoxaflor WG(7%) and was harvested at 1, 8, 15, 22 days after the final application. The residue of sulfoxaflor in Dendranthema zawadskii was analyzed by the QuEChERS method and LC-MS/MS. The limits of quantification for Sulfoxaflor, X11721061, and X11719474 were 0.01 mg/kg, and the recoveries at 0.01 mg/kg were 79.7-93.4%, 97.7-114.1%, and 84.0-90.8%, respectively. The total residue of sulfoxaflor was highest on 1 DAT after the final application at 8.69 mg/kg and decreased to 0.80 mg/kg on 8 DAT, 0.41 mg/kg on 15 DAT, and 0.40 mg/kg on 22 DAT. Linarin and Acacetin were analyzed by UPLC-DAD. The content of these two components in the untreated group was 2.29% and 1.52%, respectively. Linarin was highest at 1.03% on 22 DAT, and acacetin was highest at 1.59% on 1 DAT. Linarin decreased by an average of 61% compared to the untreated group, with values of 1.01%, 0.85%, and 0.72% on 0, 8, and 15 DAT, respectively. Acacetin decreased by an average of 65% compared to the untreated group, except for 8 DAT.

SM34 Development of an analytical method for ferimzone and tricyclazole in brown rice: Application in pesticide spraying using a multicopter, and comparison of initial concentration depending on spreader-stickers So-Hee Kim, 2271775@donga.ac.kr, munju Jeong, Woo-Seok Ahn, Yoon-Hee Lee, Hye-Ran Eun, Ye-Jin Lee, Su-Min Kim, Yongho Shin. Applied Bioscience, Dong-A U., Busan, Korea (the Rep. of) Development and validation of analytical methods for ferimzone and tricyclazole in brown rice were carried out on LC-MS/MS. The various conditions were compared to establish an efficient method for extraction, partitioning, and purification of active ingredients in samples. In the preparation step, 5 g of homogenized brown rice was saturated by 7 mL of distilled water for 15 min and extracted with MeCN/EA (1:1) containing 0.1% formic acid. The extract was distributed with QuEChERS salts (4 g of MgSO4 and 1 g of NaCl) and purified with d-SPE containing PSA and C18. The method established had a LOQ of 0.005 mg/kg and correlation coefficients greater than 0.999. The recovery and storage stability study were conducted, and the results showed a recovery rate of 90.6–98.8% (RSD ≤7.9%) at different concentrations (0.01, 0.1, 2 mg/kg). The method was reliable as it satisfied the acceptable range (70–120%, RSD ≤20%). The ruggedness of the method was demonstrated through the matrix effect of target pesticides, showing a soft matrix effect range (–3.1% to +6.5%). The analytical method was applied in a study comparing the residue levels of pesticides, which were sprayed using a multicopter with spreader-stickers in paddy fields, Buan, Republic

of Korea. Pesticide product (SC) containing 15% ferimzone and 8% tricyclazole was sprayed with spread-stickers (Cares and Gondor); it was divided into three treatment groups: (A) without spreader-sticker, (B) Cares, and (C) Gondor. After aerial spraying, the initial concentrations of ferimzone residues were found to be 0.53 mg/kg in (A), 1.26 mg/kg in (B), and 2.17 mg/kg in (C) for grains. Meanwhile, for stems, the concentrations were 1.46 mg/kg, 2.12 mg/kg, and 5.72 mg/kg, respectively. The initial concentrations of tricyclazole showed similar trends with 0.25 mg/kg (A), 0.61 mg/kg (B), and 1.15 mg/kg (C) in grains, and 0.82, 1.26, and 2.75 mg/kg in stems, respectively. It indicates that the spreader-sticker increases the initial residual concentration during aerial spraying. In the harvest season, brown rice was collected and analyzed for pesticide residues 21 days after the final spraying. Residual amounts of both ferimzone and tricyclazole were below the established MRLs in the Rep. of Korea, which are 2.0 mg/kg and 0.7 mg/kg, respectively. As a result, the addition of spreader-stickers during pesticide spraying is safe based on a toxicological perspective

SM35 Basic research on the construction of pesticide library database and suspect analysis using high-resolution mass spectrometry (LC-QTOF) Munju Jeong, 2271880@donga.ac.kr, So-Hee Kim, Woo-Seok Ahn, Yoon-Hee Lee, Hye-Ran Eun, Ye-Jin Lee, Su-Min Kim, Yongho Shin. Applied Bioscience, Dong-A U., Busan, Busan, Korea (the Rep. of) It is essential to identify residue materials including pesticides and their metabolites in food. A low-resolution mass spectrometry (LRMS) has limitations in performing qualitative analysis when no reference standards or Multiple Reaction Monitoring (MRM) transition information is available. A high-resolution mass spectrometry (HRMS), on the other hand, allows for exact mass analysis, enabling the qualitative analysis of suspect peaks using library database. In this study, a high-resolution time-of-flight (TOF) mass spectrometer was used to construct a library consisting of individual pesticides and their metabolites, and then library matching rates of target analytes were confirmed in the crops. The analysis was performed using on a Shimadzu LCMS-9030 instrument, and a library for 540 components was constructed by acquiring MS1 and MS2 spectrum data using reference standards. Data Dependent Acquisition (DDA) analysis was used, and database for the isotopic chemical species were constructed to perform MS1 full scan analysis, and their isotopic ratios were verified. In addition, an advanced MS2 database were constructed by analyzing the fragmentation patterns under various collision energy (CE) ranges. It was accomplished by conducting individual analyses using CE values ranging from 10-100 V with 10 V intervals, as well as integrated analyses using the CE spread, which covered CE values of 5-55 and 55-105 V, respectively. The mass accuracy tolerance range was set within ±5 ppm to obtain qualitative reliability. Additionally, a mixed standard solution (50 μg/mL) of 51 representative pesticides was also prepared, and the library search rates were evaluated in two crops (spinach and cabbage). The MS1 and MS2 library search rates for the analytes in spinach sample were both 90% (46 out of 51), while those in cabbage sample were 96% (49/51) and 94% (48/51), showing high matching score and similarity. In the evaluation of quantitative properties of the QTOF, the recovery range of the target compounds in the two crops was within 70-120%, and their RSDs were also ≤20%. The pesticide library and database constructed through high-resolution mass spectrometry technology were successfully applied to suspect analysis, and based on this, it is anticipated that it could be expanded to non-target analysis and utilized in pesticide residue surveys.

SM36 Encapsulating peppermint essential oil in chitosan particles to reducing macrophage inflammation Yu-hua Tu, stu382095@gmail.com, Yu-Wen Ting. National Taiwan U. Inst. of Food Sci. and Tech., Taipei Essential oils have been used for centuries in traditional medicine because of its commercial value and curative effect. Peppermint has also been reported to display several biological effects including anti-inflammatory, antimicrobial, antioxidant and antiviral abilities. However, essential oils are composed of volatile compounds, which easily evaporates or decomposes during food processing and antimicrobial film preparation by direct exposure to heat, light or oxygen. Chitosan is the second most abundant polysaccharide in the world with excellent biodegradable, biocompatible, hydrophilic, low toxicity abilities and GRAS, which show potential usage as drug delivery system. In this study, chitosan is prepared by modification of chitin, which consists of β-(1→4)-N-acetyl-D-glucosamine and the amino group on the structure provides the positive charged properties. We aim to use a chitosan particle to encapsulate essential oils. First, the chitosan solution and peppermint essential oil were fabricated into an oil-in-water emulsion with Tween80 emulsifier and negative charged sodium tripolyphosphate to formed particle by the electrostatic interaction between chitosan to encapsulate essential oils. The reaction enable to reduce the loss of essential oils as well as achieve effective controlled release. Also, the electrostatic interaction between chitosan and mucin in mucus layer can attain the purpose of particles maintain in oral cavity. Therefore, encapsulation technology improves its storage stability, realizes the retention of peppermint essential oil in the oral cavity and reducing inflammation from oral ulcer. The results showed that the weight ratios of chitosan to peppermint essential oil of 1:1.25, 1:1.5 and homogenization at a speed of 24,000 rpm for 5 min showed better encapsulation efficiency and loading capacity, which determine by UV-vis spectrophotometry and TGA.

7:00 Development of eugenol loaded active packaging patch by electrospinning technology Yen-Ting Chen, r10641006@ntu.edu.tw, Yu-Wen Ting, James Wu. Inst. of Food Sci. and Tech., National Taiwan U., Taipei The main function of food packaging is to protect food from outside contamination. With changes of consumer demands, the concept of active packaging has emerged. Active packaging can absorb or release substances and extend the shelf-life of food products. It comes in various forms, including bags, films, sachets, or patches. Using patches as active packaging could reduce the usage of antioxidants or preservatives during food processing. Eugenol is a natural compound extracted from plants with many functions, such as antibacterial and antioxidant. It is a legal food additive and has been used in the cosmetics and pharmaceutical industry for many years. However, eugenol is a heat and light-sensitive compound that may degrade when exposed to normal conditions. Encapsulation technology is necessary to increase its availability. Electrospinning technology is an easy-to-operate, low-cost, and non-thermal processing technique. By applying high voltage, the solution stretches into fibers due to electrohydrodynamic force and bioactive compound can be effectively incorporated into the fiber matrix. In this study, zein, gelatin and eugenol were used as materials for electrospinning to produce a patch as active packaging. Scanning electron microscopy was used to observe the fiber characteristics. The result showed that using 20 kV with 1 mL/hr flow rate could get average fibers. The fibers were then cut into pieces and made into patches. The encapsulation efficiency and loading capacity were measured by using the total phenol assay. The encapsulation efficiency result show from 45% to 60% and the loading capacity showed from 5% to 10%. The vapor phase DPPH assay was used to evaluate the antioxidant ability and the scavenging ability could reach about 63%. The disk diffusion method was used to evaluate the antibacterial ability of the patch against Escherichia coli and Staphylococcus aureus as representatives of Gram-negative and Gram-positive microbes, respectively.

7:00 Evaluating the effects of Taiwan lemon essential oil on skin health Zheng-Yuan Su, zysu@cycu.edu.tw, Yu-Xiang Weng. Dept. of Bioscience Technology, Chung Yuan Christian U., Taoyuan City, Taiwan The skin is the biggest organ on the human body. As a barrier between the body and the external environment, the skin is the primary line of defense against external environmental substances. Therefore, skincare is a very important issue. Studies have shown that plant essential oils are biologically active, such as antioxidants and antibacterial agents. This study aims to extract essential oil (EO) from Taiwan lemon (Citrus depressa Hayata) peel, and to further evaluate its effects on skin health. The composition of CD-EO was analyzed by GC-MS, and its main compounds were found to be (R)-(+)-limonene and γ-terpinene. In the DPPH and ABTS free radical recovery assays, the Trolox equivalent antioxidant capability (TEAC) of CD-EO was 0.28 and 2.24 mg TE/g, respectively. In the assay of the carcinogenic agent TPA inducing carcinogenic transformation of mouse epidermal cells JB6, we found that essential oil (100 μg/mL) could significantly inhibit the non-adherent growth of cells and increase the protein levels of Nrf2 and its downstream antioxidant enzymes. Furthermore, CD-EO can also inhibit the growth of pathogenic microorganisms like Candida albicans, Escherichia coli, Pseudomonas aeruginosa, and Staphylococcus aureus. As a result, CD-EO has the potential of skin health care, including antioxidants, skin cancer chemoprevention and inhibition of disease-causing microbial growth.

7:00 Reducing advanced glycation end products in bread through fortification with quercetin nanoparticles William Huang1, whuang24@lawrenceville.org, Chi-Tang Ho2. (1) The Lawrenceville School, Lawrenceville, New Jersey(2) Food Sci., Rutgers The State U. of New Jersey, New Brunswick Starch-based dough products (e.g., bread) are some of the most consumed foods in western countries. However, during the high-temperature bread baking process, certain harmful Maillard reaction products, advanced glycation end products (AGES), like carboxymethyl lysine (CML) and carboxyethyl lysine (CEL) may form in a reaction between bread proteins and reducing sugars. Long term accumulation of AGEs in human body has been shown to cause chronic inflammation and metabolic diseases. Fortification of bread products with phytochemicals is a promising choice of reducing the AGEs and the risks of some metabolic diseases. In this talk, quercetin (3,5,7-trihydroxy-2-(3,4-dihydroxyphenyl)-4H-chromen-4-one), one of the best natural antioxidants with versatile biological functions including anti-diabetic, anti-inflammation, and anti-hypouricemic activities, was selected to be fortified into bread. To enhance the water solubility and bioaccessibility of quercetin, the media milling technique has been employed to reduce the quercetin particle sizes to the nanoscale. The successful preparation of quercetin nanoparticles was demonstrated using field emission scanning electron microscopy (FE-SEM). X-ray diffraction results indicated that the crystallinity of quercetin nanoparticles was lower than that of unprocessed quercetin, suggesting the media milling process increased the composition of amorphous phase. Solid state 13C NMR results suggested that the chemical structure of quercetin was not changed by media milling process. The addition of quercetin particles strengthened the storage modulus of the dough, and quercetin nanoparticles had a larger increase in mechanical properties than the unprocessed ones. The TNO dynamic gastrointestinal model-1 (TIM-1) results indicated that bread fortified with quercetin nano particles had higher in vitro bioaccessibility than bread fortified with regular quercetin. The effect of quercetin nanoparticles on the inhibition of AGEs in bread was confirmed by the ELISA tests. Our research suggests that the fortification of bread with quercetin nanoparticles may serve as a promising approach for limiting AGE production in the baking process and decreasing the risk of many chronic diseases.

7:00 Simple proteolytic enzyme enrichment process for food and cosmetic peptide production Hesson Chung[1], heschung@kist.re.kr, Jeongae Lee[1], Ha Lim Bang[1], Yunji Kang[1], Su Yun Jang[2]. (1) Innovative Enterprise Cooperation Center, Korea Inst. of Science and Tech., Seoul, Seoul, Korea (the Rep. of)(2) JNJ Nature Cosmetic, Daejeon, Korea (the Rep. of) Ground or juiced vegetables including pineapple containing proteolytic enzymes were dialyzed to remove small molecules such as sugars and pesticides. Pineapple crown was also ground for dialysis. Purified materials in the bag were mixed with ground beans for proteolytic hydrolysis. When fresh pineapple juice mixed with carbendazim (0.2 mM) was dialyzed for 8 h, only 4 w/w% of the total mass was left in the bag with no trace of sugar or pesticide (Figure A). The yield of the soluble fraction did not change before or after dialysis indicating that enzyme molecules or the activity was not lost in the process. Pineapple crowns, known to contain bromelanin, was less efficient, but can also be used for hydrolysis after dialysis (Figure B). Total hydrolysate, soluble fraction and the solid remnants can be used in food or cosmetic applications. Ground peas, white beans, coffee beans, lentil beans, kidney beans or their mixtures were hydrolyzed with dialyzed ground vegetables including pear, papaya and kiwi fruit. Pineapple was the most effective. All the peas and beans produced 10 to 20 w/w% of soluble fraction except for the kidney bean, which was not hydrolyzed. Liposomes or transfersomes containing the soluble fraction were prepared with hydrogenated soy lecithins. The average droplet size of the liposomes was ca. 110 nm (polydispersity 0.3), which was slightly bigger than the liposomes without the soluble fraction.

7:00 In situ assessment of macro/micronutrients in soil from the PVA/starch/fertilizer system Roselena Faez1, faez@ufscar.br, Claudinei Souza2, Camila Chiaregato3. (1) DCNME, U. Federal de São Carlos - Campus Araras, SP, Brazil(2) DRNPA, U. Federal de São Carlos- Campus Araras, SP, Brazil(3) Química, U. de Sao Paulo, Brazil Concerns about the environmental and economic impacts of agrochemical usage have highlighted the importance of enhanced efficiency fertilizer materials for achieving the 2030 agenda for sustainable development. While fertilizers can increase food production using the same land space, their excess can cause soil contamination, underground water inviability, and soil acidification, underscoring the need for sustainable agriculture practices. Therefore, we prepared and evaluated a macro/micronutrient mono and multicomponent material based on poly(vinyl alcohol), KNO3, and starch/micronutrient (Mn, Fe, and Cu) microspheres. Using the time-domain reflectometry technique (TDR), which provides real-time measurements simultaneously with a non-destructible sample technique, we obtained the electrical conductivity of the soil for 80 days, providing an easy way to determine nutrient release. We observed the initial burst release 12 days earlier for the multi (macro/micro) and commercial Basacote compared to the macro-material due to the competition of diffusion of multi-elementary ions. However, after 80 days of nutrient release in the soil, the materials still contained nutrients in the composition as determined by XRD, FTIR, and SEM-EDS analysis. In addition, SEM images of the surface showed signs of deterioration, confirming their biodegradation potential over time and their similar release profile to the commercial material. These results demonstrate the potential of multi-elementary EEFs material to supply macro and micronutrients simultaneously using a single material, resulting in a cost reduction in fertilizer application. Moreover, compared to commercial materials that use non-biodegradable polymers, the developed material is more sustainable, as it has the potential to biodegrade.

7:00 Plasma activated water influenced growth and gene expression in mung bean Yu-Jou Chou, lucy840218@gmail.com, Yu-Wen Ting. Food Sci. and Tech., National Taiwan U. College of Bioresources and Agriculture, Taipei Plasma technology has become increasingly popular as a non-thermal technology for various applications, including crop growth. Studies have been conducted on the use of plasma water to improve crop growth, indicating its potential as a pretreatment technology. However, there is still limited knowledge on the effects of plasma activated water composition and crop characteristics on the growth of plants, and the underlying mechanisms are not fully understood. In this study, mung bean was used as a model crop to investigate the effects of plasma activated water produced under different gases and conditions on crop growth and gene expression. The results showed that plasma activated water can enhance the growth and germination of mung bean. Specifically, it was found that plasma activated water can promote the removal of surface microorganisms and induce an adversity response, which enables plants to grow under stress conditions. The key factors influencing gene expression were identified as phenylpropanoid biosynthesis and plant hormone signal transduction pathways in the KEGG database. This research provides valuable insights into the potential use of plasma technology to promote crop growth and offers good reference for future studies.

7:00 Site-specific carriers of neutraceuticals using pectins with different nanostructural charge distribution and structural characteristics Yang Kim, ya_kim@hotmail.com. Center for Food and Bioconvergence, Seoul National U., Gwanak-gu, Seoul, Korea (the Rep. of) Many nutraceuticals have low bioaccessibility due to their hydrophobic and/or unstable character within the human gastrointestinal tract thus adequate carriers are required for protection and efficient delivery/release. Pectin, a natural dietary fiber consisting of plant cell walls, has got great attention as a carrier material delivering bioactive compounds to the targeted digestive system since they are not digested by gastric or intestinal enzymes but totally degraded by pectinolytic enzymes produced by colonic microflora. In order to gain better insight into the effects of charge distribution and nanostructure of pectin on site-specific delivery/release and bioaccessibility of encapsulated nutraceuticals, two separate delivery systems, pectin microbeads and emulsions were developed using well-characterized pectins including a pectin modified with a papaya pectin methylesterase. Hydrophobic curcumin and hydrophilic vitamin B_{12} were encapsulated and their encapsulation efficiency, release, and bioaccessibility were investigated using in vitro simulated gastrointestinal tract model. As a result, nanostructural characteristics of pectin greatly affected the physicochemical properties of both delivery systems thus huge differences were observed in encapsulation efficiency, release, and bioaccessibility of curcumin and vitamin B_{12} ($p<0.05$). Emulsions stabilized with high (DM72) and medium (DM50) methoxy pectin showed small mean particle diameter and less zeta potential and retained initial droplet structure after in vitro mouth and stomach digestion implying higher stability of the emulsions during digestion when compared to enzyme-modified pectin. However, emulsion stabilized with modified pectin (DM50) showed higher curcumin bioaccessibility of 80% after in vitro digestion while other emulsions displayed only 76 and 65%, respectively. It is noticeable that enzyme-treated pectin with contiguous demethylesterified block showed higher encapsulation in microbeads and more extended stability and bioaccessibility of bioactive compounds in emulsion when compared to commercial pectins. The results manifested great potential for pectin to be utilized as a material for target-specific carriers of nutraceuticals within the human body.

7:00 New strategy for Omega-3 PUFAs protection and curcumin vectorization via water-in-oil gelled-in-water multiple emulsion Jose Antonio Vellido-Perez1, Edmundo Brito-de la Fuente2, Antonio Martinez-Ferez1, amferez@ugr.es. (1) Chemical Engineering, U. de Granada Facultad de Ciencias, Andalucía, Spain(2) Innovation & Development Center, Fresenius Kabi AG, Bad Homburg, Hessen, Germany A water-in-oil gelled-in-water multiple emulsion (W-OG-W) is a metastable system composed of small water droplets dispersed inside gelled oil droplets which are, in turn, dispersed in a continuous aqueous phase. This novel delivery system allows the incorporation, protection, and vectorization of interesting hydrophobic bioactive compounds such as omega-3 polyunsaturated fatty acids and curcumin. For decades, both have shown important therapeutic properties and positive health effects. Nevertheless, their low solubility in aqueous systems in addition to their low bioavailability, high chemical reactivity and instability under common ambient conditions leads to their degradation and, finally, to the deterioration and loss of product quality. This research aims to develop and optimize a W-OG-W emulsion to protect the lipid phase –composed of a gelled fish oil concentrate– against oxidation processes and, simultaneously, for curcumin transport and release. For this purpose, the water:oil ratio in the primary oleogel emulsion and the thickener concentration (xanthan gum) were fixed based on previous studies (40 and 0.31 wt.%, respectively), and a Draper-Lin design was carried out to evaluate the effect of six factors: total emulsifier concentration (Cet), the hydrophobic:hydrophilic emulsifier ratio (φOE/WE) in the primary emulsion, the total oleogel concentration (φ(W1/O)/W2), the hydrophilic emulsifier concentration in the secondary emulsion (Ce2) and the homogenization speed for each emulsion (HSs and HSm for each emulsion, respectively). We found that the total emulsifier concentration drawdown in the primary emulsion is essential to decrease the lipid oxidation and, together with the hydrophilic emulsifier concentration in the multiple emulsion, are key variables to simultaneously minimize the particle size and the lipid oxidation (maximizing the curcumin retention capacity). The viscosity curves represent a pseudoplastic behaviour, typical for these structured materials. The mathematical models to predict the response variables were obtained and the results were analyzed using the multi-response surface methodology to obtain the optimal values: Cet = 8.1 wt.%, φOE/WE = 89.8 wt.%, HSs = 19600 rpm, φ(W1/O)/W2 = 5.1 wt.%, Ce2 = 9.6 wt.% and HSm = 6400 rpm. In conclusion, the unique properties of W-OG-W emulsions make them suitable for their use to stabilize and transport thermal- and photo-labile bioactive compounds to maintain their healthy properties.

7:00 Effect of iota-carrageenan and environmental conditions on the stability of oil-in-water emulsions Hanna(John) Khouryieh, hanna.khouryieh@wku.edu. Western Kentucky U. Ogden College of Sci. and Eng., Bowling Green The purpose of this research was to investigate the effect of iota-carrageenan, pH, and sodium chloride on the properties and stability of whey protein isolate WPI-stabilized oil-in-water (O/W) emulsions. The emulsions were prepared with 2% of WPI and 0.05, 0.1, 0.2, or 0.4% i-carrageenan. The stability of the emulsions to pH (3-7) and sodium chloride (0-100 mM) was determined. The results indicated that pH, NaCl, and concentration of i-carrageenan had significant impact on the stability of the emulsions. For i-carrageenan emulsions with 100 mM NaCl, the droplet charge was close to 0 mV for pH 3, 4, and 5 for all concentrations, indicating minimal electrostatic interaction. For emulsions without NaCl, only pH 3 and 4 were near 0 mV, with pH 5 being more negative without NaCl. The droplet particle size for emulsions without NaCl was lower than for emulsions with 100 mM NaCl. The particle size was lowest at pH 6 and 7 for both with and without NaCl, which may be due to high electrostatic interaction decreasing flocculation. Emulsions containing 0.1, 0.2, and 0.4% i-

carrageenan with 100 mM NaCl were fully stable at pH 6 and 7 which displayed no creaming at all. The addition of NaCl significantly decreased the emulsions viscosity with those containing 0.4% ι-carrageenan has the highest viscosity. The results of this research have an important implication for the design of delivery systems of dairy emulsions and may lead to the development of food products with improved stability to environmental stress.

7:00 Engineering of isoprenoid pathway for production of (–)-α-Bisabolol in metabolically-engineered Saccharomyces cerevisiae Hoon Hwangbo, Hee Kook Yang, Tae-Yeob Kim, Ye-Gi Lee, Yong-Cheol Park, ycpark@kookmin.ac.kr. Kookmin U. College of Science and Tech., Seongbuk-gu, Seoul, Korea (the Rep. of) An isoprenoid of (–)-α-bisabolol is an essential component in an oil-extract of German chamomile and a potent cosmetic ingredient with whitening, skin-smoothing, antibacterial and anti-inflammentary activities. In this study, metabolic engineering strategies were attempted to produce (–)-α-bisabolol in Saccharomyces cerevisiae. The codon-optimized MrBBS gene coding for (–)-α-bisabolol synthase from Matricaria recutita was expressed in S. cerevisiae for (–)-α-bisabolol production. The resulting strain (DM) produced 9.5 mg/L of (–)-α-bisabolol in 24 h of batch culture. Additionally, the mevalonate pathway was intensified by introducing a truncated HMG1 gene coding for HMG-CoA reductase and ERG10 encoding acetyl-CoA thiolase. The resulting strain (DtEM) produced a 2.9-fold increased concentration of (–)-α-bisabolol than the DM strain. To increase the acetyl-CoA pool, the ACS1 gene coding for acetyl-CoA synthetase was also overexpressed in the DtEM strain. Finally, the DtEMA strain produced 124 mg/L of (–)-α-bisabolol with 2.7 mg/L-h of productivity in a fed-batch fermentation, which were 13 and 6.8 times higher than the DM strain in the batch culture, respectively. Conclusively, these metabolically-engineered approaches might pave the way for the sustainable production of other sesquiterpenes in engineered S. cerevisiae

7:00 Production of azelaic acid from nonanoic acid and its esters by whole cell biocatalyst of Candida tropicalis Eun-Young Jeong, Jinwoong Hong, Ji-young Kim, Min-woo Jeon, Ye-Gi Lee, Yong-Cheol Park, ycpark@kookmin.ac.kr. Kookmin U. College of Science and Tech., Seongbuk-gu, Seoul, Korea (the Rep. of) A α,ω-dicarboxylic acid of C5-azelaic acid has multiple applications in plastic and cosmetic industries. Chemical oxidation of oleic acid with ozone (called ozonolysis) allows the production of both azelaic acid and a major byproduct of nonanoic acid. To increase the total yield of azelaic acid in the ozonolysis, in this study, sustainable biotransformation process using a whole cell biocatalyst was developed to directly convert nonanoic acid and its esters to azelaic acid. Candida tropicalis ATCC20962 immediately cleaved ethyl nonanoate to nonanoic acid after ethyl nonanoate addition, and then converted nonanoic acid into azelaic acid with the aid of nonane addition and continuous glucose supply. Finally, a fed-batch biotransformation by continuous feeding of pure nonanoic acid resulted in the production of 30.1 g/L azelaic acid with 0.30 g/L-h productivity and 90% molar yield. By combination of the ozonolysis and our process, a maximum of 95% molar carbon yield of azelaic acid from oleic acid was estimated. This is the first report that nonanoic acid and its esters were directly and biologically transformed to azelaic acid with over 90% yield, and would be a groundwork for the biotransformation of fatty acids with under nine carbons to the corresponding α,ω-dicarboxylic acids.

7:00 Microcapsules produced with polymer blend improve the viability of probiotics and oxidation stability Hsieh Shan-Ni, shanni9994@gmail.com, Yu-Wen Ting, James Wu. National Taiwan U., Taipei Probiotics is getting more and more attention nowadays. However, viability of probiotics was significantly decreased by the harsh environment during conventional processing, transportation, storage and digestion. Omega-3 rich oil is defined as "candidate prebiotic" by International Scientific Association for Probiotics and Prebiotics (ISAPP). Many studies demonstrated omega-3 rich oil co-encapsulated with probiotics could enhance viability of probiotics. But this co-encapsulation system was unstable since omega-3 rich oil is apt to oxidize. At present study, polymer blend used as shell materials would retard oxidation of microcapsules with omega-3 rich oil. Therefore, the aim of this project was to investigate that using dextran/whey protein as shell materials in microcapsules co-encapsulated omega-3 rich oil and probiotics whether could improve oxidation stability and viability of probiotics. This project also found optimal addition level of omega-3 rich oil. The method used in this project was coaxial electrospraying. After treatment, the oxidation stability was measured by testing thiobarbituric acid value (TBA value). The viability of co-encapsulated probiotics was evaluated by inoculating in MRS agar followed by culture at 37 degrees Celsius and 24 hours. Electrospraying parameter and dextran/whey protein ratio were depending on the encapsulation efficiency of probiotics and oil. With the co-encapsulated system, we delivered these health-promoting bioactives simultaneously in one food system to obtain their advantages and synergistic benefits. We also expected the co-encapsulated system could enhance the functionality of probiotic food products.

7:00 Developing water-in-cocoa butter emulsions using cellulose nanofibers hydrogel Wei-Ying Chou, connie991203@gmail.com, Yu-Wen Ting, James Wu. National Taiwan U., Taipei Food that are high in saturated fat could cause health problems. Recent studies use water-in-cocoa butter emulsions produced with polyglycerol polyricinoleate (PGPR) to replace cocoa butter in chocolate. However, the emulsions were unstable during processing. To overcome the problem above, there are also studies show that increasing the viscosity of the water phase dispersed in cocoa butter can form fat-reduced chocolate with regular glossy appearance, proper melting and rheological properties and can also increase mechanical strength to improve processing stability, increase structural rigidity with less sugar content. Cellulose nanofibers (CNFs) are clean-labelled, eco-friendly and plant-derived. Additionally, CNFs can not only increase dietary fiber content in food, inhibit fat digestion but also become a potential material to form tangled 3D network due to abundant hydroxyl groups and high aspect ratio to improve the melting and rheological properties of fat-reduced chocolate. The objective of this study is dispersing CNFs hydrogel in cocoa butter to develop stable cocoa butter emulsion with glossy appearance and better storage stability. The conductivity of cocoa butter emulsions will be zero which indicates the forming of water-in-oil emulsions, the droplet size will decrease by the water phase proportion and form stable cocoa butter emulsions with the water phase more than 40% by homogenization of 24,000 rpm for 5 mins. Then, the glossy appearance can be observed through microscopy and SEM and proper stability through storage stability test when the water phase of the cocoa butter emulsions is more than 40%.

7:00 Effect of argon plasma pretreatment on drying rate and qualities of green tea Yu-Ting Lin, r10641027@ntu.edu.tw, Yu-Wen Ting, James Wu. Graduate Inst. of Food Sci. and Tech., National Taiwan U., Taipei According to The Food and Agriculture Organization (FAO), green tea is one of the most famous non-alcoholic beverages in the world and the consumption continues to increase because of the pleased flavors and health benefits. Conventionally, the green tea processing is including blanching, rolling and drying. To remove the water and prolong the

shelf life, drying is a necessary step during tea making. However, the high temperature use in the drying process could result in the degradation of active compounds such as catechins and polyphenolics The aim of this study is to investigate a pretreatment to reduce the drying time of green tea and analyze its qualities. Cold plasma (CP) is considered the fourth state of matter, which consists of reactive species such as charged ions, free radicals, electrons and ultraviolet photons at room temperature. In this study, green tea was pretreated with different power of Argon CP to figure out the influence of etching effect from CP on the tea leaves. The results showed that 22% of the drying time of green tea was reduced and the average drying rate increase 18% after argon cold plasma pretreatment at 100 W for 20s. The total phenolic content and total catechin content of the tea extract were increase by 19.5% and 9.5% respectively. For colors, pH value and DPPH free radical scavenging activity, there is no significant change between the control and experimental groups. Hence, cold plasma technology has good potential to be applied to tea processing that reduce the drying time while retain more of phytochemical.

7:00 Protective effects of annatto-extracted tocotrienols on brain nerve injury in mice Hui-Yun Tsai2,4, Ying-Ling Lin1, Han-Wei Liao1, Chung S. Yang3, Yu-Kuo Chen1, chenyk@mail.npust.edu.tw. (1) Dept. of Food Sci., National Pingtung U. of Science and Tech., Pingtung, Taiwan(2) Dept. of Nutrition and Health Science, Fooyin U., Kaohsiung City, Taiwan(3) Dept. of Chemical Biology, Rutgers The State U. of New Jersey, New Brunswick (4) Aging and Disease Prevention Research Center, Fooyin U., Kaohsiung City, Taiwan Alzheimer's disease (AD) is a progressive brain disease culminating in cognitive decline, memory impairment, emotional disturbances, and language dysfunction. The pathological features of AD are the production of a large number of amyloid plaque deposits and neurofibrillary tangles in the brain. Studies have shown that AD is highly related to diabetes, and that diabetic patients have a higher risk of developing AD or other dementias compared with healthy people. It was also found that the concentration of methylglyoxal (MG) in the blood of diabetic patients is higher than normal, and MG is the neurotoxic mediator of oxidative stress in the progression of AD. Vitamin E is a collective term that is composed of tocopherols (TP) and tocotrienols (TT). TT is thought to have more potent antioxidant and anticancer properties than TP. The unsaturated side chain of TT allows them to penetrate more efficiently into brain. Therefore, in this experiment, TT was used as a sample to explore the protective effects of 40 and 80 mg/kg annatto-extracted TT on MG-induced brain nerve damage in mice. It can be observed in the Morris water maze test and the novel object recognition test that the administration of TT improved MG-induced spatial learning impairment and memory decline symptoms. In the open field test, mice in the MG group had anxiety similar to those with AD symptoms, while the mice given TT tended to reduce anxiety symptom. The results of histopathological examination showed that the administration of TT reduced the neuronal damage induced by MG, and immunohistochemical staining also indicated that the administration of TT reduced the hyperphosphorylated tau proteins induced by MG. In summary, TT possesses the potential to protect MG-induced cognitive impairment and brain nerve damage in mice.

7:00 Using calcium-chelated soy protein isolate as emulsifier to improve the quality of almond milk Ching-Ting Wei, tiffanywei0215@gmail.com, Yu-Wen Ting, James Wu. National Taiwan U., Taipei Milk is considered a source to provide calcium that are important for human. Calcium plays an important role in strengthening bones, regulating muscle contractions and assisting nerve function. The growing demand for plant-based milk substitutes is a result of the enhanced environmental awareness, health issues caused by milk consumption, and the popularity of vegetarian diet. Almond milk is one of the popular plant-based milk which hold the second place of market share in global dairy alternative market. Although almond milk is environmentally sustainable, cholesterol-free, and rich in antioxidants, it is still in low micronutrient content, such as calcium, and its high fat content may be unstable when emulsified with mechanical shear only. To solve this problem, we aimed to use calcium-chelated soy protein isolate as emulsifier to fortify calcium and keep the emulsion system stable. Soy protein isolate was phosphorylated by sodium trimetaphosphate (STMP). CaCl2 would then react to form calcium-chelated soy protein isolate. After preparation, different amounts of emulsifiers would be added to the almond milks respectively and treated with the high speed homogenization method. The concentration of calcium in almond milks was measured using Arsenazo III. Moreover, the stability of an emulsion determined by the particle size and zeta potential over 14 days, and was studied by Zetasizer. The optimized parameter regarded to the highest content of calcium and smallest particle size. According to this experiment, people could complement calcium through drinking plant-based milk substitutes and extended the shelf life of the products by stabling the emulsion system with the novel emulsifier.

7:00 Accurate and Reliable Analysis of Food Samples using ICP-MS Sukanya Sengupta1, Bhagyesh Surekar2, Richard Fussell3, Daniel Kutscher1, Andy Fornadel1, andy.fornadel@thermofisher.com. (1) Thermo Fisher Scientific, Bremen, Germany(2) Thermo Fisher Scientific Inc, Bremen, Germany(3) Thermo Fisher Scientific, Hemel Hempstead, United Kingdom Food is subject to regular analysis for potentially harmful contaminants, including screening for pesticides, typical contaminants and also toxic metals. This task is commonly fulfilled by analytical testing laboratories, often specialized particularly on the analysis of foods, which turn over a large number of different sample types to provide rapid answers to manufacturers and regulatory authorities. For elemental analysis, the use of inductively coupled plasma mass spectrometry (ICP-MS) is widespread due to the outstanding detection limits that can be achieved. Although ICP-MS is known as an analytical technology unaffected by matrix effects, this may still be an issue when testing large amounts of potential different sample types. Matrix effects could be observed when samples contain differing amounts of major elements, or when the digestion procedure may result in different acid concentrations. Although internal standardization provides a means to account for the changing responses, due to the stringent QC requirements applicable in regulated laboratories, even small differences in the samples may cause the need to isolate a particular sample, dilute and re-run, which creates additional labor and cost for the laboratory. This presentation will highlight how ICP-MS can be used for the high throughput analysis of food samples using automated dilution of the samples with argon gas directly in the instrument. The method was fully characterized and initially validated using a certified reference material as well as spiking experiments, and has proven to provide accurate and reliable results.

7:00 Extraction of diatom fucoxanthin with supercritical carbon dioxide optimized by response surface method Su-Yuan Lai2, You-Ding Li3, Chen-Hao Lin1, Yi-Fang Cheng1, Min-Ying Wang1, mywang@dragon.nchu.edu.tw, Hou-Chien Chang3. (1) Graduate Inst. of Biotechnology, National Chung Hsing U., Taichung, Taiwan(2) Dept. of Food Sci. and Tech., Central Taiwan U. of Science and Tech., Taichung(3) Dept. of Chemical Engineering, National Chung Hsing U., Taichung, Taiwan Fucoxanthin is the most abundant and representative carotenoid in diatoms. Due to its wide variety of health-promoting biological activities, the total global fucoxanthin market increases every year. Diatoms are single-

celled eukaryotes with rich and diverse species. In this study, diatoms (Halamphora coffeaeformis and Hyalosynedra toxoneides) were produced for the extraction of fucoxanthin. Among various extraction methods, supercritical carbon dioxide extraction is well recognized as the least toxic and most environmentally friendly one. The yield of fucoxanthin in supercritical fluid extraction depends on a variety of physicochemical factors, among which temperature, pressure, and the flow rates of the co-solvent and carbon dioxide are selected as the variables in this work to elucidate their effects in the extraction process. Box-Behnken design (BBD) is adopted as the design of experiment (DOE) to retrieve the results with statistical analysis. Response Surface Methodology (RSM) is employed to analyze the data and to quantify how these factors influence the yield of fucoxanthin extracted from Halamphora coffeaeformis and Hyalosynedra toxoneides. For Halamphora coffeaeformis, the best yield is 2.21 mg/g (the amount of fucoxanthin divided by the dry weight of diatom) corresponding to the optimal parameter combination of 5779.7 psi of pressure, 42.7 degree C of temperature, and 3.1 ml/min of co-solvent flow rate. Based on these results, how pressure, temperature, the flow rates of carbon dioxide, influence the yield of fucoxanthin extracted from Hyalosynedra toxoneides will also be reported.

7:00 Acceleration of phytoestrogen accumulation in soy plants (Glycine max L.) by 1-aminocyclopropane-1-carboxylic acid (ACC) Seunghwan Lee1, dlalwl1996@daum.net, Jeong Ho Kim1, Cha Young Kim2, Ki Hun Park1. (1) Division of Applied Life Science (BK21 plus), IALS, Gyeongsang National U., Jinju, Gyeongsangnam-do, Korea (the Rep. of)(2) Biological Resource Center, Korea Research Inst. of Bioscience and Biotechnology, Jeongeup, Korea (the Rep. of) The bottleneck of functional food industry is a lack of bioactive metabolite contents in target plants. Thus, dramatic enhancement of bioactive metabolite contents is an essential step and an innovative challenge in functional food field. Recently, we have paid attention to 1-aminocyclopropane-1-carboxylic acid (ACC). ACC is well known as the precursor of ethylene and more than just the precursor of ethylene, but there is no influential report regarding a role of ACC for metabolite changes and activation of specific genes corresponding the metabolites production. The low levels of bioactive metabolites in target plants present a bottleneck for the functional food industry. The major weakness of soy leaves is the low phytoestrogen content in spite of enriched source of flavonols. In our study, the simple foliar spraying of ACC significantly enhanced the phytoestrogen contents in the whole soy plant, including its leaves (27-fold), stalks (3-fold), and roots (4-fold). Particularly, ACC continued to accelerate the biosynthesis pathway of isoflavones in the leaves for up to 3 days after treatment to be 15,439 μg/g from 580 μg/g. The detailed changes in the levels of this metabolite in soy leaves are disclosed by quantitative and metabolomic analyses based on HPLC and UPLC-ESI-TOF/MS. The PLS-DA score plot, S-plot, and heatmap provide comprehensive evidences to discriminate ACC treatment. ACC was also proved to activate a series of structural genes (CHS, CHR, CHI, IFS, HID, IF7GT and IF7MaT) along the isoflavone biosynthesis pathway time-dependently. In particular, ACC oxidase (ACO) genes were turned on 12 h after ACC treatment, which was rationalized to start activating the synthetic pathway of isoflavones.

7:00 Strategy for the development of plant-based high-protein foods Hiroyuki Yano, hyano@affrc.go.jp. Food Research Inst., National Agriculture and Food Research Organization, Tsukuba, Japan A strategy for the development of plant-based, high-protein foods as well as the examples of such food materials are introduced. In respect of food materials, proteins from sustainable plants are recommended. Hemp is considered one of the most suitable plants as the seed has high nutritional value comparable to soy and the stalks are available for fiber/construction materials. Moreover, hemp requires less pesticides or water in growth compared to cotton, a representative fiber plant. For the development of foods, especially for elderly people, not only swallowable/digestible characteristics but also with “foody” appearance/texture to fulfil the appetite are one of the indispensable factors for the pleasure of food, a significant part of the quality of life. In the construction of food structures and textures, evidences are accumulating to suggest that intermolecular disulfide crosslinking between proteins plays critical roles. Therefore, exploring the suitable combinations of the plant proteins respectively working as “donor” and “recipient” of sulfhydryl (SH) groups for the acceleration of disulfide network formation should be effective for the development of foods with unique structure/texture. In this research examples of such high-protein food materials are introduced with the background of hypothetic mechanisms.

7:00 Narirutin-rich Celluclast extract from mandarin (Citrus unshiu) peel with anti-obesity potential Seung Tae Im2, lama1010@naver.com, Hyeon Kang2, Wook chul Kim2, Seung-Hong Lee2,1. (1) Dept. of pharmaceutical engineering, Soonchunhyang U., Asan, Chungcheongnam-do, Korea (the Rep. of)(2) Dept. of medical science, Soonchunhyang U., Asan, Chungcheongnam-do, Korea (the Rep. of) Mandarin peel, a main by-product of the processing of citrus juice, is rich in various bioactive substances, like polyphenols. However, this by-product has been regarded as waste, and has provoked environmental issues. The previous study suggested that the enzymatic extract of mandarin peel (MPCE) using Celluclast possesses inhibitory effects on lipid accumulation and differentiation in adipocytes. However, to obtain a potential therapeutic agent of MPCE to attenuate obesity, the anti-obesity effect of MPCE needs to be further elucidated by in vivo model. Therefore, the aim of the study was to evaluate the effect of MPCE on obesity in high-fat diet (HFD)-induced obese mice. The quantitative analysis by high-performance liquid chromatography (HPLC) revealed that narirutin and hesperidin are the main active components of MPCE. The results showed that oral administration of MPCE of (125 and 200) mg/kg bw/d for 11 weeks) reduced HFD-induced body weight gain and adiposity. MPCE also decreased the levels of triglyceride, leptin, ALT, and AST in the serum of HFD induced obese mice. Moreover, MPCE significantly inhibited hepatic lipid accumulation by reduction of the expression levels of critical enzymes in the lipogenic pathway proteins. Furthermore, MPCE significantly decreased the adipocyte size and expression levels of key adipogenic-specific proteins in the white adipose tissue (WAT) of HFD-induced obese mice. In addition, MPCE significantly activated AMPK and lipolytic enzyme in the WAT. The current findings demonstrate that MPCE ameliorated HFD-induced obesity, and could be used as a potential ingredient in functional food to ameliorate obesity and related diseases.

7:00 Fucoidan extracted from Ishige okamurae ameliorates non-alcoholic fatty liver in high-fructose diet-fed mice by modulation of lipid metabolism and gut microbiota Seung Tae Im1, lama1010@naver.com, Hyeon Kang1, Wook chul Kim1, Yun Su Lee2, Seung-Hong Lee1,2. (1) Dept. of medical science, Soonchunhyang U., Asan, Chungcheongnam-do, Korea (the Rep. of)(2) Dept. of pharmaceutical engineering, Soonchunhyang U., Asan, Chungcheongnam-do, Korea (the Rep. of) Recently, a new mechanism has revealed that gut microbiota plays a pivotal role in metabolizing fructose to acetate that facilitates hepatic lipogenesis. Therefore, our study investigated the role of microbiome on abnormal lipid synthesis in the presence of fructose and identified attenuating effects of fucoidan extracted from Ishige okamurae (IOF) against fructose-induced fatty liver. The results indicated that oral administration of IOF (150 and 300 mg/kg/day for 12 weeks)

significantly reduced both gut microbiota-mediated and -non-mediated hepatic lipogenesis simultaneously triggered by fructose metabolism. IOF reduced hepatic triglyceride accumulation and expression levels of key enzymes for glucolipid metabolism. In addition, IOF regulated fatty acid synthesis, β-oxidation, and improved hepatic inflammation. Furthermore, IOF inhibited direct fructose-to-acetate conversion and altered the compositions of gut microbiota. These findings suggest that IOF might serve as a potential prebiotic dietary supplement by ameliorating fatty liver through dual regulation of classical lipogenic pathway and gut microbiota.

7:00 Obtention of antioxidant peptides from pork liver through enzymatic hydrolysis with ultrasounds pretreatment Blanca Rubio1, Leticia Mora1, Fidel Toldra1, Milagro Reig2, mareirie@upvnet.upv.es. (1) Instituto de Agroquímica y Tecnología de Alimentos (CSIC), Paterna, Valencia, Spain(2) Instituto de Ingeniería de Alimentos para el Desarrollo, U. Politècnica de València, Spain Meat industry generates many by-products that are expensive to manage and with a high impact on the environment. Nowadays, there is an increased interest to give an added value to these by-products, therefore increasing the sustainability of the meat industry and improving the circular economy of the sector. This study is focused on the use of ultrasounds treatment to increase the amount of antioxidant peptides generated in pork liver hydrolyzates. Ultrasounds at 35 kHz were used at different times to improve the performance of enzymatic hydrolysis of pork livers with different proteolytic enzymes (Alcalase and Alcalase with Protana prime). The hydrolyzates with the generated peptides were deproteinized and then further purified by reversed-phase HPLC chromatography. The eluted peptides were collected and antioxidant activity was assayed in each fraction by using the DPPH radical scavenging activity, Ferric reducing antioxidant power and ABTS radical scavenging assay. The sequences of peptides in the most active fractions were analyzed using a nanoESI qQTOF 6600 plus TripleTOF mass spectrometer (ABSCIEX). Peptide hydrophobicity was evaluated with the Peptide 2.0 database. Main results showed that those samples with 60 min ultrasound treatment provided a higher degree of hydrolysis (20-23 %), although non-significant changes were observed in DPPH and Ferric reducing power. However, the ABTS antioxidant capacity increased after 30 min of US treatment in Alcalase hydrolyzates, reaching 1000 mmol/mL of sample. The use of a second enzyme resulted in a significant increase of both, the hydrolysis degree and the antioxidant activity in all cases. The antioxidant activity of HPLC-fractionated samples was measured and fractions 4 and 16 were those showing the highest activity in Ferric reducing power (absorbance of 0.98) and ABTS capacity (820 mmol/mL of sample), respectively. Once peptides in those fractions were identified by MS/MS, the obtained sequences were analysed in silico to determine their potential as antioxidant compounds as well as to evaluate its toxicity, allergenicity, and cell-penetrating capacity. In this work, pig liver was used to obtain peptides with high antioxidant capacity through the use of ultrasounds pretreatment and enzymatic hydrolysis, concluding that pork liver hydrolyzates constitute a good source of antioxidant peptides.

7:00 Metabolomic approach of azole fungicides in radish (Raphanus sativus): Perspective of functional metabolites Ji-Woo Yu, uzu1030@gmail.com, Min-Ho Song, Young-Soo Keum, Jiho Lee. Konkuk U., Gwangjin-gu, Seoul, Korea (the Rep. of) This research focused on exploring the harmful effects of three types of azole fungicides, namely diniconazole (DIN), metconazole (MET), and tebuconazole (TEB), on the leaves and roots of radish plants. The analysis was done through targeted metabolomics using gas chromatography-mass spectrometry (GC-MS/MS), with a special emphasis on the changes in functional chemicals such as phytosterols and glucosinolates. The radish samples were collected after 7 and 14 days of exposure to the fungicides, and the experimental groups were clearly distinguished in PCA and PLS-DA score plots. The results indicated that the fungicides caused significant changes in the levels of phytosterols and glucosinolates, affecting the primary and secondary metabolism of the plants. Overall, the study revealed that the azole fungicides triggered the defense mechanisms of the radish plants, and affected multiple metabolic pathways in a similar manner regardless of the type of fungicide used. This study aimed to evaluate the correlation between fungicide application and functional metabolites changes, using toxicometabolomics approaches. These findings give fundamental data to understand effects of triazoles to plant metabolism

7:00 Using the electronic nose to help guide flavor development in chocolate protein beverages Gergana Milkova1, gergana_milkova@mccormick.com, Smaro Kokkinidou2. (1) Research and Innovation, McCormick and Company Inc, Hunt Valley, Maryland(2) Starches, Sweeteners and Texturizers North America, Cargill Inc, Minneapolis, Minnesota The electronic-nose (e-nose) is an analytical instrument that analyzes and compares the aromatic profiles of food and beverages. Similar to how the human brain creates fingerprint profiles for different aromas, the electronic nose generates unique profiles based on chemical composition for each food or beverage product. The electronic nose utilizes gas chromatography-flame ion detection (GC-FID), two unique column chemistries and is coupled with proprietary flavor libraries to analyze the volatile profiles. Multivariate statistics is additionally used to identify the unique components of different food matrices. Coupling analytical data along with consumer insights research and sensorial data can provide a data-driven approach that allows the identification of drivers of liking and the opportunity to tailor flavors that improve consumer preference. In this work, the e-nose was utilized to facilitate the development of a signature chocolate flavor for a protein powder to rival the current market leaders. Based on market and consumer data research, seven main competitors were selected, two being market leaders in the chocolate protein powder space. Five cross-category chocolate-flavored products (ice creams and cakes) were also selected based on their excellent market share and consumer preference results in the indulgence product category. All samples were analyzed via static-headspace gas chromatography and principal component analysis (PCA) was performed using the chromatographic peaks as principal components. The PCA was used to the identify the flavor compounds driving sample differentiation and clustering. The flavor differentiators were used to formulate a chocolate flavor that closely mimicked the market leaders and also incorporated the chocolate profiles from cross-category indulgence products. The newly developed chocolate flavor was analyzed and found to be more similar in volatile composition to the market leaders and the chocolate ice cream samples than the original chocolate base. To validate that the new signature profile would also be favored by consumers, it was evaluated against the market leading product in a blind-consumer preference test. Panelists reported a “would purchase” intent four-times greater for the new chocolate signature flavor than the market leader. The study below demonstrates the electronic nose’s potential to be used as a tool in base optimization and flavor development.

7:00 Ameliorative effect of probiotics containing product on gastrointestinal functions in loperamide-induced constipated rats Ting-Hua LAI1, tinghualai@gmail.com, Chuang Yi-Ping1, Chung-Hsin Wu1, James Wu2, Szu-Chung Shen1. (1) National Taiwan Normal U., Taipei, Taiwan(2) National Taiwan U., Taipei Summary: Bifidobacterium spp. and Lactobacillus spp. containing probiotic product from Gia Pharmaceuticals LLC (BLPG) alleviates

loperamide-induced constipation in rats. Introduction: Constipation, with a global prevalence of 5-20%, is a common gastrointestinal disease that may cause discomfort such as rare stools, difficult defecation, pain and stiffness of human body. Constipation may also alter intestinal flora and affect the integrity of its intestinal barrier, immune and metabolic functions. Previous studies suggested that the intake of probiotics improve the intestinal bacteria phase and promote the health of their host. Method: Male Sprague-Dawley rats (6 weeks old) were adapted to the environment for 2 weeks. The rats were injected loperamide to induce constipation, and meanwhile daily orally gavaged the BLPG for 4 weeks. The relevant growth parameters of the rats were recorded every week. The rats were sacrificed at the end of trial and the relevant fecal parameters, intestinal microbiota composition and bacterial species diversity of loperamide-induced constipated rats were measured. Result: The results revealed that the high dosage BLPG (3.8 g/kg bw/day) significantly increased feces water content in loperamide-induced constipated rats ($p < 0.005$) at 4th week. The intestinal microflora analysis indicated that Bifidobacterium spp. of low (1.9 g/kg bw/day) and high dosage (3.8 g/kg bw/day) BLPG group are 5.76±0.18 and 6.25±0.24 (log CFU/g), respectively, and both of them are significantly higher than that of loperamide-induced constipated rats after 4 weeks treatment. In addition, the intestinal Lactobacillus spp. of low dosage BLPG group are 6.33±0.19 (log CFU/g) and is also significantly higher than that of loperamide-induced constipated rats. Significance The results from the present study suggest that probiotic product of Gia Pharmaceuticals LLC possesses potential to develop into a health food to improve intestinal health in the human body.

7:00 Optimizing the lignan extraction from oat using response surface methodology Yoonjeong Kim, ang1569@naver.com, Jihwan Kim, Younghwa Kim. Kyungsung U., Busan, Korea (the Rep. of) Lignans are polyphenol phytoestrogens found in various fruits and vegetables, and their most important dietary sources are whole-grain cereals and legumes. In this study, the optimal extraction condition for lignans (lariciresinol, matairesinol, pinoresinol, secoisolariciresinol, syringaresinol, and medioresinol) from oat was investigated using response surface methodology (RSM). In the results, the methanol concentration, extraction temperature and time all had significant effects on the extraction yield of lignans from oat. Then, Box-Behnken design was employed to develop the following three extracting parameters: temperature (X1: 20-60°C), methanol concentration (X2: 60-100%), and time (X3: 30-90 min). The optimum extraction conditions of total lignan contents (65.151 μg/100 g) were obtained at X1=43.03°C, X2=84.24%, and X3=56.06 min. The predicted result (65.932 μg/100 g) matched well with the experimental results obtained using the optimal extraction conditions, which validated the RSM model with a good correlation. These results may be useful for providing reliable data about the lignan content in cereal grains.

7:00 Rapid Screening of 510 Pesticide Residues in Agricultural Product by QuEChERs Method Combined with LC-QTOF and GC-QTOF Hyeong Wook Jo1, hyeongwook.jo@gmail.com, Hyo-min heo1, Kyu-Won Hwang2, Jung-Hoon Sun1, Joon-Kwan Moon2. (1) Hansalim Agro-Food Analysis Center, HKNU IACF, Suwon, Kyeonggi-do, Korea (the Rep. of)(2) Hankyong National U., Anseong, Korea (the Rep. of) For screening pesticide residues in agricultural product (rice, cabbage, apple, potato, and bean), this study was performed by QuEChRES method combined with LC-QTOF and GC-QTOF. Sample weighing (10 g) in a 50 mL conical tube, added acetonitrile (10 mL) was shaken for 10 min. And QuEChERS extraction salt (Citrated buffered, EN 15662, 4 g MgSO4, 1 g NaCl, 1 g Na3Cit.2H2O, 0.5 g Na2Cit.25H2O) were added to the sample in the 50 mL conical tube. The mixture was strongly shaken for 1 min and was centrifuged at 3,000 g for 10 min. The acetonitrile layer was purification with dSPE (150 mg MgSO4, 25 mg PSA) and was centrifuged at 13,000 g for 5 min. The supernatant was filtered with a membrane filters (pore size: 0.2 um) before analysis. ME (%, Matrix effect) for almost analytes range were -10.48 to58.1%. MLOD (Method LOD) and MLOQ (Method LOQ) was calculated by S/N ratio. MLOQs were 0.01 mg/kg. The linear correlation coefficients (r2) were > 0.99 within the range of 2 ~ 100 ug/kg for all of the 510 pesticides. The percentages (of pesticides) recovers were in the range of 65.1 ~ 110.6% (0.01 mg/kg level), 73.2 ~ 105.8% (0.1 mg/kg level) and 87.4 ~ 106.9% (0.5 mg/kg level) within the validation criteria (recover; 60-120% with RSD < 20%)

7:00 Synthesis of avenanthramides and applications on quantitation as an analytical standard Min-Ho Song, tdasgtaasf@gmail.com, Ji-Woo Yu, Lee junghoon, Hui-Yeon Ahn, Jiho Lee, Young-Soo Keum. Konkuk U., Gwangjin-gu, Seoul, Korea (the Rep. of) Avenanthramides were unique bioactive alkaloids found in Avena sativa (oats), which is a globally consumed cereal crop. These alkaloids could be classified into two groups: the C-type, which is derived from anthranilic acids and 3-phenylprop-2-enoic acids, and the A-type, which is derived from anthranilic acids and 5-phenylpenta-2,4-dienoic acid. Due to their various biological activities, numerous studies have been conducted. Most studies have been focused only on avenanthramide 2p, 2f, and 2c. The quantitative analyses of other types of avenanthramides are based on extrapolation of analytical properties of avenanthramide 2p, 2f, and 2c. However, a previous study reported that the extrapolation method gave incorrect analytical results. This study presented a simple synthetic method for A-type avenanthramides, including an efficient preparation of substituted 5-phenyl-2,4-pentadienoic acids and anthranilic acids. The whole series of avenanthramides were synthesized and characterized using HPLC-ESI-QTOF-MS and NMR. Synthetic compounds were used as analytical standards. A robust quantitative analysis of avenanthramides in oats was developed using two internal standards. The sample extraction and purification were optimized to achieve the highest sensitivity and accuracy and reduce matrix effects. The method was validated in linearity, accuracy, and precision. The recovery of avenanthramides ranged from 80% to 110%, and the relative standard deviations were below 20%.

7:00 Preparation of nanopesticides by flash nanoprecipitation using Arabic gum as green carrier Jianing Yi1, Enguang Ma2, Li Li1, Xuhong Guo1,2, guoxuhong@ecust.edu.cn. (1) School of Chemical Engineering, East China U. of Science and Tech., Shanghai, China(2) School of Chemistry and Chemical Engineering, Shihezi U., Xinjiang, China Flash Nanoprecipitation (FNP) is a simple, efficient and scalable technology to achieve rapid and controllable preparation of drug-loaded nanoparticles based on dynamic control mode. It has been widely used in agriculture, biomedicine, and chemical industry in recent years. In this study, the hydrophobic pesticide abamectin was used as the model drug and Arabic gum alone or mixed with surfactants was used as green carriers to prepare nanopesticides by FNP technology. By characterizing the structure (morphology, size, and size distribution) and drug loading rate of the nanopesticides, the influences of carrier concentration, composition of carrier, solvent ratio, and Reynolds number on structure of the nanopesticides were studied. The stability and in vitro release behavior of nanopesticides at 0 and 25 °C were further investigated. Our work demonstrates that polysaccharides like Arabic gum have great potential as green carriers of pesticides.

7:00 Residual characteristics and risk assessment of chromafenozide in perilla leaves Kim Dong Ju1, kimdj6746@naver.com, Ham

Young Jin1, Jun Young Kim1, Oh Eun Been1, Lee Chae Yeon1, Jang-Eok Kim2, Kim Tae Hwa3, Young-Soo Keum4, Kee S. Kyung1. (1) Life and Environment Sciences, Chungbuk National U., Cheongju, Chungcheongbuk-do, Korea (the Rep. of)(2) Kyungpook National U., Daegu, Daegu, Korea (the Rep. of)(3) Analysis Technology and Tomorrow, Gimcheon, Gyeongsangbuk-do, Korea (the Rep. of)(4) Konkuk U., Gwangjin-gu, Seoul, Korea (the Rep. of) This study was carried out to investigate the residual characteristics and risk assessment of the insecticide chromafenozide in minor crop perilla leaves. The test pesticide chromafenozide 5% EC was sprayed two times with a 7-day interval onto perilla leaf at 100 g a.i./ha. Samples were collected at 0, 1, 3, 5, 7 and 10 days after final spraying. Residues of the test pesticide in samples were analyzed with an UHPLC-MS/MS. Limit of quantitation of chromafenozide was 0.01 mg/kg. Recoveries of the test pesticide in the crop at 0.01, 0.1 and 4.0 mg/kg ranged from 91.6 to 110.8%. Chromafenozide residue in the crop was remarkably reduced to 0.86 mg/kg 10 days after last application and its half-life was 3.4 days. The maximum estimated daily intakes of chromafenozide in all samples were below 0.07% of its acceptable daily intake, indicating that health risk does not pose by ingestion.

7:00 Residual characteristics of boscalid in different parts of welsh onion Jun Young Kim1, tim8518@naver.com, Kim Dong Ju1, Ham Young Jin1, Oh Eun Been1, Lee Chae Yeon1, Im Moo-Hyeog2, Kim Seo Hong2, Kee S. Kyung1. (1) Life and Environment Sciences, Chungbuk National U., Cheongju, Chungcheongbuk-do, Korea (the Rep. of)(2) Dept. of Food Engineering, Daegu U., Gyeongsan, Gyeongbuk, Korea (the Rep. of) This study was carried out to investigate the residual characteristics of boscalid in different parts of welsh onion. Field trials were conducted from three fields located in major production areas of welsh onion in South Korea. Boscalid 49.3% WG was sprayed three times onto the welsh onion with 7-day interval at 0.657 kg a.i./ha according to its critical GAP in Korea. Samples were collected on the day of harvest and some of them were cut by dividing the top and bottom based on the white and the green part. Residues of boscalid in welsh onion were analyzed with an LC-MS/MS after QuEChERS extraction. The limits of quantitation of boscalid in whole welsh onion, top welsh onion and bottom welsh onion were all 0.01 mg/kg. Recoveries of boscalid in whole welsh onion, top welsh onion and bottom welsh onion ranged from 75.56-118.02, 70.03-108.77 and 70.29-107.75%; storage stabilities were from 85.32-111.63, 94.17-102.29 and 92.06-101.09%; and amounts of residue were 0.38-0.90, 0.69-1.10 and 0.02-0.13 mg/kg, respectively. The residual amounts were high in the order of top welsh onion, whole welsh onion and bottom welsh onion. These results indicated that the pesticide adhered well to the top part of welsh onion than other parts during application. Additionally, the total amount of pesticide residue on the top part was higher than the other parts.

7:00 Residual characteristics of kresoxim-methyl and pyrifluquinazon in Korean goatsbeards Oh Eun Been, gsw06059@naver.com, Kim Dong Ju, Ham Young Jin, Jun Young Kim, Lee Chae Yeon, Kee S. Kyung. Life and Environment Sciences, Chungbuk National U., Cheongju, Chungcheongbuk-do, Korea (the Rep. of) This study was carried out to investigate residual characteristics of kresoxim-methyl and pyrifluquinazon in Korean goatsbeards. Kresoxim-methyl 44.2% SC (0.0177 kg a.i./10a) was sprayed three times, and pyrifluquinazon 6.5% SC (0.0039 kg a.i./10a) was sprayed two times with a 7-day intervals onto Korean goatsbeards with different treatment dates before harvest. Samples were collected on the day of harvest. Pesticide residues were analyzed with an LC-MS/MS after QuEChERS extraction. The limits of quantification (LOQs) of kresoxim-methyl and pyrifluquinazon in Korean goatsbeards were all 0.01 mg/kg. Average recoveries of them in the crop at LOQ, 10LOQ and highest residue level ranged from 77.8 to 114.8%. The amounts of kresoxim-methyl and its metabolites (BF490-2 and BF490-9) residues were <0.01-1.51. Also, the amounts of pyrifluquinazon and its metabolite (pyrifluquinazon-1H) residues were <0.01-2.66 mg/kg. As the last application was closer to the harvest, the residual amounts of the test pesticides were higher.

7:00 Validation of QuEChERS multi-residue methods for 108 pesticides in Litopenaeus vannamei using LC-MS/MS Ham Young Jin1, youngjin0223@naver.com, Kim Dong Ju1, Jun Young Kim1, Oh Eun Been1, Lee Chae Yeon1, Park So Ra2, Moon Gwi Im2, Kee S. Kyung1. (1) Life and Environment Sciences, Chungbuk National U., Cheongju, Chungcheongbuk-do, Korea (the Rep. of)(2) Residues and Contaminants Standard Division, Ministry of Food and Drug Safety, Osong-eup, Chungcheongbuk-do, Korea (the Rep. of) This study was carried out to validate the multi-residue analytical methods for pesticides using LC-MS/MS after QuEChERS extraction developed by the Ministry of Food and Drug Safety of the Rep. of Korea. The validation of the methods was performed using Litopenaeus vannamei, a representative crustaceans. The methods were developed for monitoring and setting standards for pesticides that may unintentionally contaminated seafood through feed or the environmental factors, such as soil and water. The multi-residue analytical method for 108 pesticides was evaluated by analysis using an LC-MS/MS after QuEChERS extraction. The limits of quantitation (LOQs) of the pesticides were all 0.01 mg/kg. A recovery test with five replicates was conducted at the LOQ, 2LOQ, and 10LOQ levels. The matrix effect (ME) was calculated using the slopes of both the matrix-matched standard and the pure standard calibration curve. The r2 values of all pesticides were above 0.98 and the %ME was indicated a low or medium ME in the samples. The maximum relative standard deviation (RSD) at the LOQ level was 24.4%. In the recovery test 34, 10 and 4 pesticides at the LOQ, 2LOQ, and 10LOQ levels, respectively, were found to be unsuitable for the acceptable recovery range. The cause of unsuitable recovery at the LOQ level was attributed to the large y-intercept effect.

7:00 Enhancement of anti-adipogenic activity of mandarin peel by acid hydrolysis in 3T3-L1 adipocytes Jiye Pyeon, pyun04@naver.com, Yoonjeong Kim, Younghwa Kim. Kyungsung U., Busan, Korea (the Rep. of) Mandarin peels contain a variety of flavonoids, however, most of them are usually disposed of as agricultural waste. Glycosylated flavonoids show less biological activity compared to their aglycone forms because of reduced cellular absorption. This study aimed to investigate the effects of acid treatment in mandarin peel on lipid accumulation during differentiation of 3T3-L1 cells to adipocytes. The acid-treated mandarin peel extract (AMP) showed no cytotoxicity during adipogenesis in 3T3-L1 cells. AMP markedly inhibited lipid accumulation and suppressed the expression of adipogenic specific proteins including peroxisome proliferator-activated receptors (PPARγ) compared to control or mandarin peel extract (MP). Moreover, the treatment of AMP decreased the mRNA expression of PPARγ compared to control or MP groups. A total of 48 phenol compounds and flavonoids were tentatively identified in AMP and MP using HPLC-Q/TOF-MS. The chemical changes of AMP due to acid hydrolysis were confirmed by PLS-DA and OPLS-DA analysis. These results indicate acid-hydrolysis processing could help release flavonoids from mandarin peel and convert them into aglycone forms, leading to efficient suppression of lipid accumulation in 3T3-L1 cells.

7:00 Simultaneous LC–MS/MS quantification of 6 lignans in cereal grain, potatoes and their products Jihwan Kim, jihwn1211@naver.com, Jiye Pyeon, Younghwa Kim. Kyungsung

U., Busan, Korea (the Rep. of) Lignans are phenolic dimers found in many plant families and common foods, including whole grain cereals, nuts, seeds, legumes, vegetables, and drinks such as tea, coffee or wine. The major dietary lignans include lariciresinol, matairesinol, pinoresinol, secoisolariciresinol, syringaresinol, and medioresinol. There has been increased interest in lignans due to their potential effect in reducing the risk of developing several diseases. Therefore, the present study is conducted to the determination of total lignan contents of cereal grains, potatoes and their products consumed in South Korea. A total of 72 samples (rice, wheat, oat, sweet potato, and noodles) were used for this study. Total lignan contents were determined using a liquid chromatography-tandem mass spectrometry (LC-MS/MS) method for the quantification of 6 lignans. The linearity, limits of detection and quantification (LOD and LOQ), accuracy, and the precision of lignans were acceptable based on the AOAC guidelines. Total lignan contents of grains, potatoes and their products was in the range of 0.000-128.818 μg/100 g. The steamed sweet potato had the highest total lignan contents (128.818 μg/100 g), followed by roasted sweet potato (113.437 μg/100 g) and fresh sweet potato (99.533 μg/100 g). Lignans were found in small amounts in rice (0.195-24.011 μg/100 g). Especially, the cooking process in rice led to an increase in the content of lignan versus the corresponding raw rice. These results provide reliable data on the lignan contents of starchy foods frequently consumed in Korea.

7:00 Essential oil composition of Tetrapleura tetraptera (Schum and Thonn) fruit extracted by dichloromethane and hydro-distillation fraction of n-Hexane Omujal Francis1, fomujal@gmail.com, Joseph Okello1, Richard Komakech1, Esther Kemigisha2, Solome Kirabo3, Enock Ssekuubwa2, Mnason Tweheyo2. (1) Natural Chemotherapeutics Research Inst., Kampala, Uganda(2) Forestry and Biodiversity, Makerere U. College of Agricultural and Environmental Sciences, Kampala, Uganda(3) Chemistry, Makerere U., College of Natural Sciences, Kampala, Uganda Tetrapleura tetraptera (Schum and Thonn), family Fabacea is a deciduous tree that produces aromatic fruits that are used as medicine for various ailments and as a food spice in many African countries. Although the fruit is highly aromatic, determination of its essential oil composition is difficult since hydro distillation of its pulp does not produce oil like most plants used as spices. This study evaluated the essential oil profile of T. tetraptera fruit extracted with dichloromethane (DCM) and hydro-distillation followed by fractionation with hexane. One fruit pulp sample of T. tetraptera was macerated in direct DCM for 48 hours and another was hydro distilled for 6 hours and its distillated fractionated with n-hexane. DCM and n-hexane extracts were analyzed with the Gas Chromatography- Mass Spectroscopy (GC-MS). The number of compounds identified in DCM and n-hexane extracts were 23 and 20 respectively. The dominant compounds in DCM extract were; N-aminopyrrolidine (18.3%),2,6,10,15,19,23-Pentamethyl-2,6,18,22-tetracosatetraen-10,15-diol (15.3%), 2-methylheptacosane (8.6%) and octyl palmitoleate (8.4%), and those in hexane were; hexadecanoic acid (46.4%), octyl palmitoleate (15.6%) and 9-octadecenoic acid (10.4%). Six compounds were detected in both DCM and n-hexane extracts and they included; octyl palmitoleate, hexadecyl pentadecanoate, 1,3-benzenedicarboxylic acid, hexadecanoic acid, z-9-pentadecenol and 2-methylheptacosane. It was also found that only DCM extract contained nitrogenous compounds (i.e. N-aminopyrrolidine and 3-pyridinamine,2,6-dimethyl) that exhibit strong characteristic odor for T. tetraptera. Therefore, DCM extraction can be used to profile the essential oil compounds in T. tetraptera fruit.

7:00 Pre-processing of near-infrared spectra for multivariate calibrations Mukti Singh, mukti.singh@ars.usda.gov, Mark Berhow, Sean X. Liu. FFR, USDA Agricultural Research Service, Peoria, Illinois Near-infrared reflectance spectroscopy (NIRS) is recognized as a fast, environmentally friendly, cost-effective, and accurate technique for measuring chemical and compositional traits in food and agricultural commodities. Models describing the relationship between component concentration and scanning spectra are developed using multivariate regression analysis. Pre-processing of raw spectra is a vital component for removing unwanted variations. The choice of pre-processing methods or combination of methods strongly influence the results. NIRS spectra of 2000 ground soybean samples grown in different regions of the U.S. over several years was obtained. Five major fatty acids in soybeans were measured using gas chromatography (GC). Raw spectra were pre-processed using several methods and their combinations to offset noise, slope, baseline, and scatter effects, and normalization. Partial least squares regression (PLSR) and multiple linear regression (MLR) analysis were used to develop calibration models for each of five fatty acids using differently pre-processed spectral data and fatty acid values for soybean samples measured by a standard GC method. Correlation coefficient and root-mean-square error of calibration, prediction and cross validation were used to assess the performance of calibration models using validation and cross validation sets of data. Spectral pre-processing was found to be effective in improving the performance of the PLSR and MLR models for determining fatty acids in soybean samples.

7:00 Psidial C: Identification of absolute configuration through DFT calculation and its inhibition mechanism on PTP1B via kinetic analysis and molecular docking Dongyup Hahn, dohahn@knu.ac.kr, Thao Quyen Cao. Kyungpook National U., Daegu, Korea (the Rep. of) Protein tyrosine phosphatase 1B (PTP1B) plays a critical role in the negative regulation of insulin signaling and the leptin signaling pathway. The selective inhibition of PTP1B has drawn the attention of many scientists as a promising drug target for treating type 2 diabetes and obesity [1]. Psidial C is a sesquiterpenoid-based meroterpenoid which first isolated from the leaves of Psidium guajava L. in 2010 [2]. Up to now, there has not been any description of its absolute configuration. Besides, its potential mechanism inhibits PTP1B activity has not been investigated. In this study, psidial C was isolated from P. guajava L. and its absolute configuration was elucidated by spectroscopic analyses and quantum chemical calculations of the electronic circular dichroism (ECD) and nuclear magnetic resonance (NMR) spectra. The inhibitory activity of psidial C against PTP1B was studied by in vitro assays, enzyme kinetics, and molecular docking analysis. Psidial C exhibited a significant inhibitory effect with an IC50 value of 2.59 μM and displayed mixed-type inhibition of PTP1B. The finding observed from in vitro and in silico studies suggests that psidial C may be appropriate for future studies on the development of new diabetes inhibitors.

7:00 Testing of Per- and Polyfluoroalkyl Substances in the U.S. Domestic Meat and Poultry Supply Cristian Ochoa, cristian.ochoa@usda.gov, Randolph Duverna, Alexander Domesle. Office of Public Health Science, Food Safety and Inspection Service, Washington, DC Per- and polyfluoroalkyl substances (PFAS) are a class of highly stable chemical compounds that are used in many household and industrial appliances. As a result of their widespread usage, many PFAS persist as environmental contaminants and accumulate in water, air, soil, and plant and animal tissue. USDA’s Food Safety and Inspection Service (FSIS) conducts national-level monitoring of U.S. meat and poultry products to contribute to the understanding of the scope and distribution of these potential contaminants in the food supply. Under the U.S. National Residue Program, FSIS uses an ultra performance liquid chromatography – tandem mass spectrometer

method that screens, confirms and quantifies 16 PFAS compounds with an analytical range of 0.50-125 ng/g (ppb) in beef, swine, poultry and Siluriformes fish tissue. Data from 2020-2022 has found that < 0.2% of beef, swine and poultry samples were found to have detectable levels of PFAS. However, the PFAS perfluorooctane sulfonic acid was found in 13% of Siluriformes fish samples tested. Most (82/83) of the positive Siluriformes samples were domestic wild caught fish that were likely exposed due to living in natural waters that are subject to PFAS contamination. FSIS will continue to adapt its national-level monitoring of PFAS in meat and poultry products to best support governmentwide efforts to identify and reduce sources of PFAS exposure.

7:00 Optimization of a methodology for the extraction and quantification of policosanols by HPLC in Costa Rican sugar cane Oscar Saenz1,2, oscar.saenzrosales@ucr.ac.cr, José Castañeda3. (1) Chemistry, U. de Costa Rica, San Pedro, San José(2) Chemistry, U. Nacional de Costa Rica, Heredia(3) Analytical Applications, SCANCO, Cuidad de Guatemala, Asunción, Guatemala Policosanols are a group of solid, long-chain primary aliphatic alcohols, which have become popular because recent studies have shown benefits on cholesterol levels, some of these studies even suggest that they are more effective than synthetically derived pharmaceuticals for the treatment of high blood pressure. This study presents an optimized method for the extraction and quantification of four policosanols found in the granules and juice of sugarcane in Guanacaste, Costa Rica. For the extraction, samples of sugar cane granules and juice were taken and multiple extractions with chloroform and an ultrasonic bath were carried out, later the chloroform was evaporated with a stream of nitrogen and the sample was reconstituted in mobile phase to be analyzed by reverse phase liquid chromatography, on an Alliance HPLC system with IR detector, using primary standards of 8 different policosanols. The method proved to be effective for the analysis of sugarcane granules and juice samples from the Guanacaste area by allowing the extraction and quantification of hexacosanol, heptacosanol, octacosanol and triacontanol (the only 4 policosanols present in the cane samples from the area), however, the adequate chromatographic resolution was not obtained for heneicosanol, docosanol, tricosanol and tetracosanol, so in case of wishing to quantify them, a different optimization of the method is recommended, increasing, for example, the polarity of the mobile phase and the length of the column or by decreasing its micronage.

7:00 Capturing the quality and functional characteristics of the Greek PDO Cheese Anevato through its microbiome Konstantinos Papadimitriou1, kpapadimitriou@aua.gr, Maria Govari2,1, Dimitra Tsoliakou2,1, Maria A. Gkerekou1,2, Panagiotis Skandamis1, Marina Papadelli2, John Kapolos2. (1) Dept. of Food Sci. & Human Nutrition, Agricultural U. of Athens, Greece(2) Dept. of Food Sci. and Tech., U. of the Peloponnese, Athens, Greece Anevato is a traditional PDO cheese made in the region of Western Macedonia, Greece, which has not been extensively researched before. Cheese samples were obtained from three producers and subjected to culture-based microbiological analysis and shotgun metagenomics. The main microbial populations were found to be lactic acid bacteria (LAB) and yeasts. The shotgun metagenomics analysis allowed species-level identification such as Lactococcus lactis, Streptococcus thermophilus, Lactococcus raffinolactis, Lactobacillus helveticus, Lactiplantibacillus plantarum, and Streptococcus parauberis. The yeast species identified were present in low abundance and included Kluyveromyces lactis and Saccharomyces cerevisiae. Metagenome-assembled genomes (MAGs) were also predicted along with the presence of several potential spoilage microbes. In silico analysis was performed to find quality and functional characteristics dictated by the metabolome of the different MAGS and through the entire microbiome. The information obtained through shotgun metagenomics could be used to identify suitable starters and adjuncts for this type of cheese, standardize production, and extend shelf life.

7:00 Implications of the quality of table olive brines in supermarkets assessed by metagenomic analysis Konstantinos Papadimitriou1, kpapadimitriou@aua.gr, Dimitrios Pavlidis2, Konstantinos Panousopoulos2, Maria-Chrysanthi Kafentzi2, Athanasia Koliadima3, Marina Papadelli2, John Kapolos2. (1) Food Sci. and Human Nutrition, Agricultural U. of Athens, Greece(2) Dept. of Food Sci. and Tech., U. of the Peloponnese, Kalamata, Greece(3) Dept. of Chemistry, U. of Patras, Greece This study aimed to investigate the microbial ecosystem and safety of table olives at retail using metagenomics. Samples of Kalamata, Halkidiki, and Konservolia cultivars were obtained from Greek supermarkets, and their brines were analyzed for microbial communities using both culturable and shotgun metagenomics approaches. The microbial species identified included Lactiplantibacillus (Lb.) pentosus and Lb. plantarum for Kalamata and Konservolia cultivars, and Debaryomyces hansenii for Halkidiki cultivar. The findings were confirmed by MALDI-ToF/ToF identification of isolates from the cultivable community. The culturable approach showed negative results for hygienic indices, and these results were corroborated by shotgun data analysis. A deep search was performed to identify metabolic paths related to the fermentation process, the production of compounds related to the organoleptic characteristics of the product, and its safety. The study concludes that commercial table olives at retail could serve as a source of new starters or adjuncts in olives production. Moreover, the findings highlight the potential of next-generation sequencing (NGS) as a microbiological risk assessment approach, although the need for benchmarking of bioinformatics tools is emphasized. Overall, this research provides important insights into the microbial composition of table olive brines and can inform efforts to improve the safety and quality of table olives.

7:00 Evaluating the effect of mixing corn oil with oils high in antioxidants during deep frying Tamany M. Alanezi, Tamany.alanezi@gmail.com, Amer Abu-Ghazaleh, Namariq Dhahir. Dept. of Animal Science, Food and Nutrition, Southern Illinois U. System, Carbondale The reusing of frying oil often leads to health problems due to the buildup of oxidized products during deep frying. One way to reduce the formation of these oxidized products and extend the oil's shelf life is by mixing frying oils with oils high in antioxidants. To that end, refined corn oil (COO) was blended with black seed oil (BSO), blueberry oil (BBO), sesame oil (SSO), olive oil (OLO), and pomegranate oil (PMO) at a ratio of 85:15 (COO/BSO, COO/BBO, COO/SSO, COO/OLO, COO/PMO). The acid value (AV), peroxide value (PV), p-anisidine value (p-AV), total oxidation value (TOTOX), fatty acid composition, free fatty acids (FFA), Total Polar Compounds (TPC), and Viscosity for frying oils were determined. The COO and its blends were used to fry falafel at 175 ± 5°C for 20 min (total of 12 h and 36 cycles). At the end of the last frying cycle, oil samples were collected and stored at -20°C until analysis. The results showed that all blends led to significant decreases in PV, FFA, p-AV, TOTOX, and TPC after deep frying compared with the COO and the best results were reported for the olive, pomegranate and sesame oil blends. The TOTOX showed that the pomegranate and olive oil blends were more resistant to oxidation than the other oil blends. Moreover, frying significantly decreased the percentages of linoleic acid (C18:2), and linolenic acid (C18:3) and increased the percentage of trans-C18:1 in all oil samples but the effect was least with the olive oil and pomegranate oil blends. This study found that blending COO

with pomegranate or olive oils significantly improved the oxidative stability of frying oils.

7:00 Physicochemical and sensory properties of novel high-intensity sweetener glycosylated neohesperidin dihydrochalcone Yang Kim[1], ya_kim@hotmail.com, Seo-Jin Chung[2], Jaehee Hong[3]. (1) Center for Food and Bioconvergence, Seoul National U., Korea (the Rep. of)(2) Nutritional Science and Food Management, Ewha Womans U., Seoul, Korea (the Rep. of)(3) Food and nutrition, Seoul National U., Seoul, Seoul, Korea (the Rep. of) High-intensity sweeteners with superior sensory quality and physiological functionality have received significant attention because of low calorie and health benefits. Neohesperidin dihydrochalcone (NHDC) is a semi-natural sweetener with 1000~2000 times relative sweetness. However, it was majorly used in medicines, cosmetics, and feeds due to its low solubility and long-lasting sweet taste. Novel sweetener, glycosylated NHDC (1-(4-((2-O-[6-Deoxy-α-L-mannopyranosyl]-(4-O-α-D-glucopyranosyl]-β-D-glucopyranosyl)oxy)-2,6-dihydroxy phenyl)-3-[3-hydroxy-4-methoxyphenyl]-1-propanone) was synthesized via enzymatic glycosylation of NHDC and subjected to investigate physicochemical and sensory properties. The water solubility of glycosyl NHDC (G-NHDC) was about 6g/10mL water which is over 300 times higher than that of NHDC as determined using a spectrophotometer. Thermal stability and stability in acid and base conditions were determined by quantifying the amount using HPLC after a 2-week storage period. G-NHDC remain stable in 0.1M sodium acetate buffer (pH3) at 20C and only 10% was decreased at 60C after the storage period. However, it was completely degraded in 0.1M glycine-NaOH buffer (pH10) within 6 days. The thermal property measured by differential scanning calorimeter exhibited less enthalpy of G-NHDC than that of NHDC manifesting less thermal stability of G-NHDC. Thirty screened panelists evaluated sweetness potency relative to that of sucrose and sensory bitterness. Four concentrations of sucrose solutions (2, 3, 4, and 5%) were prepared and relative sweetness to that of 0.03% glycosylated NHDC was determined using two-alternative forced-choice tests. The relative sweetness of glycosylated NHDC was determined as 117.86 and no significant difference in sensory bitterness compared to sucrose solution was shown ($p<0.05$). From the results, G-NHDC manifested great potential as a novel high-potency sweetener revealing its superior sensory quality without bitterness showing excellent solubility in water. Further studies are required to elucidate detailed sensory characteristics to suggest its feasibility as a novel sweetener in industrial applications.

7:00 Volatile organic compounds and amino acid composition in the rinds of cantaloupe cultivars during maturity Ganga K. Sah1, sahganga92@gmail.com, Kevin Crosby2, Vikas Dadwal2, Bhimu S. Patil2. (1) Food Sci. and Tech., Texas A&M U. System, College Station(2) Dept. of Horticultural Sciences, Texas A&M U. System, College Station Cantaloupe (Cucumis melo L.) rind accounts for about 25% of the total fruit weight and is considered a waste product. However, the rind has a key role in defending against pathogens and producing aroma compounds that influence consumer preferences and contains amino acids, which have potential uses in animal feed and supplements. This study measured volatile organic compounds (VOCs) and amino acids in the rind of cantaloupe cultivars at two maturity stages. Flowers of four cultivars of cantaloupe were tagged at anthesis and fruits were harvested at 26 and 39 days after anthesis (DAA). Rinds were processed for analysis of VOCs using headspace solid phase microextraction (HS-SPME) coupled with gas chromatography-mass spectrometry (GC–MS), and amino acids were analyzed using ultra-high-performance liquid chromatography (UHPLC). The cultivars and maturity stages showed significant variation in VOCs, and partial least scores discriminant analysis (PLS-DA) models classified VOCs such as benzaldehyde, benzyl alcohol, eugenol, and decanoic acid as major markers for classifying cultivars, followed by β-cyclocitral, which is reported for the first time in cantaloupe rind. Similarly, VOCs such as (E, Z)-3,6-nonadien-1-ol and (E,E)-3,5-octadien-2-one, and δ-cadinene were identified as markers of maturity in rind of cantaloupe cultivars. Furthermore, to the best of our knowledge, amino acids were quantified for the first time in cantaloupe rind and showed significant variation during maturity stages. Correlation heatmaps illustrated the correlation between amino acids and VOCs; for example, gamma aminobutyric acid (GABA) was positively correlated with phenylacetaldehyde ($r = 0.612$) and (E)-2-octenal ($r = 0.575$). These results suggest the potential role of amino acid metabolism in VOCs biosynthesis that may contribute to the fruit aroma and defense mechanism. In conclusion, this study demonstrated that cantaloupe rinds are rich in VOCs and amino acids of biological importance that could be useful for industrial extraction of amino acids, and aroma compounds for the flavor industry, or for animal feed in reduction of food waste.

7:00 Rosé wine quality impacted by storage conditions Cristina Medina Plaza1, cmedinaplaza@ucdavis.edu, Aubrey DuBois2, Elizabeth Tomasino2, Anita Oberholster1. (1) Viticulture and Enology, U. of California Davis(2) Food Sci. & Technology, Oregon State U., Corvallis Rosé wines are bottled in clear bottles as color is an important factor in consumer preference. Bottled wine can be exposed to UV-visible light for relatively long periods of time in retail stores, restaurants, domestic settings... Exposure to light and elevated temperature can decrease the quality of the wine changing the color and producing off-odors. This research studied the impact of bottle color, light exposure, and temperature on rosé wine composition. Three rosé wines were bottled in clear and green bottles and stored at room (22°C) and cellar (15°C) temperature under three different light conditions (darkness, fluorescent and cool white LED bulbs). Wines were analyzed after 0, 3, and 6 months of storage. The color and phenolic composition were determined by RP-HPLC and spectrophotometrically. Aroma profiles were determined through volatile screening using SPME-GC-MS. Spectrophotometric analysis showed that color intensity decreased over time. Light type in combination with bottle color showed the largest impact on color. Wines stored in clear bottles showed a larger decrease in color intensity than those in green bottles. Under same temperature and bottle conditions, fluorescent light showed a larger impact than LED. Wines stored in the dark, independent of the bottle type and temperature did not show any impact. Higher temperature and/or clear glass increased the percentage of yellow and decreased the percentage of red color in the wines potentially due to oxidation. Significant changes were found between the starting wines and the different time points on aroma profiles. In this case, bottle color showed a smaller impact than temperature. Sensory studies proved that panelists were able to distinguish the wines based on their aging conditions. Overall, although all variables studied impacted rosé wine aging significantly, higher temperature in combination with clear glass bottles under fluorescent light were the most detrimental to rosé wine quality.

7:00 Production and analysis of metabolites from solid-state fermentation of Chenopodium formosanum sprouts in a bioreactor Chenche Hsieh[2], Shu-Han Yu[2], Yu-Wei Liou[1], Kuan-Chen Cheng[1,2], kccheng@ntu.edu.tw. (1) Inst. of Food Sci. and Tech., National Taiwan U., Taipei(2) Inst. of Biotechnology, National Taiwan U., Taipei The research employed fresh Chenopodium formosanum sprouts on the fourth day as a substrate for Rhizopus oligosporus fermentation. The resulting products displayed greater antioxidant capacity than those from C. formosanum grains. In contrast to traditional plate fermentation (PF), employing a bioreactor (BF)

(35°C, 0.4 vvm aeration at 5 rpm) yielded higher free peptide content (99.56 ± 7.77 mg casein tryptone/g) and enzyme activity (amylase, glucosidase, and proteinase were 2.21 ± 0.01, 54.57 ± 10.88, and 40.81 ± 6.52 U/g, respectively) than PF. Two peptides, TDEYGGSIENRFMN and DNSMLTFEGAPVQGAAAITEK, were predicted to possess high bioactive properties as DPP IV and ACE inhibitors using mass spectrometry analysis. Additionally, over twenty new metabolites, such as aromatics, amines, fatty acids, and carboxylic acids, were discovered in the BF system in comparison to the PF system. The results suggest that using a BF system to ferment C. formosanum sprouts is a suitable approach for scaling up fermentation and improving nutritional values and bioactivities.

7:00 Structure elucidation of an anthocyanin-based aluminum blue complex and monitoring the changes with pH using electrospray ionization FT-ICR mass spectrometry Xinyue Fan, fan.1079@buckeyemail.osu.edu, Monica Giusti. Food Sci. and Tech., The Ohio State U., Columbus An aluminum metal complex consisting of delphinidin-3-glucoside and 5-caffeoylquinic acid (5CQA) was reported to be responsible for the blue color of Hydrangea flower. The food industry has been searching for blue colorants from natural sources that could substitute synthetics in food applications, but this is challenging since blue edible materials are rare in nature. In this project, we formed blue colors by combining eggplant peel extract containing delphinidin-3-rutinoside (dp3rut), Yerba Mate extract containing 5CQA and aluminum sulfate at pH 4 sodium acetate buffer. Color changes were monitored when the pH was adjusted from 2.5 to 7.0. Samples were injected into the Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (ESI FT-ICR MS) in order to identify the complex and characterize the changes in different pH. The mass of a metal complex containing dp3rut, aluminum and 5CQA was found in ESI FT-ICR MS at pH 4 (Figure 1), similar to the metal complex previously reported in Hydrangea plant, this time produced using edible food sources in solution. Ratios of complex to dp3rut could explain the color changes observed with pH changes. The emerging ESI FT-ICR MS technique was able to identify and monitor the complex changes in different pH, providing insights into the complex characteristics, helping the development of a more stable blue colorant for the food industry.

7:00 Walnut skin darkening associated with heat extreme is linked to changes in its metabolites and quality Zatil Afrah, zafrah@ucdavis.edu. Food Sci. and Tech., U. of California Davis Extreme heat is an environmental factor that potentially impacts the agriculture sector, including walnut production. A few weeks before walnut harvest, heatwave occurred and it resulted in a much higher proportion of walnuts with darker skin than usual. To understand if the darkening affects the metabolite and quality parameters, we subjected 14 pairs of samples to analysis. Each pair consisted of light and dark kernels sourced from the same cultivar and orchard/handler. The lightness classification was based on L* values determined using a colorimeter with the light group having L* of 20-39 and the dark group having L* of 40-59. The sampling covered three main cultivars grown in California: Chandler, Howard, and Tulare. The analysis comprised of fatty acid profile, volatiles, oxidative stability, total fat, free fatty acid, and peroxide value. Our findings demonstrated that significant changes are observed in the fatty acid profile, volatiles, total fat, and oxidative stability. Cultivars affect how the skin darkening affects the fatty acid profile of walnuts. Dark kernels had a higher relative concentration of volatiles and oxidative stability but reduced total fat. Free fatty acid in the dark kernels is slightly higher than in the light kernels. No significant difference was observed for peroxide values. These findings demonstrate that the heat extreme, manifested in the darkening of skin color, resulted in changes in the metabolite and quality parameters of walnuts. This report is expected to add knowledge on how environmental factors affect walnut properties.

7:00 Continuous flow high-pressure homogenization is an alternative preservative technique to increase the shelf life of watermelon juice during cold storage Jayashan Adhikari1,4, jadhikari@tamu.edu, Lida Rahimi Araghi3, Koushik Adhikari2, Rakesh K. Singh3, Bhimu S. Patil1,4. (1) Dept. of Food Sci. and Tech., Texas A&M U. System, College Station(2) College of Agricultural and Environmental Sciences, U. of Georgia, Griffin(3) Dept. of Food Sci. and Tech., U. of Georgia, Athens(4) Vegetable and Fruit Improvement Center, Dept. of Horticultural Sciences, Texas A&M U. System, College Station Recently, watermelon juice consumption gained consumers' attention because of its nutritional benefits. However, watermelon juice has a short shelf life, and the traditional thermal preservation technique deteriorates its qualities. Therefore, continuous flow high-pressure homogenization (CFHPH), a novel non-thermal technology, has been investigated as an alternative to thermal processing. The CFHPH comprised of a combination of three pressures (200, 250, 300 MPa), two inlet temperatures (4 or 22 C), and three flow rates (0.75, 1.125, 1.5 L/min), while the thermal process – high temperature short time (HTST) included samples treated at 75, 85 and 95 C for 15 seconds. The watermelon juice's physicochemical attributes and nutritional qualities were investigated every 15 days over 45 days of storage at 4 C. There was no significant difference in color space, pH, and total soluble solids. The level of carotenoids and amino acids were analyzed using ultra-high-performance liquid chromatography. The total carotenoid content was >40 mg/kg fresh weight, and lycopene comprised of >80% of the total carotenoid in watermelon juice. Among 15 identified amino acids, L-citrulline content decreased till 15 days and increased to the highest level after 45 days of storage. Among all the treatments, the CFHPH treatment at pressure 300 MPa showed higher retention of carotenoids and amino acids during cold storage. The CFHPH-treated watermelon juice maintained an adequate level of health-promoting compounds, and CFHPH at 300 Mpa could be a promising alternative to increase the shelf-life of watermelon juice while maintaining its nutritional qualities.

7:00 Effect of black rice dietary fiber on the metabolism of cyanidin-3-glucoside during in vitro colonic fermentation Qin Ma1, femaqinfoodfunction@mail.scut.edu.cn, Shuai Zhang1,2. (1) Guangdong Academy of Agricultural Sciences, Guangzhou, China(2) Huazhong Agricultural U., Wuhan, Hubei, China Black rice is a good source of anthocyanins and dietary fiber and possesses various health-promoting activities. This study was aimed at investigating the modulation effect of insoluble dietary fiber (IDF) from black rice on the fermentation of cyanidin-3-O-glucoside (Cy3G) in an in vitro human colonic model. The Cy3G metabolites content, antioxidant activities and SCFAs content at different time point during the fermentation were examined. The results showed that IDF can promote the biotransformation of Cy3G into phenolic compounds with stronger antioxidant activities such as cyaniding and protocatechuic acid, and increase total SCFAs production during the fermentation of Cy3G. 16S rRNA sequencing analysis revealed that the addition of IDF modulated the microbiota structure and improved the abundance of Bacteroidota and Prevotellaceae related genera, thus potentially regulating the microbial metabolism of Cy3G.

7:00 Chemometric analysis of Mānuka honey meads Lisa Pilkington1,2, lisa.pilkington@auckland.ac.nz, Chandra Chhouk1, Rebecca Deed1. (1) The U. of Auckland, New Zealand(2) Te Punaha Matatini, Auckland, New Zealand Mānuka honey is a monofloral honey made from nectar sourced from the

Leptospermum scoparium (Mānuka) tree native to New Zealand and has sparked researchers' interest due to its notable biological properties, especially its antimicrobial and antioxidant activities. The antibacterial potency of Mānuka honey is linked to the Unique Mānuka Factor (UMF), which is determined based on the concentration of key signature markers such as methylglyoxal (MGO), MGO's precursor dihydroxyacetone (DHA), and leptosperin. Mead is an ancient, fermented drink derived from three simple ingredients: honey, yeast and water and although honey mead is well studied, little is known about the properties and characteristics of Mānuka honey mead. The aim of this research was to study the chemical signatures of Mānuka honey from different regions of New Zealand and identify how these translate to and influence the chemical profile of their resulting honey mead.As part of this investigation, Mānuka honey meads were produced (through inoculation with Saccharomyces cerevisiae or spontaneous fermentation) using a range of 45 Mānuka honeys from different regions in NZ. Once the honey mead was made, the chemical profiles of both the honey-must and honey meads were analysed to investigate the differences in the meads based on the geographical origin in the honey and fermentation inoculation source. The chemical signatures were studied using a range of chemometric techniques to explore unique and identifying chemical markers in these complex matrices. We will present the results of these statistical workflows and identify chemical markers related to Mānuka honey mead and how they relate to the composition and origin of the parent honey and the method of fermentation.

7:00 Sensitive and specific electrochemical Nano-biosensor for monitoring of bacterial contamination in wash water of fresh produce Ahmed El-Moghazy, aelmoghazy@ucdavis.edu, Nicharee Wisuthiphaet, Nitin Nitin. Food Sci. and Tech., U. of California Davis Washing fresh produce is an important step in eliminating undesired organic and inorganic particles and reducing the levels of microbes, and other contaminants that may be present on the surface of the produce. However, the wash water used to clean the produce can become contaminated with pathogenic microorganisms, such as E. coli, Salmonella, and Listeria, that can potentially transfer to multiple batches of fresh produce and cause foodborne illness. The Food Safety Modernization Act (FSMA) Produce Safety Rule has specific requirements for the testing of water used for post-harvest washing of fresh produce with no detectable generic E. coli in a 100 mL sample of water. To reduce the risk of contamination, a highly sensitive and specific electrochemical biosensor was developed for the detection of E. coli in wash water using a handheld device without the need for culturing or nucleic acid extraction. The biosensing platform was fabricated based on a unique combination of hierarchical conductive nanofibers-modified screen printed electrodes with engineered bacteriophage T7 mediated specific lysis of the target bacteria. The employment of conductive nanofibers as a sensor matrix enhanced the electroactive surface area by more than three and four times as compared to casted conductive membranes and non-conductive nanofibrous membranes, respectively. The fabricated biosensor depicted successful detection of 1 CFU/mL of E. coli BL21 in simulated wash water within 3 h. With applying enrichment time of 6 h, the developed biosensor was able to detect E. coli at a concentration of 1 CFU/100 mL of wash water. Furthermore, the developed biosensor demonstrated the ability to detect the active E. coli only as well as high specificity toward the E. coli in the presence of other common bacterial contaminants.

7:00 Benzenethiols with smoke-derived phenols causing ashy aroma and flavor in red wine Darrell C. Cerrato1, cole.cerrato@oregonstate.edu, Jenna Fryer1, Mackenzie Aragon2, Philip L. Ashmore2, Lindsay Garcia1, Thomas S. Collins2, Elizabeth Tomasino1. (1) Dept. of Food Sci. and Tech., Oregon State U. College of Agricultural Sciences, Corvallis(2) Washington State U. College of Agricultural Human and Natural Resource Sciences, Pullman Changing climates have exacerbated conditions, promoting wildfire size and intensity in areas all over the world! For decades smoke from wildfires has had a negative impact on winemakers, grape growers, and wine consumers by making wines undesirable due to unpleasant flavors and aromas. Smoke can impart undesired ashy, campfire, rubbery, and other smoky sensory characteristics after nearby smoke events. While research has associated elevated amounts of phenols derived from incomplete pyrolysis of lignin in smoke, such as guaiacol, syringol, and the cresols, the association between the smoke phenols and aroma/flavor has not been as clear. Using a 13C-labelled fuel source, barley, this study discovered a novel group of compounds that have been impacting the quality of Oregon and Washington red wines due to smoke: benzenethiols! GCMS data suggests a reaction with smoke phenols and a sulfur source to form the benzenethiols, such as 2-methoxy-benzenethiol. A sensory experiment in this study confirms the influence of benzenethiols by comparing 20 µg/L of combined smoke phenols with 1.25 ng/L combined benzenethiols separately and together. Descriptive analysis showed that the combination of phenols and benzenethiols are the cause of the ashy aftertaste in smoke impacted wines! These results will play a crucial role in future amelioration work with more targeted chemical fining of impacted wines.

7:00 Determination of carbohydrates in peanuts by HPAE-PAD Yukiko Kawahara, Yukiko.kawahara@thermofisher.com, Jeffrey Rohrer. Ion Chromatography, Thermo Fisher Scientific, Sunnyvale, California Analysis of carbohydrates can be challenging using common reversed-phase HPLC or LC-MS methods due to carbohydrates' lack of chromophores and structural similarity. In this experiment, a fast and easy method to determine carbohydrates in peanuts and peanut butter was developed using High-Performance Anion-Exchange Chromatography with Pulsed Amperometry Detection (HPAE-PAD). Samples were processed with Carrez clarification using commercially available ready-to-use reagents prior to analysis by HPAE-PAD. Carbohydrates (glucose, fructose, sucrose, raffinose, stachyose and verbascose) were separated on an HPAE column in less than 17 minutes with good reproducibility and recovery. Carbohydrates were detected without analyte derivatization (labeling) by PAD. The total amount of glucose, fructose, and sucrose was in agreement with the sugar amount listed on the nutrition label of each product, demonstrating method accuracy. Though only peanut butter and dry roasted peanuts were tested in this experiment we believe this method can be used for the carbohydrate analysis of other legumes.

7:00 Engineered yeast displaying specific norovirus-binding nanobodies for the concentration and detection of human norovirus in food matrix Xue Zhao, Tom Kasputis, R. C. Wright, Juhong Chen, jhchen@vt.edu. Biological Systems Engineering, Virginia Polytechnic Inst. and State U., Blacksburg Human noroviruses pose grave threats to public health and economy. In this study, we genetically engineered yeast (S. cerevisiae EBY 100) to display specific norovirus-binding nanobodies (Nano-26 and Nano-85) on cell surface to facilitate concentration of noroviruses for improved detection. The binding of norovirus virus-like particles (VLPs) to these nanobody-displaying yeasts was confirmed and characterized using confocal microscopy and flow cytometry. The ability of our engineered yeasts to capture norovirus VLPs can reach up to 91.3%. Furthermore, this approach was applied to concentrate and detect norovirus VLPs in a real food matrix. A wide linear detection range (10 – 105 pg/mL) was observed and the detection limit on spiked spinach was calculated as low as 0.71 pg/mL. Overall, our engineered yeasts could be a promising approach to concentrate and

purify noroviruses in food samples for easy detection, which allows to prevent the spread of foodborne virus in the food supply chain.

7:00 Gomphrenin derivatives: alternative anti-inflammatory pigments from fruits of Basella alba L. (Malabar spinach) Slawomir Wybraniec1, slawomir.wybraniec@pk.edu.pl, Renata Górska1, Ewa Dziedzic2, Monika Bieniasz2, Przemyslaw Mielczarek3,4, Lukasz Popenda5, Malgorzata Tyszka-Czochara6, Katarzyna Sutor-Swiezy1. (1) Department C-1, Cracow U. of Technology, Poland(2) Faculty of Biotechnology and Horticulture, Agricultural U. of Krakow, Poland(3) Dept. of Analytical Chemistry and Biochemistry, Akademia Gorniczo-Hutnicza im Stanislawa Staszica w Krakowie, Krakow, Małopolskie, Poland(4) Maj Inst. of Pharmacology, Polska Akademia Nauk, Cracow(5) NanoBioMedical Centre, U. im Adama Mickiewicza w Poznaniu, Poznan, Wielkopolskie, Poland(6) Faculty of Pharmacy, U. Jagiellonski w Krakowie Collegium Medicum, Małopolskie, Poland Anti-inflammatory effects were studied for gomphrenin, known for its high antioxidative potential, in relation to its acylated and decarboxylated derivatives as well as Basella alba L. fruit extracts. The most abundant natural acylated gomphrenins, 6'-O-E-caffeoyl-gomphrenin (malabarin) and 6'-O-E-4-coumaroyl-gomphrenin (globosin), were isolated from B. alba extract and decarboxylated gomphrenins were obtained by controlled thermic decarboxylation of gomphrenin in purified B. alba extract at 65-75 °C. The most abundant products of the heating process were 17-decarboxy-gomphrenin and 2,17-bidecarboxy-gomphrenin as well as their isoforms. The decisive factor in the formation of 2-decarboxy-gomphrenin was a high concentration of citrates which favored the formation of this derivative to a great extent. This effect was substantially attenuated by addition of EDTA. The effects of citric acid and EDTA on retention and reactivity of gomphrenin pigment and its acylated derivatives in B. alba extracts submitted to heating were also studied. Exploring the matrix effect on reactivity of the pigments revealed tremendous increase in the stability of all betacyanins after first stage of the extract purification on a cation exchanger in all the studied conditions and buffers. This means that much of unfavorable matrix can be removed from the extract which presumably contains reactive species that degrade the pigments. Tested compounds showed varying activity on the development of Lipopolysaccharide (LPS) induced inflammation in culture of human macrophages. The macrophages play a major role in inflammation, wound healing and the reparative process within the human body. The results of the experiments showed that malabarin and globosin inhibited the development of inflammation by reducing the levels of the pro-inflammatory cytokines TNFα, IL-1β and, in particular, IL-6 which induce a systemic response in the body. In contrast to gomphrenin, both acylated gomphrenin derivatives and 2,17-bidecarboxy-gomphrenin inhibited the secretion of the pro-inflammatory cytokine IL-18, whose overexpression in vivo may contribute to cytokine storm leading to lung tissue damage as well as rheumatic diseases. Inhibition of the activity of pro-inflammatory cytokines has recently been intensively studied as therapeutic targets in infections and autoimmune diseases and we believe that research on gomphrenin derivatives may concur to development of novel therapeutic approach in the future.

7:00 Chemical profile and antioxidant activity of sweet cherry pulp (Prunus avium L.) from the Apulian region of Italy Pasquale Crupi2, Roberta Tardugno1, roberta.tardugno@gmail.com, Marilena Muraglia1, Francesco Limongelli1, Maria Lisa Clodoveo2, Filomena Corbo1. (1) Pharmacy - Drug Science, U. degli Studi di Bari Aldo Moro, Puglia, Italy(2) Interdisciplinary Dept. of Medicine, U. degli Studi di Bari Aldo Moro, Puglia, Italy Sweet cherry (Prunus avium L.) fruits are traditionally very appreciated by consumers due to their quality characteristics and their intake has been associated with beneficial effects. The antioxidant capacity of cherry pulp extracts is strictly related to the phenolic content, starting from the hypothesis that the higher content of polyphenols corresponds to the higher antioxidant indexes in sweet cherry pulp extracts. This work aims to assess which compounds characterized three cultivars namely, Ferrovia, Sweetheart, and Lapins grown in Apulia (Southern Italy). An optimized green extraction procedure adopting water/ethanol (1:1, v/v) as solvent allowed to obtain the maximum recovery of the main phenol compounds present in the cherry pulp. The HPLC–MS/MS analyses allowed the identification of 17 flavonoids, including 4 flavan-3-ols, 8 flavonols, and 5 anthocyanins. Moreover, 25 hydroxicinnamates derivatives were also identified. The extracts were tested for their radical scavenging power by measuring their capacity to scavenge DPPH and ABTS cation radicals and their reducing power using the Folin–Ciocalteau method. Lapins and Sweetheart extracts, richer in polyphenols, returned the highest reducing power and radical scavenging capacity. Finally, a factorial analysis was applied to the collected data allowing reliable correlations between polyphenols and antioxidant indexes.

7:00 Physicochemical properties, structural features and biological activities of two fructans obtained from single-clove garlic and multiple-clove garlic: A comparison Zhichang Qiu1, zhichangqiu@126.com, Hengjun Du1, Zhenjia Zheng2, Hang Xiao1. (1) Food Sci., U. of Massachusetts Amherst(2) Food Sci. and Engineering, Shandong Agricultural U., Tai'an, Shandong, China This study aimed to compare the structural features and biological activities of polysaccharides from single-clove garlic (SGPs) and multiple-clove garlic (MGPs). Our results showed that fructans were the predominant carbohydrates in both varieties of garlic. SGPs and MGPs differed in molecular weight distributions (6.76 kDa and 5.40 kDa, respectively) but shared similar monosaccharide composition (mainly composed of fructose and glucose), functional groups and glycosidic linkage patterns (both containing →1)-β-D-Fruf (2→, →6)-β-D-Fruf (2→ and terminal α-D-Glcp (1→ residues). SGPs and MGPs showed similar thermodynamic properties and X-ray diffraction patterns as well as high stability under an in vitro simulated gastrointestinal digestion system. They could scavenge free radicals and reduce oxidized metals in a dose-dependent manner in vitro. They were effective in alleviating metronidazole-induced oxidative stress and CuSO4-induced inflammation and associated damage in zebrafish via inhibiting the over-expression of inflammation-related proteins and cytokines. Compared with MGPs, SGPs showed lower free radical scavenging activity but higher antioxidative and anti-inflammatory activities in vivo. Taken together, this study demonstrated that the molecular weight/chain length was the main structural difference between the two garlic fructans of different varieties, which was responsible for their different biological activities.

7:00 Straightforward synthesis of P-alkylphosphonamidates and bioactivity screening as herbicides or quorum sensing modulators Simon Backx[1], simon.backx@ugent.be, Andreas Dejaegere[1], Andreas Simoens[1], Jef Van de Poel[1], Dorota Krasowska[1], Emmelie De Ridder[2], Anne Willems[2], Kris Audenaert[3], Willem Desmedt[3], Christian V. Stevens[1], Sven Mangelinckx[1]. (1) SynBioC research group, Dept. of Green Chemistry and Tech., U. Gent Faculteit Bio-Ingenieurswetenschappen, Belgium(2) Laboratory of Microbiology, Dept. of Biochemistry and Microbiology, U. Gent Faculteit Wetenschappen, Belgium(3) Laboratory of Applied Mycology and Phenomics, Dept. of Plants and Crops, U. Gent Faculteit Bio-Ingenieurswetenschappen, Belgium Organophosphorus compounds are widely investigated in chemical research, thanks to their applications as pharmaceuticals, flame retardants or pesticides. Phosphonamidates have gained particular interest as bioisosteres to

carbon-based amides and their uses as prodrugs. Although these functionalities can be made via reported methodologies such as the Staudinger-phosphonite synthesis or Atherton-Todd reaction, these methodologies typically require low temperatures, multiple steps, dry conditions or synthesis of labile starting products. For this reason, we developed a room-temperature coupling method for synthesizing novel P-alkylphosphonamidates. Our protocol starts from commonly available symmetrical dialkyl phosphonates, which are first chlorinated with oxalyl chloride to avoid side reactions such as dichlorination. Afterwards triethylamine is used to reduce the inherent reactivity of the phosphonochloridates in the coupling step. Our protocol has been demonstrated on various primary amines, secondary amines and amino acids, as well as different phosphonates. As an example of possible target structures that could benefit from this synthesis route, we synthesized a library of N-acyl homoserine lactone-analogues that were evaluated for their activity as quorum sensing modulators in Chromobacterium violaceum. As a second demonstration, the synthesized compounds were evaluated as herbicides in a high-throughput precision phenotyping system. We found that several phosphonamidates showed strong herbicidal activity and may have potential as lead compounds for future herbicide development. In the future, evaluating other nucleophiles such as thiols could further extend the potential of this method.

7:00 Chitosan gel embedded with Nano S as a coating film for Phosphorus fertilizers to enhance use efficiency Edwin A. Davidson1, eadbarahona@knights.ucf.edu, Swadeshmukul Santra1, Anastasiia Peresteva2,1, Felicity Rizzi2,1. (1) Chemistry, U. of Central Florida, Orlando(2) Biology, U. of Central Florida, Orlando In the coming years, the predicted increase in the global population will impose a challenge in food security to supply the global demand. For this reason, the implementation of more efficient agricultural practices are needed to reduce the use of resources (e.g. fertilizers and pesticides) without comprising the crop's productivity. A common strategy to provide plants with Phosphorus (P) is the use of rock phosphate (RP) or mono ammonium phosphate (MAP) as fertilizers. Nevertheless, these fertilizers have concerning disadvantages such as waterborne sedimentation, run-off, and eutrophication. Initially, to address these concerns sulfur (S) coating attracted interest but their low wettability and the need for post-coating sealing were major limitations. Herein, we developed a chitosan acidic gel-based polymeric matrix with nano S as a coating agent to overcome the challenges of P fertilizer and S coating. We performed an immersion coating methodology and characterized the coating formulation with Optical microscopy, Fourier-transformed Infrared (FTIR), Scanning Electron Microscopy (SEM), X-ray diffraction spectroscopy (XRD), and Zeta potential. Additionally, we quantified the concentration of P to determine the run-off and use efficiency of post-coated fertilizers. We studied the effects on plant growth and germination of tomatoes (Solanum Lycopersicum) under greenhouse conditions. Overall, we demonstrated the potential use of nano-enabled coating technology as a promising strategy to enhance the use efficiency and controlled release of nutrients towards more sustainable agricultural practices.

7:00 Analysis of volatile phenol interaction with film coatings developed to reduce grape absorption of wildfire smoke compounds Lindsay Garcia, lindsaygarcia.lg@gmail.com, Trung T. Tran, Jooyeoun Jung, Darrell C. Cerrato, Lik R. Lim, Michael H. Penner, Yanyun Zhao, Elizabeth Tomasino. Food Sci. and Tech., Oregon State U., Corvallis Vineyards exposed to wildfire smoke can result in negative sensory qualities in the resulting wine. The lack of effective mitigation techniques to combat smoke affected grapes elicited the development of innovative film coatings to prevent smoke uptake in wine grapes. These films were made using a cellulose nanofibers base and chitosan, β-cyclodextrin or a 2:1 combination of the two. Preliminary experiments confirmed smoke volatile phenols (VPs) sorb to the film. Thus, it was necessary to determine the diffusion directionality of the VPs. The first experiment determined if the VPs desorb from the film back into the atmosphere after smoke exposure diminishes, and if so, how much. Pieces of film (30 x 30 mm) were hung in airtight containers and exposed to smoke VPs for five days. The films were aired out in a fume hood and placed in acetone twice consecutively to extract all volatile phenols still sorbed to the film. The second experiment determined if the film is permeable to VPs, which could still result in a smoky flavored wine. To test for permeability, 10 x 10 cm films were exposed to VPs in a specially designed polytetrafluoroethylene container. After several days of exposure, air samples were taken from inside the box. All samples were analyzed using GCMS. The collective results of this study show the seven volatile phenols analyzed interact differently with the film. The differences in permeability provide crucial information needed to modify the formulation. The optimization of the film coating formula will provide the wine industry with an effective strategy in minimizing the grape absorption of critical volatile phenols responsible for smoke taint in wine.

7:00 Simultaneous prediction of beta-carotene, anthocyanins, and phenolics in sweet potatoes by near-infrared spectroscopy Matthew Allan[1,2], matthew.allan@usda.gov, Ragy Ibrahem[3], Suzanne D. Johanningsmeier[1,2], Kenneth Pecota[3], Craig Yencho[3]. (1) Food Sci. and Market Quality & Handling Research Unit, USDA Agricultural Research Service, Raleigh, North Carolina(2) Food, Bioprocessing and Nutrition Sciences, NC State U., Raleigh(3) Horticulture, NC State U., Raleigh Sweet potato compositions can be predicted using near infrared spectroscopy (NIRS) models developed with samples of known composition. β-carotene and anthocyanins are of interest in sweet potatoes for their health benefits and impacts on appearance and flavor. However, predictions are conflated due to similar NIRS wavelength absorbances. Therefore, NIRS models that account for both chromophores in sweet potatoes are needed. A sample set (n=100) was selected from the NCSU sweet potato breeding program based on NIRS diversity and visual appearance. Anthocyanins and phenolic compounds were extracted using acidified methanol. Phenolic contents were measured by the Folin-Ciocalteu′s phenol assay, and anthocyanins were measured by the pH differential method. Anthocyanidin quantities (peonidin, cyanidin) from acid hydrolyzed anthocyanins were separated and quantified using high performance liquid chromatography with photodiode array detection (HPLC-PDA). β-carotene was extracted using hexane and quantified by HPLC-PDA. Partial least squares (PLS) prediction models for each measured compound were trained using 75 randomly selected samples then validated with the remaining 25 samples. Validation set range (mg/100g fresh weight) with root mean square error of prediction (RMSEP) and R^2 were the following: phenolics, 918.0 to 5343.3 ± 269.4, 0.94; total anthocyanins, 0 to 673.0 ± 10.34, 0.97; cyanidin, 0 to 769.0 ± 36.39, 0.73; peonidin, 0 to 383.5 ± 19.24, 0.73; and β-carotene, 0 to 61.4 ± 4.3, 0.94. Total anthocyanins, β-carotene, and total phenolics in sweet potatoes were accurately predicted by these models, which can be used by breeding programs to select for genotypes with specific phytonutrient profiles of interest.

7:00 Foodborne silica nanoparticles induced adverse effects differentially in obese and non-obese mice Hengjun Du, hengjundu@gmail.com, Hang Xiao. Dept. of Food Sci., U. of Massachusetts Amherst Silica (SiO2), a commonly used food additive (known as E551), contains an appreciable fraction of particles falling in the nanoscale, which has raised concerns about their unintended potential risks to human health. Accumulating evidence demonstrated that different populations have different

susceptibilities to nanoparticles, such as obese vs. non-obese and males vs. females. Herein, we determined the potential adverse effects of SiO2 NPs in non-obese and obese mice (both male and female adult mice). Mice (3-week old) were fed either a low-fat diet (10 kcal% fat, does not induce obesity) or a high-fat diet (60 kcal% fat, induces obesity) containing SiO2 NPs (20 nm, 0.1 wt%) or E551 (food-grade SiO2 additive, 0.1 wt%). The results showed that administration of E551 and SiO2 NPs led to the accumulation of SiO2 in mouse kidney and liver dose-dependently, accompanied by damage to specific cellular organelles in the renal and liver tissues. Interestingly, SiO2 NPs induced adverse effects in female mice were stronger than in male mice. Furthermore, the SiO2 NPs profoundly modulated the mRNA levels of genes involved in oxidative damage in the liver and kidney. The effects mentioned above were more pronounced in obese mice than non-obese mice. Additionally, it exacerbated the obesity-induced low-grade colonic inflammation, such as increasing inflammation-related cytokines and losing healthy colonic morphology in the colon. SiO2 NPs further reduced obesity-induced decline in the cecal levels of SCFAs, such as butyrate. The results showed that dietary SiO2 NPs led to a significant dysbiosis of gut microbiota with stronger alterations in obese mice than in non-obese mice. On the other hand, E551 and SiO2 NPs caused adverse effects on the reproductive systems of both male and female mice, such as the sperm and oocytes number decrease, sperm abnormality, pathological change of testes and ovaries, and abnormalities in sex hormone secretion. Moreover, SiO2 NPs disordered the expression of genes and proteins related to spermatogenesis, oogenesis, apoptosis, oxidative stress, and steroidogenesis in the gonads of mice, causing reproductive toxicity, especially in obese ones. Overall, these findings provided a valuable new perspective on the potential adverse effects of foodborne SiO2 engineered NPs among different populations.

7:00 Macroporous adsorbent resin debittering of HLB-affected orange juice and its impacts on consumer sensory acceptance Taylor Washington1, Fabiana Briceno1, Charles Sims1, Renee M. Schneider1, Jeffrey Brecht2, Katlyn Nau1, Yavuz Yagiz1, Liwei Gu1, lgu@ufl.edu. (1) Food Sci. and Human Nutrition, U. of Florida, Gainesville(2) Horticultural Sciences Department, U. of Florida, Gainesville HLB infection of oranges induces the biosynthesis and accumulation of bitter limonoids. The objective of this study was to debitter HLB-affected orange juice and try to preserve tasteless and health-promoting limonoid glucoside and flavanones using resin adsorption. Three resins (FPX66, PAD900, and XAD16N) were found to have higher adsorption and desorption capacity for limonin from seven selected candidates. Adsorption of limonoids rapidly increased in the first 2 hours of kinetic tests while slower adsorption kinetics were observed for flavanones. Limonin isothermal adsorption fit best with the Langmuir model, suggesting a physical, monolayer process. Dynamic adsorption showed that a fixed-bed column packed with PAD900 was able to debitter 200 bed volumes of oranges juice before limonin reached its taste threshold of 4.7 µg/mL in the eluent. Regeneration of the resin was achieved by eluting the column with 4 bed volumes of alcohol or 4% NaOH to remove adsorbed compounds from resin. Resin adsorption reduced limonin content in orange juice from 5.85 µg/mL to 1.34 µg/mL but also decreased tasteless compounds by at least 40%. A consumer taste panel gave the debittered juice a higher overall liking and preference over untreated juice. This study showed that resin adsorption is an effective approach to reduce bitterness of orange juice affected by HLB.

7:00 Determination of fatty acid composition, functional group, and compounds found in cocoplum (Chrysobalanus icaco L) seed oil using GC-FID, FTIR, and GC-MS instrument: Extractions, physicochemical and phytochemical parameters Chika E. Oyeagu1, oyelion@gmail.com, Adaora Stella S. Ezeuko2, Francis B. Lewu1. (1) Dept. of Agricultural, Cape Peninsula U. of Technology Faculty of Applied Sciences, Cape Town, Western Cape, South Africa(2) Pure and Applied Chemistry, U. of Fort Hare, Alice, Easter Cape, South Africa The cocoplum seed oil has been used as an alternative cooking oil due to its bioactive components and nutritional properties beneficial to human health. The cocoplum, a genus of Chrysobalanus icaco L, is a seed rich in oil containing dietary fatty acids to prevent oxidative damage, blood lipid, and cardiovascular diseases. This study aimed to provide information on the physicochemical parameters, percentage (%) composition of fatty acids present, functional groups assignment, compound determination using GC-MS, and phytochemistry of cocoplum seed oil. The physicochemical analysis was investigated, and the result of parameters such as the density (0.9583 g/cm3), moisture content (7.4%), refractive index (1.479 at 40 oC), acid value (5.34 mg KOH/g), saponification value (194.1 mg KOH/g), peroxide value (ranging from 3.02 to 6.50, 5.02 to 8.95 and 6.02 to 10.05 when the oil was exposed to contact air, temperature, and combination of contact air/temperature during the storage period) and iodine value (5.219 g) were obtained. The Origin Pro 2019 statistical software was used for data analysis. The oil sample extracted from the cocoplum has a golden yellow color with a pleasant odor. The oil sample has a pH of 7.23, which is safe for human consumption. The phytochemistry screening revealed that cocoplum seed oil contains flavonoids, alkaloids, terpenes, quinones, cardiac glycosides betacyanin that improve the human heart and reduce blood pressure and cholesterol level. The FTIR of the cocoplum seed oil indicated the presence of aldehydes, aliphatic hydrocarbons, and esters. The GC-FID instrument determining the % composition of fatty acids revealed that seed oil has four primary abundant fatty acids. They include stearic (24.99%), oleic (20.5%), linoleic (13.1%), and palmitic (5.99%). The compounds detected using GC-MS revealed that cocoplum seed oil contains nanocosane, n- triacontane, tritriacontane, stigmasta-5-ol, etc. These compounds play a vital role in preventing the human body from chronic diseases and other oxidative damage. Therefore, it can be concluded that cocoplum (Chrysobalanus icaco L) seed oil can be recommended as the best dietary oil due to its therapeutic properties, nutritional value, affordability, and safety.

7:00 Sustainable food processing through low-pressure membrane technologies for food quality and safety Mona Gulied, mgulied@qu.edu.qa, Fathima Sifani Zavahir, Tasneem Elmakki, Dongsuk Han. Center for Advanced Material, Qatar U., Doha, Ad Dawhah The food industry is searching for alternative food processing technologies with minimal energy requirements to maintain food quality and ensure a safe nutrient content. One of the primary operations in the food industry is the concentration of liquid foods. It is essential to dewater naturally during food processing to enhance shelf life. Recent studies have demonstrated that membrane-based dewatering technology is more efficient and less energy-demanding than conventional ones. Forward osmosis (FO) and membrane distillation (MD) have emerged as promising for food processing. However, recent reviews emphasize the benefits of the FO process over other membrane-based approaches for enriching liquid foods. This comprehensive study highlights the contributions and advancements of FO and MD in food processing and discusses their maturity and technological readiness level related to food concentration. Also, it presents tangible parameters, such as pretreatment methods, membrane cleaning approaches, and membrane configurations/modules suitable for specific types of liquid food dewatering. Most FO and MD research have been carried out primarily on a laboratory scale for concentrating fruit juice and whey. Future studies should focus on pilot-scale process development and techno-economic analysis for industrial transition.

7:00 Ice recrystallization inhibition and acceleration by cellulose nanocrystals in the presence of anionic and neutral polymers Min Li, mli63@vols.utk.edu, Tao Wu. Food Sci., U. of Tennessee, Knoxville Ice crystals over 50 µm in ice cream cause undesired icy texture, decreasing consumers' appeal. These large ice crystals result from the ice recrystallization process, which refers to the size increase of already-formed ice crystals without increasing the ice mass. Food polysaccharides, such as guar gum and locust bean gum (LBG), are used as stabilizers in ice cream to control ice recrystallization. Sometimes, mixed stabilizers, such as LBG and xanthan gum, carrageenan, and LBG or guar gum, are used, but their combined IRI effect is unknown. Cellulose nanocrystals (CNCs) are novel colloidal materials demonstrating IRI activity and potential as ice cream stabilizers. In this work, the IRI effect of CNCs in the model ice cream system – 25.0% sucrose solution was investigated in the presence of sodium alginate (SA), carboxymethyl cellulose (CMC), polyethylene glycol (PEG), and inulin. With increasing the concentrations of anionic polymers (SA and CMC), the IRI effect of CNCs was improved first and then reduced. Acceleration of ice recrystallization occurred with further increase of polymer concentration and large ice crystals with irregular morphology formed by merging of nearby ice crystals. There was little impact on the IRI effect of CNCs in the presence of neutral polymers (PEG and inulin). The addition of anionic polymer reduced the available volume and increased the effective concentration of CNCs, leading to the enhanced IRI effect. The reduced IRI effect and recrystallization acceleration might be explained by the depletion interaction that caused the aggregation of CNCs and the merging of ice crystals. The research findings in this work bettered our understanding of the IRI effect of mixed stabilizers, which is important for formulating ice cream stabilizers.

MONDAY MORNING August 14
Chemistry of Wine - Wine Aging, Sensory, and Health
8:05 What causes red wine headaches? Andrew L. Waterhouse1, alwaterhouse@ucdavis.edu, Apramita Devi1, Morris Levin2. (1) Viticulture and Enology, U. of California Davis(2) Neurology, U. of California San Francisco Some people suffer from headaches when drinking red wine, but not other alcoholic drinks. The literature is rife with speculation as to the cause, and biogenic amines, sulfites and phenolics have been suggested among other ideas. However, no pathway has been offered by which these various compounds might lead to headaches. Some people have a dysfunctional acetaldehyde dehydrogenase (ALDH2) that leads to flushing and headaches, caused by the accumulation of acetaldehyde. The abuse of alcohol is sometimes treated with disulfiram, which is a potent inhibitor of ALDH2, and headaches are one of the uncomfortable symptoms when alcohol is consumed. Red wine contains higher concentrations of phenolics which are extracted from the grape's skin and seeds during fermentation, and this includes quercetin and related compounds. We have observed that quercetin and in particular its glucuronide inhibits ALDH2. The glucuronide has been reported to be circulating after consuming red wine. Thus, we hypothesize that red wine headaches are caused by the quercetin metabolites inhibiting ALDH2, which results in elevated acetaldehyde in circulation. Testing on human subjects must be carried out to validate this hypothesis.

8:30 Chemical properties of interspecific red wines bottled with different concentrations of free sulfur dioxide Aude A. Watrelot, watrelot@iastate.edu, David Carter, Alexander D. Gapinski, Yiliang Cheng. Food Sci. and Human Nutrition, Iowa State U., Ames Sulfur dioxide (SO_2) is a common preservative in the wine industry, especially important in wine at bottling to protect wines against oxidation and microbial spoilage. However, in wine, the molecular form of SO_2 is the most effective form but is present in the least amount under acidic conditions (wine pH). A rational use of SO_2 in wine made from non-Vitis vinifera grape cultivars is challenging as the chemical composition of those wines is not well known, especially during aging. The chemical composition, including the concentrations of total phenolic compounds, tannins, anthocyanins, acetaldehyde, and free and total SO_2 concentrations, as well as color parameters were determined in three interspecific red wines after 4-months of aging. The wines were initially bottled with 30, 60 and 90 mg/L free SO_2. The highest concentration of free SO_2 at bottling in all wines negatively impacted the color intensity. In 'Crimson Pearl' and 'Petite Pearl wines', the acetaldehyde concentration was lower in the 90 mg/L free SO_2 condition and the hue and b* parameter were higher. However, no effect of the concentrations of free SO_2 added at bottling on the hue and acetaldehyde concentration was observed in 'Marquette' wines. The impact of winemaking and SO_2 concentrations on phenolic compounds and quality of wine made from interspecific grapes will be discussed.

8:55 Withdrawn
9:20 Evaluation of extraction rates of toasted-oak volatiles in model wines as a function of toast level in oak barrel alternatives Mackenzie Aragon, Thomas S. Collins, tom.collins@wsu.edu. Washington State U., Richland Oak barrel alternatives have become more widely available as a tool for providing oak character for lower price point wines. While appropriate timelines for the use of barrels for aging wines are well understood, extraction rates for toasted oak-related volatiles compounds from alternative products have been less clear. In this study, convection-toasted oak cubes, approximately 25 cm on a side, of five different toasting levels from light to heavy (1 lightest to 5 heaviest) were extracted in 15% ethanol model wine (20 g/L of cubes) over a 180-day period to determine extraction rates for five oak volatiles present in all the toast levels. Model wine extracts were sampled for analysis at 2, 4, 6, 8, 10, 15, 30, 60, 90, 120, 150 and 180 days. Concentrations of furfural, 5-methyl furfural, guaiacol, cis-oak lactone and trans-oak lactone were determined using solid-phase micro-extraction headspace gas chromatography mass spectrometry (SPME-HS/GC-MS). Extractable volatiles varied by toast level and compound. Furfural and 5-methyl furfural concentrations increased with toast level from level 1 to level 2 or 3, then declined in the heavier toast levels. Guaiacol increased from level 1 to level 5, while both cis- and trans-oak lactones decreased with increasing toast level. Concentrations for all compounds increased with time, at least initially. Concentrations of 5-methyl furfural, and cis- and trans-oak lactones peaked at 60 days, then remained stable or declined slightly. Furfural concentration peaked at 90 days and remained relatively stable after that time point. Guaiacol concentrations were consistently low in the two lightest toasting levels but increased consistently across the entire extraction period for toasting levels 3, 4 and 5. This study will be followed by a similar study using the same toast levels in a different format to evaluate the impact of shape/size on extraction rates.

10:05 Impact of micro-oxygenation in combination with barrel aging to shorten maturation time Cristina Medina Plaza, cmedinaplaza@ucdavis.edu, Lik X. Lim, Anita Oberholster. Viticulture and Enology, U. of California Davis During oak barrel maturation, the wines are enriched in aromatic compounds, the color is stabilized and mouthfeel complexity is improved. The extraction of oak phenolics has been shown to be dominated by diffusion kinetics; the rate of extraction is initially high which decreases when the concentration in the wine approaches that on the surface of the wood. The oxygen that diffuses through the barrel walls also plays an important role during barrel aging, facilitating polymerization reactions. Micro-oxygenation (MOX) in combination with barrel

maturation could accelerate aging, reducing the time that wine needs to be in barrel while still obtaining the benefit of oak aromas. In this project, a red wine blend was aged in barrel and stainless-steel vessels using different oxygen dosages (0, 1 and 2 mg/L/month). The 2 mg/L/month treatment was stopped after 3 months whereas the 1 mg/L/month treatment was applied for 6 months and the treatments without MOX continued for 12 months. Dissolved oxygen (DO), volatile acidity, free, and total SO2 levels were measured weekly. Acetaldehyde-adducts and phenolics were determined by RP-HPLC. No differences among treatments were found on DO levels although a larger decrease in free SO2 was found in those vessels with MOX treatments. Wines reached similar levels of acetaldehyde at the end of each treatment independent of MOX level. Total tannins increased overtime, particularly in the wines aged in barrels and total anthocyanins decreased overtime paired with an increase in polymeric pigments for all the wines. PCA results using all the chemical data indicated that the 6 months oxygen treatment at 1 mg/L/month showed similar ageing to the barrel treatment without MOX after 12 months. When consumer studies were carried out, there were no significant differences on ranking suggesting that MOX could be used to shorten aging time in barrel.

10:30 Detection and identification of modified tannins evolved during red wine aging Apramita Devi1, aprdevi@ucdavis.edu, James F. Harbertson2, Andrew L. Waterhouse1. (1) Viticulture and Enology, U. of California Davis(2) Viticulture and Enology, Washington State U., Pullman Condensed tannins are the important molecules associated with wine astringency. During wine aging, the tannins undergo many modifications by reacting with other chemical constituents in wine such as sulfur dioxide, anthocyanin, and acetaldehyde. The modifications appear to affect the physical and chemical properties of tannin with potential impact on the character of wine astringency in aged wines. This work aimed to discern the presence of modified tannin in aged red wines and understand the chemistry of their formation in the oenological conditions. First, a database of modified tannins, based on those reported in literature was created. The database mainly includes the sulfonated tannins and anthocyanin-tannin adducts. Second, the modified tannins were detected and identified in the aged wines (10 years old or more) using LC-Q-TOF MS. In addition, one of the modified tannins i.e., sulfonated tannins, was prepared by reaction of commercial grape tannins with SO2. From the reaction, epicatechin sulfonate is the major monomeric flavanol sulphonates produced, as epicatechin is the predominant extension unit in tannins. The effect of temperature (23, 35 and 45 °C) and pH (2, 3 and 4) on the reaction indicated that sulfonation is favored by low pH and high temperatures. Based on the reaction rates, we estimated that 2% of the tannin in red wine would react in a year to produce sulfonated tannins at wine pH and normal storage temperature. Hence, during the normal aging of tannic red wine, the conversion of tannin via sulfonation may be significant and could contribute to the modification of astringency observed in aged red wines. Future synthesis and characterization of modified tannins will make it possible to better measure the impact of these modifications on the sensory qualities of wine.

10:55 Modeling wine aroma perception from Key odorant composition and psychophysical measurements: using odor detection probability Terry E. Acree, tea2@cornell.edu, Yao Jiang, Tiffany Hsu. Food Sci., Cornell U., Ithaca, New York Some of the most potent odorants, i.e. Key odorants (KOs), chemically detected in wine are neither detected individually by the nose nor do they modulate the configuration created by the mixture. This lack of a consistent functional relationship between the smell of a mixture challenges attempts to predict wine aroma from it's analytical chemistry. Furthermore, the fact that human smell responses are highly idiosyncratic makes predicting wine odor perception even less accurate. This presentation will discuss of the psychophysical features that must be accounted for while modeling wine perception from chemistry. For example, how does peri-threshold levels of TDN (1,1,6-trimethyl-2,2-dihydronapathalene) create Riesling aroma from an odorant mixture that would otherwise be a perfumy floral wine.

Advances in Food Chemical Informatics, Knowledge Bases and Databases

8:05 Navigating the nexus: AI, data science, and the future of Food Sci. and informatics David Wild1,2, djwild@indiana.edu, Brian D. Guthrie3. (1) Luddy School of Informatics, Computing and Engineering, Indiana U., Bloomington(2) Data2Discovery Inc., Bloomington, Indiana(3) Cargill Inc, Minneapolis, Minnesota As the world population grapples with the consequences of climate change and the rapid evolution of societal norms and needs, the challenges of producing affordable, healthy, and appealing foods continue to escalate. Concurrently, recent breakthroughs in technologies such as artificial intelligence (AI) and data science promise transformative capabilities that hold the potential to accelerate research, enhance discovery, and unlock solutions to previously intractable problems in the realm of Food Sci. and informatics. This talk will provide an overview of significant trends in informatics, AI, and data science, including how these technologies might be poised to revolutionize the field of Food Sci. and informatics over the next decade. We will delve into the potential applications of these advancements in areas such as sustainable food production, personalized nutrition, and food safety, showcasing how AI and data-driven innovations can help tackle the pressing challenges of our time.

8:35 Using cheminformatics to speed up the full clarification of the chemobiological space of food compounds Gonzalo Colmenarejo, gonzalo.colmenarejo@imdea.org, Irem Kaya, Andres Sánchez-Ruiz. Biostatistics and Bioinformatics Unit, Instituto Madrileno de Estudios Avanzados, Madrid, Spain Food compounds are extremely important for health. Their molecular mode of action is being extensively studied through biochemical and cellular assays aiming at characterizing their interactions with human targets. They have also been studied as sources of scaffolds for drug discovery (e.g. caffeine). Our group has been using chemoinformatic methodologies to a) systematically identify all published interactions of food compounds with human targets and extract patterns front it in terms of enriched compound class vs target class combinations and scaffolds; b) predict putative assay interference substructures and aggregating compounds prone to yield false positives in assays; and c) predict a large number of putative interactions of high likelihood of success with human targets. These efforts are expected to speed up the full clarification of the chemobiological space of food compounds by providing a lot of new opportunities for fast focused screens in previously unmapped regions, as well as improving the awareness of experimentalists on putative false positives in their assays. All these efforts will be discussed in this presentation

9:00 Exploring the backbone of Nature’s chemical space as the primordial source of biological-driven structural diversity Stefan Furrer2, stefan.furrer.sf1@givaudan.com, Ioana M. Ungureanu2, Cristian G. Bologa1, Jeremy J. Yang1, Jason Timm1. (1) Translational Informatics Division, U. of New Mexico Health Sciences Center, Albuquerque(2) Science & Technology, Givaudan Flavors Corp, Cincinnati, Ohio Natural products have a great diversity of biological functions and properties; the intricate relationships between structural features and biological activities is at the core of many life science research fields, from pharmacology

to flavor and fragrance research to mention just a few. Central to the structural diversity of natural products is a limited set of well-defined organic frameworks. These scaffold are defined by biosynthetic pathways, some ubiquitous, some very specific to a particular organism. Further functionalization of these scaffolds provides an ever expanding pool of biologically active compounds that are in need of a systematic exploration. With this study we are taking a first step in systematically exploring the biodiversity of natural products, namely the in-depth study of scaffolds as the origin of a vast chemical space and associated biological activities. We are building on an extensive cheminformatics analysis of natural products, their associated scaffolds and their biosynthetic origin. The importance of such a study is twofold: making the comprehensive exploration of the natural chemical space an achievable goal and supporting further expansion into white spaces of natural products. This type of study has the ultimate goal of supporting uncovering previously unknown, meaningful biological activities.

9:25 Structured Taxonomies for food and flavor databases Andreas Dunkel, a.dunkel.leibniz-lsb@tum.de, Guangjuang Luo. Leibniz-Institut fur Lebensmittel-Systembiologie an der Technischen U. Munchen, Freising, Bayern, Germany Food composition and flavor databases are critical resources required by professionals from food regulatory agencies, food manufacturers as well as researchers working e.g. in nutrition medicine, flavor analysis, and product development. Although a large number of databases in the food sector was developed over the last decades, comprehensive, easily accessible and reliable high quality information are still difficult to obtain. For a successful development of an integrated and comprehensive knowledge portal facilitating a systems biology approach for food systems, several gaps need to be addressed. Besides the development of objective quality criteria for classification of literature data on food composition, a direct connection of molecules on the one hand to their food concentrations and on the other hand to the associated biochemical function and receptors is mandatory for the target-oriented reformulation of foods. To structure this information, suitable hierarchical taxonomies for various data types are required for effective filtering and analysis of the complex and interdisciplinary data sets. The presentation will summarize approaches for classification of food items, molecular entities, receptors, sensory qualities and other physiological functions. While food information can be categorized using a standardized controlled thesaurus, individual molecules are evaluated on the appropriate chemical space using e.g. MESH vocabulary, CHEBI terms and the ClassyFire approach.

10:00 Valuable tool for flavor scientists: The Leibniz-LSB@TUM odorant database Veronika Mall, v.mall.leibniz-lsb@tum.de, Johanna Kreissl, Petra Steinhaus, Martin Steinhaus. Leibniz Inst. for Food Systems Biology at the Technical U. of Munich, Freising, Germany The aroma of food greatly influences appetite, eating pleasure, and thus food preferences in humans. The molecular basis of aroma is odor-active compounds, volatile chemicals that can be detected by our olfactory system in the nose with its ~400 olfactory receptor proteins. While most of the volatiles in a food are not odor-active, a few so-called key odorants significantly contribute to the overall aroma. The identification of the KFOs is part of the sensomics approach, also known as molecular sensory science. Sensomics is the comprehensive scientific study of chemical processes involving sensory active molecules in foods, their raw materials, the human body, and the environment. The identification of the KFOs in a given food is typically divided into seven consecutive steps including i) the gentle and artifact-avoiding isolation of the volatiles, ii) the screening of the volatiles for odorants by gas chromatography-olfactometry (GC-O), iii) structural assignment of the odorants, iv) precise quantitative measurements, v) calculation of odor activity values (OAVs) to approximate the odor potency of the individual compounds, vi) validation of the findings by aroma reconstitution, and finally vii) omission tests to assess the importance of the individual odorants for the overall aroma. To facilitate the identification of key food odorants, flavor scientists in research and development require an elaborate compilation of i) reliable data on retention behavior and odor properties of previously identified food odorants to derive structure proposals after GC-O, and ii) reproducibly determined odor threshold concentrations in different matrices for the calculation of OAVs. From an in-house data compilation generated over the years in parallel to our steadily increasing experience in the field of sensomics, we recently developed the Leibniz-LSB@TUM Odorant Database available on the internet fully open access. The current version of the Leibniz-LSB@TUM Odorant Database contains retention indices on different GC stationary phases, odor descriptions, and odor threshold concentrations of ~1700 odorants extracted from >700 scientific papers.

10:20 Food chemicals in epigenetic targets: towards an epi food chemical database Karina Juárez Mercado, kaeuridice@gmail.com, Juan Felipe Avellaneda-Tamayo, Jose L. Medina-Franco. Pharmacy, U. Nacional Autonoma de Mexico, Mexico City There is an increasing awareness of the importance of epigenetics to understand disease etiologies and develop novel therapeutics. Concomitantly, the renewed interest in epigenetic processes and their relationship with food chemicals have been reflected by an increasing number of publications in the past few years. However, there is a lack of a recent systematic and quantitative study that accounts for the most recent advances in the area associating the chemical structures of the food and natural product components with their biological activity. Here, we review the most recent advances and discuss the status of food chemicals and their intersection with natural products in epigenetic research with focus on disease prevention and drug discovery. We discuss the most investigated diseases and potential therapeutic applications associated with food chemicals and natural compounds ingested in the diet. Using chemoinformatics approaches, we compared quantitatively the chemical contents, structural diversity, and coverage in chemical space of food chemicals reported with epigenetic activity with reference libraries including libraries designed de novo, drugs approved for clinical use, and synthetic libraries focused on epigenetic targets As part of this work, we built and curated a compound database of food and natural product chemicals annotated with structural information; epigenetic target activity profile; main source of the food chemical or natural product, among other relevant features. The compounds are cross-linked with identifiers from other large major public databases such as FooDB and the COlleCtion of Open Natural ProdUcTs (COCONUT). The outcome of this work represents a further development of the field of foodinformatics contributing to systematic study, including epigenetic activity profiling, of food chemicals.

10:40 Natural products magnetic resonance database (NP-MRD): An essential resource for food chemical informatics John R. Cort1,2, john.cort@pnnl.gov. (1) Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington(2) Inst. of Biological Chemistry, Washington State U., Pullman NMR spectroscopy is essential to discovery and structure elucidation of novel natural products and specialized metabolites, as well as to the identification and quantification of known molecular components present in complex mixtures via NMR metabolomics methods. However, a lack of availability of NMR data for known natural products and mixtures hinders rapid progress in these endeavors.

Currently, chemical shift assignments are scattered throughout the scientific literature and several incomplete chemical shift databases. Historically, most raw data (FIDs) used to determine structures of natural products and characterize mixtures has not been archived and is largely unavailable. To address these inadequacies, the Natural Products Magnetic Resonance Database (NP-MRD, np-mrd.org) has been established with a goal to be comprehensive, searchable, connected, and open database and repository resource for all natural products NMR data. The NP-MRD contains derived (e.g. chemical shift assignments), raw (FIDs), and predicted NMR data, as well as simulated spectra. The database also provides tools and links to other databases, and public deposition interfaces to fulfill new requirements from journals and funding agencies for raw data deposition. NP-MRD facilitates dereplication, correction of erroneous or missing chemical shift assignments, structure validation/revision, and mixture analysis. The database also creates opportunities: for example, in developing new artificial intelligence-based approaches for structure determination, quantitative mixture analysis, chemical shift or spectral prediction, and probably additional presently unforeseen applications of any such database resource. The mission of NP-MRD is to benefit research through engagement and partnership with the worldwide natural products community.

11:00 Make flavor molecules FAIR (FAIRification) Guangjuang Luo, g.luo.leibniz-lsb@tum.de, Veronika Somoza, Andreas Dunkel. Leibniz-Institut fur Lebensmittel-Systembiologie an der Technischen U. Munchen, Freising, Bavaria, Germany The Food Systems Biology Database (FSBI-DB) is an open-access integrative repository of flavor compounds characterizing their functional properties, such as sensory activity, their occurrence in food, and their associated chemosensory receptors. It supports a targeted reformulation of food products to provide healthy and sustainable food choices with high consumer acceptance and optimized sensory profiles. However, this unique collection of interdisciplinary datasets needs to be created with longevity in mind, providing other researchers with access to the data facilitating knowledge building and transfer as well as improving research transparency and reproducibility. With the guidance of FAIR principles (Findability, Accessibility, Interoperability, and Reuse of digital assets), we describe how research data should be organized to be more easily accessed, understood, exchanged, and reused. Critical factors for a successful implementation are to prepare rich metadata, to use a publicly accessible repository with version control, to add appropriate licenses, to register the code in a community register, and to streamline the citation of the digital product. Consequently, the FSBI database, with its fair compliance, ensures the availability of consistent, high-quality information to a broad research community.

11:20 Building food composition and discovery databases in the Periodic table of food initiative (PTFI) Steven Watkins1, steve@versobio.com, Chi-Ming Chien1, Tracy Shafizadeh1, Jessica Prenni2, Selena Ahmed3. (1) Verso Biosciences, San Francisco, California(2) Colorado State U. College of Agricultural Sciences, Fort Collins(3) American Heart Association Inc, Dallas, Texas The Periodic Table of Food Initiative (PTFI) is a worldwide, non-profit project committed to creating publicly accessible food composition databases. These databases document the chemical composition of diverse foods using both targeted and untargeted omics approaches. The initiative strives to enable analytical laboratories across the globe to contribute analyses of local foods, leading to a comprehensive and varied repository of food chemical compositions. During the initial phase of PTFI development, emphasis was placed on designing and standardizing methods for metabolomics, lipidomics, ionomics, and other compositional aspects. This was achieved by developing innovative standardized reagent mixtures and centralized data pipelines. Collaborating laboratories are now employing these techniques to analyze food samples from approximately 1,500 "inspirational foods," selected by an international committee. The data will contribute to the establishment of two databases: a traditional food composition database with named and quantified compositional elements, and a discovery database featuring time-aligned MS, MS/MS, and collisional cross-section information for each mass spec feature in every food. These databases will be made available to the public as data resources and through user interfaces. This presentation will provide an overview of the methodologies, databases, and data pipelines created in support of the PTFI, while also discussing the project's future goals.

11:40 Discovery framework for natural food chemical activities Daniel Biber1, dan@d2discovery.com, Joel Duerkson1, Brian Foote1, David Wild1,2, Brian D. Guthrie3. (1) Data2Discovery Inc., Bloomington, Indiana(2) Luddy School of Informatics, Computing and Engineering, Indiana U., Bloomington(3) Cargill Inc, Minneapolis, Minnesota Data-driven scientific discovery of bioactive compounds in food is a promising avenue for developing new functional ingredients and nutraceuticals that can benefit human health. However, traditional methods of food compound discovery miss notable state of the art tools most notably found in drug discovery. To address this challenge, we have developed the Food Likeness Chemical Discovery Framework (FLC-DF) that enables rapid identification of bioactive compounds in food. The framework’s database contains approximately 300M compound structures combined with meta-data obtained from more than 90 public databases. Capabilities to dynamically update, harmonize and normalize data is built-in as source databases are versioned or updated. In addition to this integrated dataset, we developed and evaluated several key food-related metrics including toxicity prediction, natural product likeness and food likeness. The framework allows researchers to score and evaluate metrics in several key areas including: commercial availability, toxicity, natural product likeness, enzymatic production likelihood, and food likeness.

Biotechnology and Synthetic Biology for Sustainable Foods, Food Ingredients, and Flavor

8:05 Flavor sustainability and biotechnology: A review Xiaofen Du, xdu@twu.edu, Mindy Davila. Nutri. and Food Sci., Texas Woman's U., Denton With an ever-growing global population, flavor sustainability is more important now than ever. A larger population will demand a larger quantity of flavor ingredients. Currently, there are two standard methods for obtaining flavor compounds: extraction from natural sources and chemical synthesis, but both are lacking in long-term sustainability. Flavor biotechnology is poised to solve the dilemma of satisfying customers with natural flavors while keeping natural resources plentiful and protecting the environment. Flavor biotechnology has been defined as using whole or partial living organisms to create new products or alter existing ones, to enhance existing plants or animals, or to develop microorganisms for a particular use. A large portion of current biotechnology research aimed at food flavor sustainability is the utilization of intact microbe cells, namely whole yeast, bacterial, and fungi cells for the biotransformation of natural precursors; experimentation has been done with their genetic modification as well. In essence, this talk will cover the major research progress on biotech flavorings for different groups of compounds derived from their various bio pathways; their advantages and disadvantages will also be discussed. On a global scale, more than 20 flavor biotechnology companies have cumulatively produced an excess of 100 commercial flavor

chemicals. The present discussion will additionally encompass examples of those commercialized chemicals as well as major challenges and future perspectives for the flavor biotechnology as a whole. The major challenges to be overcome include regulatory issues, knowledge gaps, and technical issues. In the future, there will likely be advances in bio-aroma technology, knowledge, interest, and cost-competitiveness, leading to an overall increased market share.

8:35 Integrated chemical and biological platform for on-demand food production from minimal resources Ting Lu, luting@illinois.edu. U. of Illinois Urbana-Champaign Food is the most fundamental human need. Using a multidisciplinary approach, we are building a programmable food production platform that uses air, water, and electricity to produce delicious food with a complete nutrient profile in a portable way. The platform combines electrochemistry and plasma technology to fix carbon dioxide and nitrogen from air into organic substrates. These substrates are then used to grow engineered microorganisms to produce biomass with customized nutrient profiles including protein, lipid, carbohydrate, and fiber. Additionally, microbial biomass contains flavor and texture compounds, which can be tailored to meet consumer preferences, and can be processed to produce nutritious and safe foods in different formats. By using carbon dioxide and nitrogen as carbon and nitrogen sources, our platform has the potential to reduce greenhouse gas emission, making it an environmentally friendly alternative to traditional food production practice. Furthermore, our food production platform is portable, eliminating the need for lengthy food transportation and storage.

9:05 Assessing the flavor generation of cultivated beef Curtis R. Luckett, curtis@scififoods.com, Dongjun Zhao. Food Sci., SCiFi Foods, San Leandro, California As cultivated meat companies begin to scale up and take steps towards commercialization, research will shift to improving the consumer experience of slaughter-free meat. In the short term, hybrid products where cultivated cells and plant-based ingredients are blended to form a food product are likely to dominate the market due to the high cost of cultivating mammalian cells. However, there are no published data on how cultivated cells interact with a plant-based matrix upon cooking. This study aimed to characterize the flavor contribution of the contribution of bovine fibroblasts when incorporated into a plant-based matrix. The bovine fibroblasts were incorporated into a plant-based matrix at 6% (w/w). We also included a positive control (ground beef) and a negative control (plant-based matrix only).The samples were cooked and analyzed via SPME GC-MS in triplicate. Additionally, the samples were analyzed for fatty acid composition and taste-active mononucleotide content. With regard to the volatile profile maillard reaction products tended to be higher in the plant based and hybrid product. However, many key lipid-derived volatiles were more prominent in the conventional beef sample. The cultivated bovine cells were found to help bridge the gap between the plant-based sample and the conventional beef sample for key compounds such as 1-octanol, 2-ethyl-1-hexanol, and 1-octen-3-ol. Additionally, adding cultivated beef cells to the plant based burger was able to reduce hexanal, a common off-flavor of soy protein, to levels closer to conventional beef. As has been previously reported, the taste-active mononucleotides were lower in the cultivated beef, when compared to conventional beef. By using the fatty acid profile of the samples we were able suggest some possible explanations for differences in lipid-derived volatile expression between cultivated and conventional beef. Our findings highlight the need to assess the flavor generating capabilities of cultivated beef in a relevant food matrix and provide insights to generating tailor-made cells, designed for maximal beef flavor to produce the next generation of alternative protein foods.

9:35 Biotechnological production of dihydromenthofurolactones by basidiomycota Holger Zorn1,2, holger.zorn@uni-giessen.de. (1) Food Chemistry and Food Biotechnology, Justus-Liebig-U. Giessen Fachbereich 08 Biologie und Chemie, Hessen, Germany(2) Bioresources, Fraunhofer-Institut fur Molekularbiologie und Angewandte Oekologie IME, Giessen, Nordrhein-Westfalen, Germany In recent years, basidiomycota have emerged as a promising source for natural flavorings. The aroma compounds formed by these organisms cover a broad range of different substance classes, including terpenes and terpenoids. With more than 80,000 known representatives, the latter compounds represent an enormously broad class, with many mono- and sesquiterpenoids being known as aroma-active. Surprisingly, a number of highly aroma potent bicyclic benzofuran derivatives, namely dill ether, wine lactones and dihydromenthofurolactones (DML) have been identified in submerged cultures of basidiomycetes recently. The formation of dill ethers and wine lactones has been described for Pleurotus sapidus (PSA), a close relative of the oyster mushroom. Using multidimensional gas chromatography, two rarely occurring stereoisomers of each dill ether and wine lactones, both with an enantiomeric excess (ee) of ee ≥ 99.9, were identified. Supplementation studies using 2-13C-D-glucose showed that both, dill ether and wine lactones, were formed de novo by the fungus. The same stereoisomers of dill ether (ee ≥ 99.9) were identified in submerged cultures of Cystostereum murrayi (CMU), a fungus which is known for its coconut-like odor. For the identification of key aroma compounds, an aroma dilution analysis was performed. After isolation and structure elucidation by NMR experiments, the three compounds with the highest FD factors (29, 212, and ≥ 218) were identified as two diastereomers of DML and as the corresponding C3-unsaturated lactone, respectively. These compounds have not been previously described for CMU or any other basidiomycota. Moreover, the semi-quantitatively determined concentrations (8-86 mg/L) were surprisingly high. Supplementation studies with 2-13C-D-glucose indicated that the lactones as well as dill ether are formed de novo by CMU.

10:30 Genome-edited yeast strains to modulate the tastes and flavors of fermented foods Chan Woo Kim1,4,2, Ye-Gi Lee1,3,4, Keith R. Cadwallader1, Yong-Su Jin1,2, ysjin@illinois.edu. (1) Food Sci. and Human Nutrition, U. of Illinois Urbana-Champaign(2) Carl R. Woese Inst. of Genomic Biology, U. of Illinois Urbana-Champaign(3) Dept. of Bio and Fermentation Convergence Technology, Kookmin U., Seoul, Korea (the Rep. of)(4) Rural Development Adminstration, National Inst. of Agricultural Sciences Dept. of Agrofood Resources, Wanju, Korea (the Rep. of) Amino acids and esters are known to provide the umami and fruity characteristics of fermented foods, but the amounts of amino acids and esters produced during food fermentation are often insufficient to satisfy the consumer's preference. In this study, we isolated a Saccharomyces cerevisiae strain from Korean Nuruk and conducted genome-editing to modulate the taste and flavor profiles of Makgeolli, a traditional Korean rice wine. Specifically, we deleted URE2 coding for a transcriptional regulator of nitrogen catabolite repression (NCR) to increase the production of savory amino acids. Secondly, we overexpressed ATF1 coding for alcohol acetyltransferase to boost the production of ester-based flavor compounds, Lastly, we deleted IAH1 coding for esterase to increase the stability of the esters produced. When the resulting genome-edited strains were used for making Makgeolli, the concentrations of amino acids and esters increased more than the threshold levels of them. Our findings demonstrate that genome-edited strains might be employed for producing fermented foods with diverse tastes and flavors. As genome-edited yeast strains contain no heterologous

DNA, they can be used to improve fermented foods with no subjection to GM regulation.

11:00 Transforming toxic djenkolic acid in djenkol beans into bioactive and flavorful organopolysulfides by utilizing C-S lyase from stink beans Molan Zhang, e0511872@u.nus.edu, Dejian Huang. Food Sci. and Tech., National U. of Singapore Ingestion of the djenkol bean (Archidendron pauciflorum, Native to Southeast Asia) may lead to kidney stone due to crystallization of djenkolic acid abundantly found in the bean. Report here in a natural way to utilize djenkolic acid in djenkol bean as a natural source of aroma active cyclic organopolysulfides, which are slow H2S donors (for health promotion benefits). We optimized the utilization of C-S lyase in stink bean by adjusting the ratio of stink bean to djenkol bean. Three main organosulfides, including 1,2,4-Trithiolane, 1,2,4,6-Tetrathiepane, and 1,3,5,7-Tetrathiocane, were identified using GCMS and ESI MS in DCM extracts. The content and proportion of cyclic organosulfides extracted varied significantly under different pH conditions. As the pH increased, the main product shifted from 1,2,4-Trithiolane to 1,2,4,6-Tetrathiepane. Elemental analysis indicated that the extract at a pH of 7.5 had the highest proportion of sulfur-containing compounds, while the sulfide content was substantially reduced under weakly alkaline conditions due to the instability of cyclic organosulfides. Our finding proves the feasibility of a way to obtain natural organopolysulfides for flavor and nutracetical use.

11:30 Comparison of flavor potentials of yeast extracts produced from acetate versus glucose grown biomass Keith R. Cadwallader, cadwlldr@illinois.edu, Nagiat Hwisa, Yong-Su Jin, Chan Woo Kim. Food Sci. and Human Nutrition, U. of Illinois Urbana-Champaign Yeast extract (or yeast hydrolysate) is a popular flavoring agent used to add aroma- and taste-active components and flavor precursors to savory food products. It is typically produced via autolysis, physical disruption or enzymatic hydrolysis of brewer's yeast to yield free amino nitrogen substances, sugars, vitamins, and trace elements. Acetate is considered a universal carbon source, supporting the growth of numerous microorganisms, including yeast. However, yeast metabolism of acetate as the sole carbon (energy) source compared with sugar (glucose) may result in the production of different metabolites, thus producing different flavor and flavor precursor profiles of yeast extracts. The present study focused on the comparison of yeast extracts produced by two methods (autolysis and physical disruption) from Saccharomyces cerevisiae biomass grown on either acetate or glucose as sole carbon source in a minimal salts/nutrient medium. Comparisons were made for total amino nitrogen components and selected aroma (odor)- and taste-active components. Gas chromatography-mass spectrometry-olfactometry (GC-MS-O) was used to determine potent odorants, of which the sulfur-containing odorants methional and 2-methyl-3-furanthiol were predominant. Results indicated that, in general, yeast extracts from glucose grown yeasts contained only slightly higher levels of flavor relevant constituents. Therefore, yeast extracts produced from acetate grown yeast are a viable alternative to traditional yeast extracts as a flavoring agent.

Virtual Session - Forever Chemicals in the Environment, Distribution and Risk

10:05 Phthalates: Effect on and transformation promotion of rhizosphere bacterial community Quan-Ying Cai1, caiqy@jnu.edu.cn, Hai-Ming Zhao1, Hui-Xiong Lü2, Yan-Wen Li1, Ce-Hui Mo1, Lei Xiang1, Qing X. Li3. (1) Jinan U., Guangzhou, Guangdong, China(2) South China Agricultural U., Guangzhou, Guangdong(3) U. of Hawaii at Manoa, Honolulu Phthalates (PAEs) are prevalent in agricultural soils and pose adverse effects. Rhizospheric degradation is a green and in situ strategy to accelerate dissipation of organic pollutants in soils. However, the response of rhizosphere bacterial community and promotion mechanism on PAE microbial degradation in rhizosphere are still unclear. We analyzed the bacterial community and function genes in bulk soils and root-associated niches of maize and rice plant exposed to di-(2-ethylhexyl) phthalate (DEHP) by 16S rRNA, metagenomic sequencing and quantitative PCR. The results demonstrated a significant increase in DEHP dissipation in maize rhizosphere compared with bulk soils. The response of bacterial community to DEHP stress was influenced by plant genotypes and root-associated niches. The bacterial community diversities significantly decreased along bulk soil - rhizosphere - rhizoplane - endosphere. DEHP stress significantly reduced bacterial community diversities in both rhizosphere and rhizoplane, and changed their composition, enrichment, and depletion process. The bacterial community structures were shaped mainly by root-associated niches, DEHP pollution and rice genotypes, with significant differences in rhizosphere and rhizoplane between different rice cultivars. Both rhizospheric and pollution effects augmented more PAE-degrading bacteria than in bulk soil, and exhibited significantly higher expression of PAE-degrading genes than in bulk soil, which played important roles in degradation of PAEs in rhizosphere. Bacterial metagenomic analysis and PAE degradation pathway construction through the identified PAE intermediates demonstrated that PAE-degrading bacteria degraded PAEs through cooperation with PAE-degrading and non-PAE-degrading bacteria. Furthermore, inoculating endophytic PAE-degrader Bacillus subtilis N-1-gfp colonized well in soil-crop systems, which shifted indigenous bacterial community and enhanced the removal of phthalates. Bacterial promotion of PAE removal from agricultural soil is of significance in ensuring soil health and food safety.

10:35 Functional endophytic organic fertilizer alleviates the burden of phthalates and promotes vegetable growth Bowen Huang, Pei Wang, Ya Wang, Jing Ge, cherrygejing@126.com, Yong Li, Jinjin Cheng, Xiangyang Yu. Jiangsu Academy of Agricultural Sciences, Nanjing, Jiangsu, China Phthalates (PAEs) have become one of the main pollutants threatening the safety and quality of vegetable production. Application of bio-organic soil amendments is a promising approach to eliminate the pollutants and improve the vegetable quality. In the present study, we constructed a functional endophytic organic fertilizer (EOF) with a PAEs degrading endophyte Bacillus subtilis strain HB-T2, which had the ability to eliminate PAEs both inside the vegetables and in the surrounding soil. A pot experiment conducted to investigate the effect of EOF on PAEs degradation, rhizosphere microbiota, vegetable quality and soil fertility, the results were also compared to chemical fertilizer (CF), organic fertilizer (OF, sterilized EOF) treatments. The EOF containing HB-T2 significantly increased the elimination of PAEs in soil (up to 70%) and vegetables (up to 50%). Both OF and EOF treatments significantly ($P < 0.05$) increased soil fertility and enzyme activities compared to the chemical fertilizer treatment. The EOF treatment had the highest elimination rate of PAEs in soil and vegetables. The correlation analysis showed that the degradation of PAEs was related to the increase of the dominant rhizosphere bacteria, especially Sphingomonas. The efficiency of EOF was also evaluated under practical condition. The biomass and the quality of the vegetables were significantly improved and the human health risks were significantly reduced.

11:05 Remediation of PFAS from a variety of environmental matrices Jay Meegoda, meegoda@njit.edu. CEE, New Jersey Inst. of Technology, Newark Per- and polyfluoroalkyl substances (PFAS) are a large and complex class of anthropogenic compounds. Due to their persistence and potential toxicity to human and ecological receptors, PFAS have generated a strong public and

regulatory response to their ubiquitous presence in the environment. The need for the remediation of per- and polyfluoroalkyl substances (PFAS) is growing as a result of societal and regulatory awareness in the wake of rapidly evolving toxicology research on this class of contaminants. Major sources of PFAS released to the environment include fire training/ fire response sites, industrial sites, landfills, and wastewater treatment plants/biosolids. Per- and polyfluoroalkyl substances (PFAS) are widely distributed in the environment, and they are detected at low concentrations in surface and groundwater at thousands of locations in the USA and around the world. The current state of practice for treating PFAS contaminated water uses interim technologies (e.g., ion exchange, reverse osmosis), which result in secondary waste, as PFAS contaminants are not destroyed but rather concentrated. High-concentration PFAS waste is incinerated at off-site facilities, an expensive and energy-intensive approach. Also, potential emission of PFAS byproducts such as fluorinated and mixed halogenated organics are causing health concerns in neighboring communities. Emerging destruction technologies gaining attention include electrochemical oxidation, plasma, and sonolysis. Electrochemical and plasma treatments are actively transitioning from laboratory-scale to field pilot demonstrations. The application of ultrasound waves (i.e., sonolysis or sonochemical degradation) is shown to be both an effective and relatively fast method of mineralization of PFAS to . Bench-scale tests have shown that sonolysis is effective over a wide range of concentrations from 10 nM to 460 µM for PFAS compounds in water. The mechanism of sonolytic degradation of PFAS has been suggested to be high-temperature pyrolysis at imploding bubble surfaces or the reaction with radicals, such as the solvated electron emanating from plasma formation during bubble collapse. Thus, unlike the other emerging technologies that follow sequential defluorination pathways resulting in short-chain PFAS molecules that resist further treatment, the sonolytic decomposition of PFAS has been demonstrated to completely mineralize PFAS without accumulating short-chain PFAS.

11:35 Phthalate exposure leads to detrimental effects on preimplantation embryo development and viability Romana Nowak, ranowak@illinois.edu, Lydia Yuliana Parra-Forero. Animal Sciences, U. of Illinois Urbana-Champaign The incidence of infertility and reproductive failure among women is a significant concern with The Centers for Disease Control reporting that 12-15% of US women between the ages of 14-44 suffer from infertility. Several factors may contribute to reproductive failure, among them exposure to environmental toxicants, particularly endocrine disrupting chemicals (EDCs). Phthalates are EDCs and phthalate contamination is present in air, soil, water, and food sources due to their incorporation into the plastics we use daily. Our lab is investigating the effects of phthalate exposure on preimplantation embryo development in a mouse model. We carried out a series of in vitro studies treating mouse embryos from the one-cell to hatched blastocyst stages with a phthalate mixture (DEP, DEHP, DBP, DiNP, DiBP, and BBzP) at environmentally relevant doses (0.001 to 1.0 ug/ml). Results showed that the phthalate mixture significantly decreased embryo development from the 8-cell stage to hatched blastocyst stage at several concentrations. Moreover, phthalate exposure caused an increase in fragmentation and micronucleation in early embryos and markedly decreased expression of E-Cadherin, a protein important for embryo compaction. We then performed an in vivo study in which adult female mice were exposed to DEHP (0, 20, 200, or 2000 ug/kg body weight/day) by oral gavage for four weeks. After this treatment period mice were superovulated and placed with males for mating. Mice were sacrificed 96 h later and blastocysts collected from the uterine horns for analysis. Results showed that DEHP exposure of dams led to a higher number of early blastocyst stage embryos at 96 h suggesting a delay in development. DEHP exposure at the two higher doses led to increased percentages of blastocysts with poor quality inner cell mass and trophectoderm as well as decreased expression of Oct-4 and CDX-2 developmental genes. These findings are significant as both in vitro and in vivo studies showed that phthalate exposure at early stages of embryo development, prior to implantation, has a negative impact on embryo development and viability. Embryos exposed to phthalates showed reduced expression of several key proteins important for development of the inner cell mass and trophectoderm along with a higher incidence of morphologic abnormalities. Future studies will utilize an extended blastocyst culture system to examine later stages of development.

12:10 Return of trifluoroacetic acid as an environmental concern Thomas M. Cahill, thomas.cahill@asu.edu. School of Mathematical and Natural Science, Arizona State U. West Campus The first perfluorinated acid of concern was trifluoroacetic acid (TFA) back in the mid 1990's. At that time, it was mainly expected to form from the degradation of hydrofluorocarbon (HFC) refrigerants that replaced the ozone-depleting chlorofluorocarbons. Interest in TFA faded quickly upon the discovery of the more toxic and bioaccumulative PFOS and PFOA. However, TFA never disappeared and its sources continue to rise. This warrants a return to the topic of TFA to see what has changed over 20+ years. The first project re-sampled the exact same streams along a transect through the Bay Area to the Tahoe Basin as was done in 1998. This showed an increase in concentrations of approximately 6-fold over the 23 intervening years. The second project involved determining the toxicity of TFA in desert plants that might bioconcentrate TFA. The results showed LD50 for Joshua tree seedlings to be 48 mg TFA/kg of soil and a bioconcentration factor of 4090 (g plant/g soil). Three other short-chain perfluorocarboxylic acids were likewise tested and found to have similar toxicity. The last project is re-sampling terminal lakes (endorheic basins) that are expected to concentrate TFA. This part of the research is ongoing.

12:35 Biostimulating Acidimicrobium sp. Strain A6 in PFAS impacted soils and soil-column experiments to achieve PFAS defluorination Peter R. Jaffe[1], jaffe@princeton.edu, matthew sima[1], Jinhee Park[1], Shan Huang[1], Bruce E. Koel[2], Charles E. Shaefer[3]. (1) Civil and Environmental Engineering, Princeton U., New Jersey(2) Chemical and Biological Engineering, Princeton U., New Jersey(3) Bellevue Research & Testing Laboratory, CDM Smith, Bellevue, Washington Acidimicrobium sp. Strain A6 (A6) is an autotroph that oxidizes NH_4^+ while reducing iron, a process referred to as Feammox. It has been shown that during the Feammox process, A6 is also capable to defluorinate PFAS, including PFOA and PFOS. A6 is relatively common in acidic, iron rich soils, where it is usually present at low numbers. Hence, acidic soil samples from several DoD PFAS impacted sites were collected, and DNA extracted to quantify A6 numbers via qPCR. Although A6 numbers were low, it was detected in all samples. 30-day batch incubations to which ferrihydrite was added showed a significant increase in A6 numbers, removal of NH_4^+, and production of Fe(II) and F^-, while no changes were observed in control incubations. Ferric minerals (i.e., ferrihydrite, goethite) are positively charged at ambient pH values, and are therefore not transportable in soils, which are predominantly negatively charged, hence supplying and distributing an Fe(III) phase to soils and groundwaters is a challenge. To overcome this challenge, nanosized ferrihydrite and/or goethite particles were treated with polyacrylic acids (PAAs) to change their zeta potential to negative, making them transportable in soils. Columns were filled with soils from two of the DoD sites. A solution containing NH_4^+ was pumped through them. To one set of columns for each soil, the solution also contained PAA-treated goethite. Pumping was discontinued after goethite breakthrough was observed, after which

the columns were allowed to rest for 50 days. Pumping was then resumed to sample the column effluents, showing a significant removal of NH_4^+ and production of F^- in the columns to which the PAA-treated goethite was applied, while no changes were observed in the controls. These results indicate that A6 can be biostimulated at many acidic PFAS impacted sites to enhance PFAS defluorination. Further analyses/evaluations are under way.

1:00 Determination of plasticizers in PVC and non-PVC food contact materials Katherine Carlos, katherine.carlos@fda.hhs.gov, Lowri Dejager, Timothy Begley. Office of Regulatory Science, Center for Food Safety and Applied Nutrition, College Park, Maryland PVC is a food contact material that can be plasticized to increase its flexibility. Phthalates are one of many chemical compounds that are used as plasticizers in PVC. They may be used in packaging materials for foods and can be found in components of food processing equipment such as conveyor belts, tubing and hoses. In recent years, there has been renewed interest in understanding the potential health effects of phthalates, as well as the possible human exposure levels. However, there is limited information available about the major routes of exposure to phthalates. A recent study investigated the plasticizers currently used in fifty-six different samples of PVC food packaging and food processing materials available for purchase in the U.S. Nine plasticizers including three phthalates, diethylhexyl phthalate (DEHP), diisononyl phthalate (DINP), and diisodecyl phthalate (DIDP), were identified in the products tested. The plasticizer concentrations ranged from 1- 53% depending on the types of food contact materials and the type of plasticizer. Overall, and consistent with past testing, manufacturers are switching away from phthalates as their primary plasticizer to alternate compounds such as ESBO, ATBC, DEHT, DINCH, DEHA and DINA. An additional study investigates the phthalate concentration of non-PVC packaging. A liquid extraction method was adapted for use with paper, paperboard and cardboard. The samples were extracted with dichloromethane and hexane before injection into the GC-MS/MS. Limits of detection for the method ranged from 0.10 to 0.40 mg/kg depending on the type of plasticizer. The plasticizer concentrations were investigated in 23 different fast food packaging samples with printed and unprinted portions analyzed separately. These studies will provide the Agency important information on potential routes of phthalate exposure to consumers via food consumption.

1:25 Uptake and translocation of perfluorooctanoic acid and perfluorooctane sulfonate in lettuces (lactuca sativa L.) Lei Xiang1, wuxian622622@163.com, Peng-Fei Yu1, Hai-Ming Zhao1, Yan-Wen Li1, Quan-Ying Cai1, CEHUI MO1, Qing X. Li2. (1) Dept. of Ecology, Jinan U., Guangzhou, Guangdong, China(2) Dept. of Molecular Biosciences and Bioengineering, U. of Hawaii at Manoa, Honolulu Perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) are perfluorinated alkyl substances (PFASs) widely used in industrial and domestic products. They are highly bioaccumulative in crops, posing risk to human health. The European Food Safety Authority have lowered the reference doses (RfDs) for PFOA and PFOS 240−2400-fold in 2020, which arise serious concerns since some intakes of PFOA and PFOS exceeded the RfDs. The new RfDs, therefore, call for re-evaluation of potential human health risks from PFOA and PFOS via food consumption. Cultivation of low-accumulating crop varieties has been considered as a practical solution to ensure the food safety via reducing pollutant accumulation in edible parts of crops. We identified the PFAS low-accumulating lettuce varieties that are loose-leaf lettuces. PFOA/PFOS concentrations of the low-accumulating lettuce were 3.7–5.5-fold lower than those of high-accumulating lettuce. Rhizospheric activation, uptake, translocation, and compartmentalization of PFOA/PFOS are the key factors governing low accumulation. Root exudates, especially oxalate can effectively reduce PFOA/PFOS sorption to soils by decreasing hydrophobic force, electrostatic attraction, ligand exchange, and cation-bridge effect, because oxalate enhances dissolution of metallic ions, iron/aluminum oxides, and organic matters from soils and forms oxalate−metal complexes. PFOA/PFOS root uptake is governed by the transporter-mediated processes that are related to aquaporin (PIP1−1 and PIP2−2) and rapid-type anion channel genes (ALMT10 and ALMT13). Concentrations of oxalate in root exudates and expression of these genes are directly related to root uptake of PFOA/PFOS into lettuce. Furthermore, low-accumulating lettuce varieties showed the characteristics of high deposition of PFOA/PFOS in the root cell walls and low root-to-shoot translocation of PFOA/PFOS in comparison with the high-accumulating ones. These findings provide new insights into the uptake and accumulation of PFASs, and reveal the multi-process mechanisms underlying absorption and translocation of PFASs in vegetables, which is of significance in ensuring food safety and protecting human health.

MONDAY AFTERNOON

Artificial Intelligence (AI) Applications for Food and Agriculture

2:05 Computer vision and NIR spectroscopy: an intelligent solution to optimize the fresh fruit bunches quality assessment in the Colombian oil palm agroindustry Cesar A. Diaz, cadiaz@cenipalma.org, Jesus A. Garcia-Nunez, jgarcia@cenipalma.org. Bogota, Investigacion e Innovacion Tecnologica en Palma de Aceite, Colombia Achieving high palm oil efficiencies requires strict control of FFB (fresh fruit bunches) as well as efficient control during the oil extraction process. One of the main routine activities carried out in the mills is FFB quality assessment. Currently, FFB inspection is carried out visually by workers, considering previously established ripeness criteria. However, results obtained by worker inspection are subject to human bias, and changes in lighting conditions among other factors. Low sample representativeness per shipment (5%) is another major drawback of traditional human inspection. Thus, improvement opportunities in terms of subjective quality measurements and statistical representativeness have been identified. Cenipalma has been developing prototypes and automated qualification systems based on two fundamental pillars of Data Science: Computer Vision (artificial intelligence) and NIR spectroscopy (NIRS). In the Computer Vision pillar, algorithms based on image segmentation and classification have been developed. Simultaneously, based on NIR technology, prediction models are being developed for variables associated with the evaluation of oil content, moisture, and other conditions related to the FFB ripeness scale. Currently, there is already a prototype of this system under real-time training and improvement in one of the POMS in Colombia. Therefore, this innovation project aims to allow the establishment of dynamics of negotiation and continuous improvement on reliable criteria based on sufficient quantity and quality of information between plantations and POM. Please consider downloading this presentation: https://shorturl.at/msxR9 This is a video of a prototype: https://shorturl.at/ADF45

2:30 Protein language model-based universal deep learning architecture for bioactive peptide discovery Zhenjiao Du[1], zhenjiao@ksu.edu, Xingjian Ding[2], Yonghui Li[1]. (1) Grain Science & Industry, Kansas State U., Manhattan (2) Computer Science, Kansas State U., Manhattan Identification of potent peptides through model prediction can reduce benchwork in wet experiments. However, the conventional process of model building can be complex and time-consuming due to challenges such as peptide representation, feature selection, model selection, hyperparameter

tuning, etc. Recently, advanced pre-trained deep learning-based language models (LM) have been released for protein sequence embedding and applied to structure and function prediction. Based on these developments, we have developed UniDL4BioPep, a universal deep-learning model architecture for transfer learning in bioactive peptide binary classification modeling. It can directly assist users in training a high-performance deep-learning model with a fixed architecture and achieve cutting-edge performance to meet the demands in efficiently novel bioactive peptide discovery. To the best of our best knowledge, this is the first time that a pretrained biological language model is utilized for peptide embeddings and successfully predicts peptide bioactivities through large-scale evaluations of those peptide embeddings. The model was also validated through uniform manifold approximation and projection analysis. By combining the LM with a convolutional neural network, UniDL4BioPep achieved greater performances than the respective state-of-the-art models for 15 out of 20 different bioactivity dataset prediction tasks. The accuracy, Mathews correlation coefficient, and area under the curve were 0.7-7%, 1.23-26.7%, and 0.3-25.6% higher, respectively. A user-friendly web server of UniDL4BioPep for the tested bioactivities is established and freely accessible at https://nepc2pvmzy.us-east-1.awsapprunner.com. The source codes, datasets, and templates of UniDL4BioPep for other bioactivity fitting and prediction tasks are available at https://github.com/dzjxzyd/UniDL4BioPep.

2:55 Developing an automated pipeline for the discovery of flower-specific honey markers via non-targeted LC-MS analysis Shawninder Chahal1, shawninder.chahal@mail.mcgill.ca, Lei Tian1, Shaghig Bilamjian1, Ferenc Balogh2, Tarun Anumol3, Daniel Cuthbertson3, Stephane Bayen1. (1) Food Sci. and Agricultural Chemistry, McGill U. Faculty of Agriculture and Environment, Sainte-Anne-de-Bellevue, Quebec, Canada(2) Mathematics, CEGEP John Abbott College, Sainte-Anne-de-Bellevue, Quebec, Canada(3) Agilent CrossLab Group, Agilent Technologies Inc, Santa Clara, California The increasing complexity of the global food supply chain has made it difficult to guarantee the authenticity of food once they reach buyers. For instance, bees can use nectar from a variety of flowers to make honey. Some flowers produce unique flavours attracting higher demand and market prices. This has led to honey being one of the most frequently frauded food items today, leading to negative economic and health impacts on buyers and consumers, respectively. Therefore, there is a need to identify flower-specific markers to authenticate honey and prevent fraud. Herein, we perform a non-targeted liquid chromatography–mass spectrometry (LC–MS) analysis of 270 honey samples self-reported as monofloral blueberry, buckwheat, clover, goldenrod, linden, or other. Recursive feature elimination with hyperparameter optimization was performed using machine learning classifiers (logistic regression, support vector machine, and PLS-DA) to determine the smallest subset of features needed to accurately identify the floral origin of a honey sample. This typically led to the isolation of 4 – 40 candidate markers, depending on the floral origin, from the 1500 – 6000 features identified from non-targeted screening. Features were also evaluated on their ability to classify honey samples based on their presence, absence, whether an intensity threshold can separate one flower from the rest, or whether a ratio of feature intensities fall within an interval unique to a specific flower. This work presents an automated pipeline, developed using open-source libraries in Python, for the discovery and visualization of unique markers of authenticity for a variety of flowers used in the production of honey. The comparison of three different linear models, each optimized via a different loss function, will shed light on the strengths and weaknesses of each model. In future work, this pipeline can readily be applied towards the discovery of markers of authenticity in other food groups.

3:20 Direct recognition of zearalenone and related metabolites using Raman spectroscopy Michael Appell2, michael.appell@gmail.com, Bosoon Park1. (1) Quality and Safety Assessment Research Unit, USDA, Agricultural Research Service, U. S. National Poultry Research Center, Athens, Georgia(2) Mycotoxin Prevention and Applied Microbiology Research Unit, USDA, Agricultural Research Service, National Center for Agricultural Utilization Research,, Peoria, Illinois Foodborne pathogens reduce commodity values and pose serious health risks to consumers of food and feed, including humans and other animals. Sensitive analytical tools are needed to quantify contaminant levels efficiently through real-time monitoring. Raman and ultraviolet spectroscopy were employed with modeling methods to systematically evaluate spectroscopic properties and distinguish between the regulated mycotoxin zearalenone and its metabolites that can contaminate commodities. In addition, Raman-based methods were applied to identify and differentiate between several ferulic acid derivatives that are important for plant health. Machine learning chemometric data analysis of variations in spectral parameters of the Raman spectra enabled rapid determination and identification of contaminants and plant components. These portable Raman spectroscopy methods provide label-free tools to distinguish between structurally related plant components and pathogens and related metabolites.

4:00 AlphaFold 2-based stacking deep learning model for protein solubility prediction and food application Hyukjin Kwon, john94kwon@gmail.com, Zhenjiao Du, Yonghui Li. Dept. of grain science and industry, Kansas State U., Manhattan Protein solubility is an important physicochemical property in Food Sci.. Accurate prediction tools for solubility are in demand, as they can be used for screening food protein candidates. This study aims to build a state-of-the-art (SOTA) protein solubility prediction model with molecular descriptors extracted from predicted protein structures. Based on a solubility dataset of 3001 E. coli proteins, AlphaFold 2 was employed to generate 3D structures of the corresponding proteins. From the acquired structures, 22 structure-level features, three residue-level descriptors, and protein contact maps were extracted. A multilayer perceptron (MLP) model was then created using the 22 structure features as input. Moreover, using the residual features and contact maps, a graph convolutional network (GCN) model was constructed. Finally, the two models were treated as meta-predictors, whose outputs were input into a support vector machine (SVM) for the stacking model. Model performances were evaluated with an independent E. coli protein test dataset and an external S. cerevisiae dataset. In both datasets, the stacking model achieved great performances: R2 of 0.494 and 0.410 with RMSE values of 0.228 and 0.225, respectively. To assess the applicability of the model in the food industry, a wet-chemistry validation is also conducted using food proteins. This work shows the potential of applying deep-learning techniques in Food Sci. as well as providing a SOTA regression model for exact protein solubility prediction.

4:25 Rapid quantitative analysis of olive oil fraud using recurrent neural network and Raman spectroscopy Weiming Song, Keng Chou, kcchou@chem.ubc.ca. Dept. of Chemistry, U. of British Columbia, Vancouver, Canada This study investigates the application of recurrent neural networks (RNNs) and Raman spectroscopy for determining the oil types and percentages in fraudulent olive oils. RNNs are commonly used for temporal problems, such as speech recognition. Here we consider a Raman spectrum as sequential data and carry out regression using RNNs. Extra virgin olive oils were mixed with 7 other edible oils, including sunflower, soy, peanut, corn, canola, grapeseed, and avocado oils.

RNNs and Raman spectroscopy allowed us to obtain a continuous regression for the adulterant percentage in olive oil. Our approach identifies both the adulterant oil types and their percentages with an average error of ~2% (root mean square), which is within the AOAC standard of 5% for Non-Targeted Testing of Ingredients for Food Authenticity/Fraud Evaluation of Extra Virgin Olive Oil.

4:50 Foodborne bacteria classification using imaging spectroscopy with Fusion-nets deep learning Bosoon Park, bosoon.park@usda.gov, Taesung Shin. US National Poultry Research Center, USDA Agricultural Research Service, Athens, Georgia Artificial intelligence (AI) for big data analytics will play an important role in the future of agri-food systems, especially food safety and quality with imaging spectroscopy and deep learning. Since a series of foodborne outbreaks often threaten the public, early and rapid detection technology is essential. A hyperspectral microscope imaging (HMI) technique is the potential to classify foodborne pathogens as it generates hyperspectral big data both in spatial and spectral domains from bacteria samples at the cellular level, yet conventional machine learning methods are limited to analyze such a big data. In this presentation, HMI hypercube acquisition with Fabry-Perot interferometer (FPI) and multiple advanced deep frameworks including long-short term memory (LSTM) network, deep residual network (ResNet), and one-dimensional convolutional neural network (1D-CNN) will be introduced for classification of foodborne bacteria at the cellular level.This presentation expands advanced imaging spectroscopy with integration of microscopy and deep learning algorithms for food safety.

Biotechnology and Synthetic Biology for Sustainable Foods, Food Ingredients, and Flavor

2:05 Withdrawn

2:30 Withdrawn

2:55 Chemistry of puerarin metabolism by human gut bacterium Jaehong Han, jaehongh@cau.ac.kr. Metalloenzyme Research Group and Plant Science and Tech., Chung-Ang U., Anseong-si, - Select State/Province -, Korea (the Rep. of) Puerarin is an isoflavone C-glycoside natural product and phytoestrogenic effect have been observed. Gut metabolism of puerarin is believed to be responsible for the formation of phytoestrogenic metabolites in human gut. Human gut bacterium, Dorea sp. MRG-IFC3, converting puerarin to daidzein was isolated and chemical reaction mechanism of glycosidic C-C bond cleavage was studied by whole cell biotransformation and enzyme catalysis. The metabolic intermediate, 3”-oxo-puerarin, was identified during the formation of daidzein. Along with the complete gut metabolism of puerarin, the possible reaction mechanism of C-C bond cleavage reaction was discussed.

3:20 Genetic basis of fruit texture in cucumber Yiqun Weng1,2, yiqun.weng@usda.gov, Xiaofen Du3, Cassidy N. Duan3, Oyindamola Akinpelu3, Pratigya Thapaliya3, Junyi Tan2, Thi Nguyen2. (1) Vegetable Crops Research Unit, USDA-ARS, Madison, Wisconsin(2) Horticulture Department, U. of Wisconsin-Madison(3) Texas Woman's U., Denton Cucumber (Cucumis sativus L.) is an important fruit vegetable crop that is appreciated by consumers for its unique flavor and texture. Cucumber fruit texture-related attributes may include fruit firmness, crispiness or juiciness which are associated with consumer acceptance for fresh consumption, processing quality in pickling, or post-harvest storage or shelf life. There is a wide variation in fruit texture attributes among cucumber varieties due to long-term selection and breeding adapting to different environments, production systems, market groups, post-harvest use, or consumer needs. Studies on the genetic and physiological mechanisms of fruit texture in cucumber are sporadic, which seem to suggest that fruit texture attributes are under the control of quantitative trait loci (QTL). In this talk, we will review the literature of current knowledge on the genetic basis of traits related with fruit texture in cucumber. We will also present results from our preliminary work on QTL mapping of fruit firmness in biparental segregating populations and genomewide association analysis (GWS) in natural populations. Overall, we found that fruit firmness in cucumber is controlled by a few (3 to 4) QTL with major or moderate effects. With further fine mapping, the major-effect fruit firmness QTL ffm1.2 on Chromosome 1 was narrowed down to a small region allowing identification of a candidate gene for this QTL. This work provides novel insights into the genetic and molecular control of fruit firmness in cucumber which may contribute to manipulation of this important trait through biotechnological approaches in the future.

4:10 Identification of compounds contributing to the umami and bitter attributes of pea protein isolates Paulina Ongkowijoyo, Edisson Tello, Devin Peterson, peterson892@osu.edu. The Ohio State U., Columbus The utilization of plant proteins in food products is limited by the presence of aversive flavor attributes such as beany, grassy, bitter, umami, and astringent. The aim of this project was to identify non-volatile compounds that elicit (off)-taste attributes in pea protein isolates (PPI). In the first phase of this project, prep-LC sensory-guided fractionation of a 10% aqueous PPI solution revealed one well-known umami taste compound, monosodium glutamate (MSG), however, it was reported at a subthreshold concentration. Umami-enhancing compounds 5’-adenosine monophosphate (5’-AMP) and 5’-uridine monophosphate (5’-UMP) were further identified after the LC fractions were re-evaluated with MSG. Sensory recombination studies confirmed 5’-AMP and 5’-UMP were umami enhancers of MSG and contributed approximately 81% of the perceived umami intensity of the PPI. In the second phase, compounds contributing to the bitter perception of pea protein isolates (PPI) were investigated. Off-line multi-dimensional sensory-guided Prep-LC fractionation of the PPI solution revealed one main bitter compound that was identified by fourier transform ion cyclotron resonance (FT-ICR) and high resolution de novo MS/MS sequencing as the 37 amino acid peptide PA1b from pea albumin and further confirmed by synthesis. Quantitative LC–MS/MS analysis reported the concentration of the bitter peptide was 129.3 mg/L which was above the determined bitter sensory threshold value of 3.8 mg/L and in agreement with the perceived bitter taste of the sample. Understanding compounds that impact the flavor quality of PPI provides an improved basis for breeding and processing optimization to increase product utilization and promote sustainable agricultural practices.

4:35 Development of a novel, rapid assessment method for pectin structure and functionality Wei Zhao1, wei.zhao@usda.gov, Yang Kim2, Randall G. Cameron1. (1) USDA-ARS, US Horticultural Research Laboratory, Fort Pierce, Florida (2) Seoul National U., Center for Food and Bioconvergence, Seoul, Korea (the Rep. of) Pectin is a complex polysaccharide that has numerous applications in the food and pharmaceutical industries due to its gelling, thickening, and stabilizing properties. Pectin’s functional properties as a gelling agent are determined primarily by the structural properties (degree and pattern of methyl-esterification) of its homogalacturonan (HG) backbone. Currently, pectin's commercial functionality is defined by lengthy, laborious and operator-dependent tests. Here, we report the development of a novel, rapid assessment method to detect and assess pectin structural properties that are related to its functionality. The new method is a lateral flow assay (LFA) system, which includes three different capture antibodies immobilized on a test strip and two detection antibodies labeled with different colors of Gold NanoParticles in a small vial.

The antibodies in the system are pectin HG recognizing antibodies with different preferences for degree and/or pattern of pectin methyl-esterification. The new method is very user-friendly. A user needs only to drop a pectin sample (~20 μL) into the small vial and insert the test strip into the vial, then wait 5 min to obtain results. With a detection limit of 0.02 μg/mL of pectin, the developed method can discern pectin's degree and pattern of methyl-esterification. The reliability of the method has been validated by testing a series of known experimental and commercial pectins. The technology can be easily scaled up to high-volume manufacturing. The convenience of such a quick test would benefit the entire spectrum of the pectin utilization chain, from producers and ingredient suppliers to food formulators and those in the medical and personal care industries.

5:00 Combination of novel extraction methods and natural, deep eutectic solvents as a greener solution for the recovery of anthocyanins and antioxidant activity from blackberry (Rubus spp) Oscar Zannou1,2, zannouoscar@gmail.com, Ilkay Koca2, Salam A. Ibrahim3. (1) Faculty of Agricultural Sciences, Universite d'Abomey-Calavi, Cotonou, Littoral, Benin(2) Dept. of Food Engineering, Ondokuz Mayis U., Samsun, Turkey(3) Food and Nutritional Sciences Program, North Carolina Agricultural and Technical State U., Greensboro Blackberry fruit (Rubus spp) is a rich source of a wide range of natural compounds including natural antioxidant compounds that contribute to human health. The objective of the present study was to combine novel extraction methods and deep eutectic solvents for the efficient recovery of anthocyanins from blackberry fruit. Ultrasound-assisted extraction (UAE), homogenate-assisted extraction (HAE) and stirring-assisted extraction (SAE) were combined with deep eutectic solvents constituted by choline chloride-glycerol (CHGLY) and choline chloride-acetic acid (CHAC) in order to determine the antioxidant properties and anthocyanins of blackberry fruit. The results showed that the total phenolic content (TPC), total flavonoid content (TFC), total anthocyanin content (TAC), antioxidant activity and anthocyanin composition varied significantly depending on the extraction method and solvents ($p<0.05$). TPC, TFC and TAC ranged from 8.18±0.25-12.81±0.91 mg GAE/g, 119.62±1.03-320.07±9.25 mg ECE/100g and 102.19±6.15- 136.97±4.61 mg CGE/100g, respectively. The DPPH radical scavenging activity, ferric reducing power (FRAP) and ABTS were 120.99±4.02-164.85±0.60 mmol TE/g, 120.92±0.35-180.27±1.58 mmol ISE/g and 38.06±3.68-66.68±0.03 mmol TE/g, respectively. CHGLY combined with UAE was found to be the most efficient system for enhancing the antioxidant properties of blackberry fruit. Cyanidin-3-glucoside was the most abundant anthocyanin in blackberry, followed by cyanidin-3-rutinoside, cyanidin chloride and pelargonidin-3-glucoside, respectively. The combination of UAE, HAE and SAE with deep eutectic solvents was thus shown to be an effective, reliable and greener method for the recovery of target antioxidants, and particularly anthocyanins, from blackberry fruit.

5:25 Characterization of aroma-active compounds in raw grains and grain distillate by gas chromatography-olfactometry dilution analysis and odor activity value Di Chen1, chendi@wuliangye.com.cn, Kangzhuo Yang1, Zhanglan He1, Zhipeng Liu1, Jia Zheng1, Michael C. Qian2. (1) Wuliangye Yibin Co Ltd, Yibin, Sichuan, China(2) Oregon State U., Corvallis As the main material of Baijiu, grain gives an important contribution to Baijiu flavor. Aroma-active compounds of raw grains (the mixture of sorghum, wheat, corn, rice and glutinous rice) and grain distillate (based on a Baijiu distillation model with simulated ethanol content, acidity and filling power) were extracted and analyzed by aroma extract dilution analysis (AEDA) and odor active values (OAVs) on a polar and a non-polar column, meanwhile, GC-MS, heart-cut gas chromatography mass spectrometry and comprehensive 2D gas chromatography–time-of-flight mass spectrometry were synergistically employed for identification. The result showed that both raw grain (36 compounds identified) and grain distillate (48 compounds) had similar aroma-active compounds, mainly including aldehydes, aromatics and phenols. 2-furaldehyde diethyl acetal, 1,1-diethoxynonane, tetrahydrolinalool, isobutanoic acid, 1-phenyl-1-methylethanol, β-lonone, thymol and 4-propylphenol were reported in grain flavor for the first time. Hexanal, 1-octen-3-one, methional, (E)-2-nonenal, (E,Z)-2,6-nonadienal, (E,Z)-2,4-nonadienal, benzeneacetaldehyde, (E,E)-2,4-decadienal, guaiacol and 2-methoxy-4-vinylphenol were proved to be the key aroma-active compounds in grain distillation flavor, and quantification revealed that saturated aldehydes and acids increased obviously during the distillation. This work can provide reference for the formation of grain fragrance in Baijiu distillation.

Bioproducts from Biomass

2:05 Synthesis of mixed chitin esters with thermoplasticity Jun-Ichi Kadokawa, kadokawa@eng.kagoshima-u.ac.jp. Kagoshima Daigaku Kogakubu Daigakuin Rikogaku Kenkyuka, Kagoshima, Japan Cellulose and chitin are widely distributed on the earth and very important biomass resources. Cellulose has been used in a wide variety of practical applications. For example, cellulose acylates are used as practical thermoplastic materials. Different from cellulose, chitin is mostly unutilized as practical materials, because it forms strong hydrogen bonding, mainly between acetamido groups. Therefore, the chitin chains construct stiff fibrous crystalline structure, resulting in its poor solubility and processability. Accordingly, there had not previously been many reports on the efficient acylation methods of chitin. Over the past two decades, ionic liquids have been identified as powerful solvents for natural polysaccharides with poor solubility. For example, in 2009, the author found the dissolution of chitin in an ionic liquid, 1-allyl-3-methylimizazolium bromide (AMIMBr). The following study achieved to develop the efficient acylation of chitin using acyl chlorides in the presence of pyridine and N,N-dimethyl-4-aminopyridine in AMIMBr, which produced chitin acylates (ester derivatives) with high degrees of derivatization. In this presentation, the author reports to exhibit thermoplasticity from mixed chitin esters with long (stearoyl) and bulky (benzoyl) substituents, which were synthesized according to the above acylation procedure in AMIMBr (Scheme). The derivatives mainly composed of stearoyl groups accompanied with a small ratio of benzoyl groups formed the highly controlled crystalline alignment from stearoyl chains, which thus exhibited melting point. Owing to this character, the derivatives formed melt-pressed films, suggesting their thermoplastic nature.

2:25 Developing integrated chemical and biological processes to produce 2-Pyrone-4,6-Dicarboxylic Acid (PDC) from lignocellulosic biomass Canan Sener1, csener@wisc.edu, Steven D. Karlen1, Christos Maravelias2, John Ralph1, Timothy J. Donohue1, Daniel Noguera1. (1) U. of Wisconsin-Madison(2) Princeton U., New Jersey In our previous work, we used chemical and biological upgrading in tandem to convert a fraction of lignin to high value 2-pyrone-4,6-dicarboxylic acid (PDC). Reductive Catalytic Fractionation (RCF) was used to liberate lignin from the biomass and simultaneously depolymerize the lignin. Using an engineered strain of Novosphingobium aromaticivorans DSM12444, the RCF product mixture can be upgraded to PDC. By applying RCF to the poplar with Pd/C as catalyst and methanol as solvent; we were able to have increased monomer/oligomer product yield and the PDC yield on a per kg of biomass basis compared to a stepwise lignin isolation followed by hydrogenolysis of fractionated lignin. Furthermore, the sugar stream of the lignocellulosic biomass which was preserved after RCF process, was subjected to enzymatic and

microbial digestion to produce liquid fuels. Combined, we produced value added products from both the lignin (phenolics) and polysaccharide fractions.
Technoeconomic analyses of our processing chain indicated that the RCF stage is costly because of the high-pressure reaction conditions due to low boiling point of methanol. Changing the solvent from methanol to a higher boiling point one will not only improve the process economics but also improve the safety of process operation. For this purpose, ethylene glycol, ethanol and ethanol-water mixture were tested. In our processing chain, using these solvents with reduced reaction pressure have shown that similar lignin monomer yields with methanol as solvent can be achieved. Initial experiments showed that these solvents are not detrimental to microbial upgrading and similar PDC yields could be obtained. Further process optimization was performed by varying the reaction time, solid concentration, biomass/catalyst ratio, and the effect of these changes on the microbial funneling to PDC was determined.

2:45 Valorization of agricultural byproducts - ultrafiltration and dialysis separation of myrosinase Andrea Wade2, Mark Blakeley2, Inna E. Popova1, ipopova@wisc.edu. (1) U. of Wisconsin-Madison(2) U. of Idaho, Moscow Mustard seed meal is a low value by-product of oil extraction. However, yellow (Sinapis alba) and brown (Brassica juncea) mustard seed meals have a high potential of valorization due to the presence of endogenous enzyme myrosinase. Myrosinase is a beta-thioglucosidase enzyme that catalyzes the hydrolysis of glucosinolates to release a range of biologically active compounds. Glucosinolate hydrolysis products such as allyl isothiocyanate and ionic exhibit antimicrobial, pesticidal, and anticancer properties and have potential applications in multiple industries. However, the availability of an economically feasible procedure for recovering myrosinase from mustard seed meal is still limited. Here we present a comparison of two approaches for separation of myrosinase from yellow (Sinapis alba) and brown (Brassica juncea) mustard seed meals using ultrafiltration and dialysis. For ultrafiltration, hallow membranes with cut of size in the range of 10-500 kDa were used to separate and concentrate myrosinase. For dialysis, 300 kDa cut of membranes were evaluated. Based on the yields and normalized activity of myrosinase in the obtained concentrates, both methods were determined to be viable for separation of myrosinase. In general, myrosinase isolated from yellow (Sinapis alba) mustard seed meal had significantly higher activity than myrosinase isolated from brown (Brassica juncea) mustard seed, thus being a preferable feedstock for myrosinase isolation.

3:05 Novel cocoa-derived ingredient towards circular economy and sustainability in the chocolate industry Christiano P. Guirlanda2, Izabela D. Alvim3, Márcio T. Pereira4, Jacquiline Aparecida Takahashi1, jacqueline@ufmg.br. (1) Chemistry, U. Federal de Minas Gerais, Belo Horizonte, MG, Brazil(2) Food Sci., U. Federal de Minas Gerais, Belo Horizonte, MG, Brazil(3) Instituto de Tecnologia de Alimentos, Campinas, São Paulo, Brazil(4) Centro de Desenvolvimento da Tecnologia Nuclear, Belo Horizonte, MG, Brazil The processing of cocoa for chocolate production generates a significant number of agricultural residues mainly barks and pulps, in addition to cocoa honey, a transparent liquid of exotic flavor with chemical and sensory characteristics similar to those of cocoa pulp. This byproduct is undervalued due to its rapid degradation, but it has huge potential to be incorporated into the production chain increasing the sustainability and value of cocoa production. The global cocoa products market size is expected to reach $30.2 billion in 2026 and the large markets demand innovative products. The objective of this work was to study stability and physicochemical characteristics of cocoa honey over time, after being subjected to refrigeration (4 °C), freeze-drying, conventional (65 °C, 30 min) and microwave (1300 W, 90 °C, 12 s) pasteurization, and gamma irradiation (3, 5 and 10 kGy). Cocoa honey was also processed by spray dryer (0.75 bar, 600 L/min) using maltodextrin (15 and 30%), methylcellulose (15%), and whey protein isolate (1, 5 and 10%) as carriers. Pasteurization decreased the content of bioactive compounds, while treatment with gamma irradiation, although efficient at stabilizing cocoa honey, resulted in color change, making the liquid brown. Spray dryer processing was the most efficient process for stabilization, with recovery of cocoa honey powder between 30.08 and 46.51%. The combined use of maltodextrin 20% and WPI 1% led to the best yield of dehydrated cocoa honey, without significant loss of antioxidants. Physicochemical data such as moisture contents, hygroscopicity, aW, particle size by laser diffraction, micromorphology and total phenolic compounds showed that the byproduct became stable as a powder, maintaining nutritional, color, flavor and functional attributes. Cocoa honey powder is therefore a promising new food ingredient and its incorporation into the chocolate production chain can contribute significantly to the circular economy and agricultural sustainability of cocoa production.

3:25 Producing a portfolio of commodity chemicals from lignin bound p-hydroxybenzoate Steven D. Karlen, skarlen@wisc.edu, Vitaliy Tymokhin, Canan Sener, Justin K. Mobley, John Ralph. U. of Wisconsin-Madison College of Letters and Science Finding abundant renewable sources for common commodity chemicals and pharmaceuticals is one of the great challenges of the day. One potential chemical is p-hydroxybenzoic acid which is found in Salicaceae trees (e.g., poplar, willow, aspen, and cottonwood) and in Arecaceae (e.g., oil palm and date palms) and can be up to 3wt% of the woody biomass. Though a commodity chemical on its own, p-hydroxybenzoic acid can be converted to a portfolio of high value commodity chemicals that are precursors to textiles, pigments, resins, and biodegradable plastics. We constrained our process to fit the following criteria, 1) Start from woody biomass or isolated lignin. 3) Produce 4-aminophenol and paracetamol in high yield. 3) Utilize inexpensive isolation and purification techniques. and 4) Produce a pure colorless solid product. Here in we will report our progress on developing a three-step process for the making paracetamol from lignin bound p-hydroxybenzoates via the Hoffman rearrangement. We cover some of the issues associated with the process and our strategies to address those challenges.

3:45 Production, characterization, and applications of functional components of wheat grains processing by-product Madhav P. Yadav1, madhav.yadav@usda.gov, Amritpal Kaur2, Balwinder Singh3, Brajendra Sharma1, Majher I. Sarker1. (1) USDA, ARS, Eastern Regional Research Center, Wyndmoor, Pennsylvania(2) Dept. of Food Sci. and Tech., Guru Nanak Dev U., Amritsar, Punjab, India(3) Dept. of Biotechnology, Khalsa College, Amritsar, Punjab, India Water soluble arabinoxylans (Hemicellulose B) and water insoluble fibrous cellulose rich arabinoxylan (CAX) were isolated from wheat brans by an alkaline treatment. The wheat brans are low-value by-products obtained from processing of wheat grains for making food products. The Hemi-B isolates from wheat brans were purified, characterized and their functionalities were studied. The lipids and phenolic compounds contained in these brans and in the hemicellulose B isolated from them were also investigated. It was found that the bound phenolic content in wheat bran was higher (1160–2848.88 microgram gallic acid equivalents per gram (GAE/g)) than free phenolic content (564.17–724.72 microgram GAE/g). The bound phenolics had a higher antioxidant activity than the free phenolics. The total antioxidant activity (TAA) of wheat brans varied from 11.76 to 13.01 micromole trolox equivalents (TE)/g. Understanding the functional properties of the wheat grains

processing by-products will be beneficial for their processors and wheat growers.

4:15 Synthesis of Branched triester for Potential Biolubricant Majher I. Sarker, majher.sarker@usda.gov, Helen Ngo, Brajendra Sharma. USDA-ARS-ERRC, Wyndmoor, Pennsylvania Two methyl-branched triesters, trimethylolpropane-triisostearate (TMP-ISA) and trimethylolpropane-triisooleate (TMP-IOA) have been synthesized via esterification of trimethylolpropane with isostearic-acid and isooleic-acid, respectively. Isostearic-acid and isooleic-acid have been previously produced through skeletal-isomerization reaction of naturally derived oleic acid using the reusable zeolite catalyst. TMP-ISA and TMP-IOA are characterized with FTIR, NMR, GC-MS and LC-MS for their structural determination. Physicochemical and tribological analysis reveal, TMP-ISA or TMP-IOA exhibits higher oxidative stability, viscosity index, anti-wear property, lower cold flow properties when compared to either high-oleic sunflower oil or polyalphaolefin. Blending with high-oleic sunflower oil or polyalphaolefin shows different properties expanding their platform of potential application as biolubricant.

4:35 Upcycling of sorghum distillers grains towards quality sorghum protein materials Bingnan Mu1, bingnan.mu@huskers.unl.edu, Xiaoqing Yu1, Lan Xu2, Yiqi Yang1,3. (1) Textiles, Merchandising and Fashion Design, U. of Nebraska-Lincoln(2) Dept. of Agronomy & Horticulture, U. of Nebraska-Lincoln(3) Biological Systems Engineering, U. of Nebraska-Lincoln We have developed a new technology for producing flexible, biodegradable materials using sorghum protein extracted from distillers grains. Sorghum protein exhibits dense crosslinkages, high content of hydrophobic amino acids, and a high molecular weight, making it a promising candidate to replace unsustainable petroleum-based products. However, previous attempts to develop desirable protein materials have been hindered by difficulties in protein dissolution and regeneration, even with reinforcements such as plasticization, blending, and grafting. We have developed a protein extraction system for sorghum distillers grains that yields 75% of all major proteins, including kafirin and glutelin, with a protein purity of 92% and retention of cysteine content. We have also developed an aqueous system to regenerate proteins and fully stretched both kafirin and glutelin simultaneously, improving interactions between protein molecules. Via the optimization of ratios between kafirin and glutelin, desirable molecular entanglement was achieved. As a result of our protein extraction and dissolution techniques, we were able to produce flexible protein films from sorghum distillers grains without requiring additional treatments such as plasticization, blending, or grafting.

4:55 Nitrate adsorption on biochar pyrolyzed using concentrated solar radiation Simeng Li, sli@cpp.edu, Talar Galoustian. Civil Engineering, California State Polytechnic U. Pomona Biochar has been recognized as an effective soil amendment for reducing nitrogen leaching in agriculture, but its large-scale implementation is impeded by the costly production process due to high energy requirements for thermal decomposition of feedstock. This study aimed to develop a novel pyrolysis system utilizing concentrated solar radiation to produce biochar. Results showed that the solar-pyrolysis biochar exhibited a maximum adsorption capacity of 35.59 mg/g for nitrate, significantly higher than two out of three other commercially available biochars in America. The Fourier-transform infrared (FTIR) analysis suggested a greater number of polar functional groups present in the solar-pyrolysis biochar, which enhances its affinity for nitrate and other hydrophilic ions. The scanning electron microscopy/energy dispersive spectroscopy (SEM/EDS) analysis revealed a higher weight percentage of silicon in the solar-pyrolysis biochar, indicating more thorough thermal decomposition of feedstock than two of the three other biochars produced via traditional pyrolysis methods, as confirmed by X-ray diffraction (XRD) analysis. The porous structure of the solar-pyrolysis biochar suggested a larger specific surface area, which could benefit adsorption. Although further experiments are required to determine the stability and cost-effectiveness of a scaled-up solar-pyrolysis apparatus, these findings provide hope for a more sustainable and high-performing biochar production process in the future.

5:15 Combinatorial enzyme technology for production of bioactive oligosaccharides from libraries of converted agricultural fibers Sarah B. Batt Throne, sarah.batt@usda.gov, Dominic W. Wong, William J. Orts. USDA-ARS Western Regional Research Center, Albany, California "Combinatorial enzyme technology (1,2,3)" applies the concept of combinatorial chemistry to enzyme technology, using enzymes to convert a complex parent molecule into libraries of diverse digestion products that are screened for desirable properties. The novel technique of combinatorial enzyme technology is a powerful approach for transforming plant biomass into value-added products because of the large number of diverse candidate molecules that can be created and then screened using high-throughput methods. Combinatorial enzyme technology was used to obtain bioactive oligosaccharides from wheat insoluble fiber and citrus pectin, which were selected as promising substrates because they are composed of complex biopolymeric backbones with a variety of side groups. Enzymes were used to degrade the main chains and selectively remove side groups and side group combinations to create libraries of oligosaccharide fragments with diverse structures and functional properties. High-throughput screening was used to discover pectic oligosaccharides and feruloyl oligosaccharides with antimicrobial properties.

5:35 Sequential pretreatment of bamboo to maximize the fermentable sugar yield for the production of biofuels and bioproducts Ali Salifu1, ali.salifu@bc.edu, Nneka Ekwe2, Maksim Tyufekchiev3, Klaus Schmidt-Rohr4, Zhaoxi Zheng4, Alex Maag5, Geoffrey Tompsett5, Wole Soboyejo5, Michael T. Timko5. (1) Boston College, Chestnut Hill, Massachusetts(2) African U. of Science and Tech. (AUST), Nigeria(3) Northwestern U., Evanston, Illinois(4) Brandeis U., Waltham, Massachusetts(5) Worcester Polytechnic Inst. School of Engineering, Massachusetts Alternative feedstock should be explored to diffuse the food versus fuel conflict in the use of food crops such as corn for biofuel production. Utilizing non-edible plants, like bamboo, that grow well on marginal lands is crucial to diffusing this conflict. In this work, we investigated the effects of sequential pretreatment of bamboo prior to enzymatic hydrolysis to maximize the fermentable sugar yield and make it a cost-effective renewable carbon source to produce biofuels and bioproducts. Bamboo was ball milled for up to 60 minutes (BM60) and also subjected to a sequential pretreatment where delignification pretreatment preceded ball milling for 60 minutes (DL-BM60), or delignification pretreatment succeeded ball milling (BM60-DL). Afterward, we carried out enzymatic hydrolysis of the pretreated bamboo samples using cellulase enzymes in citrate buffer for 72 hours and analyzed the hydrolysates using HPLC. XRD and solid-state 13C NMR analysis revealed that ball milling for 60 minutes resulted in a near-complete cellulose amorphization, translating to a recovery of 62% of the available carbohydrates in bamboo as fermentable sugars (glucose and xylose) after enzymatic hydrolysis. This was followed by an evaluation of sequential pretreatment (DL-BM60 or BM60-DL) to address two critical factors affecting the enzymatic saccharification of lignocellulosic biomass – cellulose crystallinity and lignin content. Sequential pretreatment resulted in sugar yields up to 97 ± 4 %, with

a clear preference for delignification followed by amorphization, i.e., DL-BM60. Further solid-state NMR and XRD analyses revealed why the order of sequential pretreatment was crucial for maximizing the sugar yield. Finally, techno-economic analysis for bamboo conversion to sugars indicated that a biorefinery based on the preferred sequential pretreatment (DL-BM60) was economically viable with a positive projected net present value. These findings support further investment in bamboo as a renewable carbon source to decarbonize transportation fuels and chemical production without competing with food.

Virtual Session - Food Security: The Role of Alternative Protein Sources in Addressing World Hunger

3:05 New approaches to enhancing protein functionality and digestibility in plant-based foods Harjinder Singh, H.Singh@massey.ac.nz. Massay U., Riddet Inst., Palmerston North, Manawatu-Wanganui, New Zealand Increasing consumer awareness of the environmental impacts of intensive animal production systems, ethical concerns around animal welfare, and health issues are driving the global food industry to develop alternatives or substitutes to animal-based products. As a result, the category of protein alternatives has experienced exceptional growth over the past decade, with the most rapid advances in the use of plant-based materials to match the properties of animal protein products. However, there are many scientific and technological challenges that need to be overcome: many plant protein sources are limiting in some of the essential amino acids, are hard to digest and have high potential for allergenic responses. Protein functional properties, such as solubility, emulsification, foaming, water holding, fat binding, viscosity and rheology, thickening, and gelling are highly associated with their suitability in food systems. Unfortunately, the current plant protein products have highly variable functional properties and compositions, due to the source and processing techniques used in their isolation and fractionation. Physical, chemical, and biochemical approaches are being investigated to further enhance plant protein functionality and utilization. As many of the plant protein sources used in food formulations are relatively new, there is a lack of fundamental understanding of the intrinsic properties, interactions, and functionality of these proteins in food systems. Building this understanding will allow the development of specific protein structures that have superior functionality and physiological benefits. This presentation focuses on current state of knowledge on plant protein sources, structures, and their modification during processing. New approaches to enhancing protein functionality and digestibility will be discussed.

3:30 Micronutrient variation of plant-based milk alternatives: Influence of formulation and processing Benjamin Redan, benjamin.redan@fda.hhs.gov. US FDA, Bedford Park, Illinois Over the past several years, there has been an increase in the consumption of plant-based foods that are marketed and sold as alternatives for milk (plant-based milk alternatives or PBMAs). A variety of product types and brands are marketed to meet the consumer demand. However, there are limited publicly available data on the nutrient content of the various types of PBMAs and the effect of formulation and processing on these nutrients. This presentation will present data from a market basket study we conducted to determine the amount and variability of key nutrients across eight PBMA types. Types included in the analysis were produced from almond, cashew, coconut, hemp, oat, pea protein, rice, and soy. We also conducted trials in a pilot plant to determine the effect of high-temperature short-time (HTST) processing on the content of key nutrients in an in-house formulated almond PBMA. We found that a majority of PBMA types differed in the amount of target nutrients across brands. The processing experiments indicated that while thiamine levels significantly decreased during processing, levels of other target nutrients, such as vitamins A and D, were not affected. These results indicate that PBMA formulation is a significant driver of PBMA nutrient content, and that processing may affect levels of micronutrients that are very heat sensitive.

3:55 Alternative proteins: Food safety risks and their mitigation Louise Manning, LManning@lincoln.ac.uk. Lincoln Inst. for Agri-food Technology, U. of Lincoln College of Science, Lincolnshire, United Kingdom Food Science has focused in recent decades on developing a range of ‘alternative’ proteins with the intention of substituting animal-derived proteins in the human diet. Alternative proteins are currently being sourced from plants, algae, fungi, insects, and through the development of fermentation techniques and tissue culture. This study considers the potential food safety risks associated with these alternative proteins and the mitigation activities required when they are used as ingredients in food products to ensure food safety. Many of the alternative protein sources are declarable allergens (e.g. soy, almonds, crustacea) and there have been cases of allergenic reactions where dairy milk has been found in these products which has not been declared. There is concern associated with chemical, biological and radiological (CBR) food related hazards and increasing focus on the need to develop appropriate food control management systems to mitigate, and where possible eliminate the potential risk. This work is of interest as policy makers, food businesses and individuals seek to reduce the environmental footprint of the food products consumed and simultaneously assure access to safe, nutritious food.

4:40 Analysis of insect cross-reactivity with crustacean allergen detection methods Anne Eischeid, Anne.Eischeid@fda.hhs.gov, Rakhi Panda, Chung Cho, Sarah Stadig. Center for Food Safety & Applied Nutrition, U.S. FDA, College Park, Maryland In recent years, insects have come to be seen as a potentially important high value food source which can help sustainably meet the world population’s growing demand for food. Increasing consumption of insects has led to an increased focus on potential associated food safety concerns such as allergic reactions. In the US, the Food, Drug, and Cosmetic Act (FD&C Act) includes crustacean shellfish as a major food allergen group. Insects, like crustacean shellfish, are arthropods, and clinical cross-reactivity between the two groups has been demonstrated. The goal of this work was to establish whether clinical cross-reactivity translates into analytical cross-reactivity. We tested edible insect samples using both protein-based immunological methods and DNA-based polymerase chain reaction (PCR). Specifically, we examined the responses of enzyme-linked immunosorbent assay (ELISA), Multi-Analyte Profiling Food Allergen Detection Assay (xMAP FADA), Western blot, and real time PCR to a convenience sampling of commercially available edible insect samples to evaluate cross-reactivity levels and proteins involved in cross-reactivity. Both crustacean ELISA as well as the crustacean beadset in the xMAP FADA showed some level of cross-reactivity to nearly all insect samples. Western blot confirmed tropomyosin, an arthropod pan-allergen, as its major source. Real time PCR assays had markedly lower levels of cross-reactivity than immunological methods. Results varied across insect species but without a clear pattern. Lower levels of cross-reactivity observed in real time PCR support its use as a confirmatory method to help distinguish crustacean and insect signals. These results confirm that edible insects show analytical cross-reactivity with crustacean allergen detection immunoassays. Confirmation using real time PCR, which shows little to no cross-reactivity, may be helpful in clarifying ambiguous results.

5:05 Proteomics in alternative protein research – evaluating protein food safety and quality Michelle L. Colgrave,

Michelle.Colgrave@csiro.au. Agriculture and Food, Commonwealth Scientific and Industrial Research Organisation, Brisbane, Australian Capital Territory A major challenge facing the world is providing protein security in the face of a growing global population. To this end, we have started exploring different crops and food sources from pulses to insects to algae and more. As we pivot towards these under-utilised resources, potential exists for increasing prevalence of allergy or cross-reactivity. Soy is a mainstay of the plant protein ingredient market, but new plant protein sources are emerging. For instance, lupin seeds possess high protein content (35-44%) and many health-promoting benefits (lowering cholesterol and blood pressure, managing glucose levels). But lupin also contains proteins that can trigger life-threatening anaphylaxis. Another complementary, sustainable source of protein to feed the world's growing population is insects. Insects have been consumed by people for millennia, but belong to the arthropod family, like crustaceans. Crustacean (shellfish) allergies are both relatively common and potentially severe; hence, the cross-reactivity of the immune system with insect proteins (e.g., tropomyosin and arginine kinase) is a potential health concern. The development of insects for food requires technology to explore their allergenic potential. In this presentation, the role of proteomics as a powerful tool to characterise both nutritional and antinutritional proteins in emerging protein sources will be discussed.

5:30 Regulation of protein-based food ingredients in the US Jason Dietz, jason.dietz@fda.hhs.gov. Center for Food Safety and Applied Nutrition/Office of Food Additive Safety, FDA, College Park, Maryland Food innovation has never moved more quickly than today. An important element of innovation and product development is understanding the regulatory requirements for the food product you intend to market. Innovation in today's food technology space ranges from cultured animal cell foods to food ingredients produced using new methods (e.g., precision fermentation) to novel food packaging materials. Many of these products fall under the regulatory purview of FDA's Office of Food Additive Safety (OFAS). Food producers have a legal obligation to market only safe and lawful foods. To assist companies seeking to safely bring new food ingredients or food contact materials (or new uses of existing substances) to market, OFAS offers several premarket regulatory programs. The OFAS premarket programs include a notification process for food contact substances, petition programs for food additives and color additives, and a notification program for Generally Recognized as Safe substances (GRAS). Other programs include consultation programs for food from new plant varieties and foods derived from animal cell-culture. This talk will provide some examples of products appropriate for evaluation in each program and general safety considerations. Attendees will learn how they can begin engaging with OFAS to get a jump start on the applicable premarket regulatory process early in the product development process.

Virtual Session - Graduate Students Symposium in Asia-Pacific Region on Agricultural and Food Chemistry

5:35 Impact of ultrasound treatment on structural, emulsifying, and rheological properties on ultrasound treatment of oxidative oat (Avena sativa L.) protein Xu Yue[1], xuyue122112@163.com, Yang Yang[1], Chunmin Ma[1], Xin Bian[1], Likun Ren[1], Baoxiang Liu[1], Lianzhong Ai[2], Na Zhang[1]. (1) Harbin U. of Commerce, Heilongjiang, China(2) U. of Shanghai for Science and Tech., China The specific aim of this study was to explore the mechanism of ultrasonic improving oxidative oat protein aggregates (OOPA) emulsifying properties by analyzing the changing pattern in structure and emulsifying properties of OOPA by ultrasound treatment at different lasted times (5, 10, 15, 20, 25, and 30 min). Based on the physical structure analysis, ultrasound treatment at 25 min improved the as evidenced by the reduced particle size and disulfide bonds (S-S) content, exposure of the hydrophobic group, an increase of ζ-potential absolute value. The Fourier transform infrared (FTIR) spectroscopy analysis and atomic force microscopy (AFM) observation also suggested ultrasound-induced depolymerization behavior, improvement of flexibility, and reduction of the roughness of OOPA. The emulsifying properties were optimized when ultrasound treatment lasted for 25 minutes; the emulsifying activity (EAI) and emulsifying stability (ESI) increased by 2 times and 1 time, compared with the OOPA. Then, viscosity curve and frequency sweep oscillatory experiments proved the ultrasound improved the rheological properties of OOPA and the observations of the confocal laser scanning microscope (CLSM) further provided visual evidence. Finally, the correlation analysis was applicated to establish the structure-activity association between the structure and emulsifying properties of OOPA under ultrasound. In general, these results further confirmed a role of ultrasound in promoting the emulsifying properties of OOPA.

5:45 Withdrawn

5:55 Effects of different commercial mixed lactic acid bacteria on physical and chemical properties of soy protein yogurt Xinyue Xu, 13604980243@163.com, Huaitian Cui, Jiaxin Xu, Zhiheng Yuan, He Liu. Bohai U., Jinzhou, China In this study, the effects of different commercial mixed lactic acid bacteria on the physical and chemical properties of soy protein yogurt were studied using soy powder, soy protein isolate powder, soy umbilical powder and soy whey as the main raw materials. The results showed that different combinations of probiotics had significant effects on physical and chemical properties of soy protein yogurt. The pH variation trend of soy protein yogurt D fermented by commercial mixed lactic acid bacteria Danisco was significantly different from other samples. Soy protein yogurt D and F fermented by commercial mixed lactic acid bacteria Danisco and Kefir respectively have higher hardness and elasticity, but lower adhesion. Rheological analysis showed that the apparent viscosity of soy protein yogurt D fermented by the commercial mixed lactic acid bacteria Danisco was the lowest and showed weak elastic and viscous behavior. The internal structure of soy protein yogurt D was relatively compact and uniform, and its free water content was the lowest, and the water fluidity was the least. The volatile flavor substances of soy protein yogurt D and F fermented by Danisco and Kefir were more abundant, which had significant positive correlation with umami and richness. Moreover, the contents of soy isoflavone and equal in soy protein yogurt D were higher. This study not only realized the high value-added utilization of soy whey, but also developed a nutritious and healthy plant-based soy protein yogurt.

6:10 Typical emulsions as probiotic food carrier: Effect of cells position on its viability Mengfan Li1,2, mengfanli94@163.com, Filip Van Bockstaele2, Wen-Yong Lou1. (1) South China U. of Technology, Guangzhou, Guangdong(2) Dept. of Food Technology, Safety and Health, U. Gent, Belgium The development of probiotics-encapsulated emulsions that maintain the viability of probiotics during processing, storage and human gastrointestinal (GI) tract environment, receives great scientific and commercial interest. In this study, typical W/O and O/W emulsions with and without oil gelation were used to encapsulate L. plantarum. The effects of emulsion types on the viability of L. plantarum during storage and GI tract were investigated. Besides, the position of L. plantarum in emulsion system and its number of viable cells when threating by adverse environment was correlated in order to figure out which type of emulsion is more suitable as food carrier for probiotics encapsulation and protection. As a result, probiotics tend to migrate from oil to water phase due to the natural hydrophilicity, however, it's harmful for cells viability when surrounding by water

for a long time. Oil gelation in emulsions is one of the promising strategies for inhibiting the cells mobility and decreasing the contact with adverse factors (e.g., water, exogenous enzymes and gastric acid), thus enhancing the number of viable cells that enough to exert its beneficial effects in host.

6:20 White-light crosslinkable milk protein hydrogels with ultrafast gelation for first-aid wound treatment
Qinchao Zhu, 1285307720@qq.com. Zhejiang U., Hangzhou, China Uncontrollable massive hemorrhage following trauma or occurring during surgery accounts for a significant proportion of annual mortality worldwide. The traditional mechanical products and technologies for wound closure require a mass of user training and proper equipment and the process is also time-consuming. In-situ gels that are flexibly adapting to the wound shape have a promising potential, but their gelation and adhesive properties are often regressive in the presence of blood. Here, a white-light crosslinkable natural milk-derived casein hydrogel bioadhesive with fast gelation rate is presented for the first time. Benefiting from abundant tyrosine residues, casein molecule chains can bind to each other and tissue surface by forming di-tyrosine bonds under white light with a ruthenium-based catalyst. Gelation is initiated with an outdoor flashlight, a cellphone flashlight, or an endoscopy lamp, which facilitates its use during first-aid and minimally invasive operations. The rapid gelation enables 3D printing of the casein hydrogel and excellent hemostasis even during liver hemorrhage due to section injury. The covalent binding between casein and tissue enables robust adhesion which can withstand more than 180 mmHg blood pressure. Moreover, the casein-based hydrogel can facilitate post-traumatic wound healing due to trauma for its biocompatibility. Casein-based bioadhesives developed in this study pave the way for broad and practical application in emergency wound management.

6:30 Formation and characterization of oleogels derived from emulsions: Evaluation of polysaccharide ratio and emulsification method Lihua Huang1,2, hlh5213@163.com, Yongjian Cai1, Mouming Zhao1, Qiangzhong Zhao1, Paul Van der Meeren2. (1) School of Food Sci. and Engineering, South China U. of Technology, Guangzhou, Guangdong(2) Faculty of Bioscience Engineering, U. Gent, Belgium In the present work, highly oil-binding oleogels were fabricated by two polysaccharides (insoluble soybean fiber (ISF) and hydroxypropyl methylcellulose (HPMC)) using an emulsion-templated method. The polysaccharide-based network was developed by oven-drying ISF and HPMC co-stabilized emulsions to obtain the oleogels and two emulsification methods were compared. The aqueous polysaccharide mixtures displayed an increased particle size but decreased viscosity with increasing proportions of ISF, leading to a reduced interfacial tension. Increased HPMC reduced the droplet size of emulsions while it improved the apparent viscosity and loss modulus. Emulsions prepared by high-pressure homogenization displayed a smaller droplet size and lower viscosity while the oleogels exhibited abundant liquid oil. By contrast, emulsions prepared by high-speed shearing presented a larger droplet size while the oleogels exhibited well-structured semi-solid oil. The oleogels were endowed with stronger gel strength (increased to 184g and 461g, respectively) and hardness from increased HPMC, resulting in a decreased oil loss. Increasing the HPMC content contributed to a more compact structure of the oleogels and emulsions whereby emulsions with a too small droplet size were difficult to be fully converted into gel-like semi-solid oil. Results indicate that ISF and HPMC can be applied in structuring oleogels as substitutes for solid fats.

6:45 Physical treatment synergized with natural surfactant for improving gas-water interfacial behavior and foam characteristics of α-lactalbumin Jinzhe Li, nhljz_0410@163.com. Northeast Agricultural U., Harbin, China The purpose of this study was to investigate effect of physical treatment (ultrasound, U / high pressure homogenization, H / combined treatment, UH or HU) and surfactant (Mogroside V, Mog) on air/water interface adsorption and foaming properties of α-lactalbumin (ALa). Firstly, the binding of Mog and all physical-treated ALa was a static quenching process. Mog had the greatest binding affinity for HU-ALa among all treated samples. U or H treatment could change surface hydrophobicity of ALa/Mog complex. Secondly, at the molar ratio (ALa:Mog) of 1:50, foaming ability (FA) of all ALa samples got the maximum. The sequence of FA in ALa and ALa/Mog complex was listed as follow: HU > U > H > UH. Moreover, foaming stability (FS) of HU-ALa was the highest, followed by H-ALa, U-ALa and UH-ALa. Meanwhile, low concentration Mog increased FS of ALa or UH-ALa, but it reduced FS of H-ALa, U-ALa and HU-ALa. Quartz crystal microbalance with dissipation monitoring (QCM-D) experiment indicated that ALa/Mog complex after U or H treatment was quickly absorbed at air/water interface, compared with the treated ALa, and HU-ALa/Mog had the largest frequency shift. In addition, HU-ALa had the thickest bubble membrane and the highest dissipation shift in all samples, indicating that the absorbed membrane thickness and viscoelasticity of samples was correlated with foam stability. Therefore, U and H treatment synergism with Mog was an effective approach to enhance foam properties of ALa, which indicated that HU-treated ALa/Mog complex could be viewed as the safe and efficient foaming agent applied in food processing.

6:55 Food-grade seamless capsules loaded with probiotics: gastrointestinal protection and long-term storage Kui Zhang, zk244833@163.com, Chenlu Ma, Jian Zhang, Ying Liu, Liqiang Zou. Nanchang U., Jiangxi, China Probiotics have many beneficial physiological effects, such as enhancing immunity and regulating intestinal microflora. However, low pH in the stomach, various digestive enzymes and bile salts in the intestine threaten their viability and function. In this study, we developed a novel probiotic delivery system to encapsulate probiotics into a seamless capsule formed by a pH-responsive wall material and a lipid core material that isolates water and oxygen. The probiotic viability in the prepared capsules exceeded 9.7log CFU/g, and the size of the capsules could be adjusted within 2-8mm as needed. Laser confocal microscopy showed that probiotics were evenly distributed in the inner lipid layer. Simulated in vitro digestion results showed that after 2h incubation with simulated gastric juice (SGF) and simulated intestinal juice (SIF), the survival rate of probiotics in seamless capsules exceeded 90%, while the survival rate of unencapsulated probiotics did not exceed 1%. Furthermore, after 30 days of storage at 4 ° C, the probiotic viability in the capsules decreased by only less than 0.1 log CFU/g. The capsules can be taken directly or applied to solid beverages, which can provide additional ideas for the development of probiotic functional foods.

7:05 Exploration of interaction between α-lactalbumin and β-lactoglobulin under dUHT treatment and storage: Experimental and molecular dynamics study Tai Zhang1,2, tyzhang@stu.ouc.edu.cn, Yisuo Liu1,2, Pengjie Wang3, Yixuan Li3, Fazheng Ren3,2, Huaxi Yi1,2. (1) Ocean U. of China, Qingdao, Shandong, China(2) Food Laboratory of Zhongyuan, Luohe, China(3) China Agricultural U., Beijing Direct ultra-high temperature (dUHT) milk is considered as the next generation of liquid milk product because it keeps more nutritional ingredients and better flavor than UHT milk. However, sedimentation and age gelation are urgent problems to develop dUHT milk. The role of whey protein interaction in the destabilization of dUHT milk is rarely reported. In this study, the interaction between α-lactalbumin (α-La) and β-lactoglobulin (β-Lg) was investigated by thermodynamics, spectroscopy and silico approach at 75°C (preheat), 145°C (dUHT) and 37°C (storage). The

results showed that α-La could interact with β-Lg via hydrophobicity along with exothermic reaction. During dUHT and storage, the average molecular weight (MW) distribution of α-La/β-Lg complexes increased from 20.3 kDa to 274.4 kDa. The particle size increased from 135.53±5.26 nm to 153.50±3.83 nm and the zeta potential decreased from -27.80±5.90 mV to -7.73±2.65 mV. Fibrous cluster-like protein bridges promoted the formation of α-La/β-Lg aggregates. The interaction mechanism between α-La and β-Lg was explored by molecular docking and dynamics simulations. It was found that heat treatment reduced the binding free energy of α-La and β-Lg and promoted the formation of α-La/β-Lg complexes. Electrostatic and van der Waals were the main energy contributors to the binding. UHT treatment increased the number of hydrogen bonds and weakened the hydrophobic interaction. These findings indicate that the interaction between α-La and β-Lg forms aggregates during heat treatment and storage, which help to optimize the manufacture and storage of dUHT milk.

7:20 Metabolic diversity in fermented milk of Lactococcus lactis isolated from naturally fermented dairy products Weicheng Li, liweicheng0011@163.com, Zhihong Sun. Key Laboratory of Dairy Biotechnology and Engineering, Ministry of Education, China, Huhhot As an important microorganism in the food industry, Lactococcus (L.) lactis subsp. lactis is widely used as a starter culture in fermented dairy products due to its ability to improve the structure and sensory properties of these products. Although the genetic diversity and strain heterogeneity of L. lactis subsp. lactis are high, there is limited knowledge about the metabolic differences in strains with different fermentation rates or isolate sources. To address this, we analyzed the fermentation capacity and metabolic profiles of 17 L. lactis subsp. lactis strains using ultra-performance liquid chromatography coupled with quadrupole-time-of-flight mass spectrometry. Our results showed that there were significant differences in metabolites between fast-fermenting strains (fermentation time < 16 h) and slow-fermenting strains (fermentation time ≥ 16 h), with the former enriched in peptides and lipids. We identified several biomarkers, including peptides, esters, and tributyrin, which could distinguish between the two groups, with tributyrin playing a role in regulating strain growth. We also characterized the volatile flavor compounds produced by L. lactis subsp. lactis strains isolated from sour milk, sour goat milk, and cheese, and found that different strains from different isolates had different contributions to fermented milk flavor. For example, compared to sour milk isolates, L. lactis subsp. lactis isolated from sour mare's milk was more conducive to the production of alcohol metabolites, while L. lactis subsp. lactis isolated from sour goat milk was more favorable to the production of ketone and aldehyde metabolites. Overall, our study provides novel insights into the metabolic causes of different acid production rates and isolate sources among L. lactis subsp. lactis strains.

7:30 Withdrawn

7:45 Prevention of loperamide-induced constipation in mice and alteration of 5-hydroxytryotamine signaling by Ligilactobacillus salivarius Li01 Bo Qiu, 22118248@zju.edu.cn, Mingfei Yao. Zhejiang U. First Affiliated Hospital State Key Laboratory for Diagnosis and Treatment of Infectious Diseases, Hangzhou, Zhejiang, China Although Ligilactobacillus salivarius Li01 (Li01) has shown much promise in preventing multiple gastrointestinal diseases, the potential of the probiotic in alleviating constipation and the related mechanisms remain unclear. In this study, the effects of Li01 were evaluated in a loperamide-induced constipation mouse model. The results indicate that Li01 intervention can alleviate constipation symptoms by improving water content, quantity, and morphology of feces, as well as by modulating gut motility (gastrointestinal transit rate). Additionally, Li01 can down-regulate the expression of aquaporins associated with fluid transit, decrease levels of vasoactive intestinal peptide and substance P, and increase levels of somatostatin in serum. Constipation significantly increased the levels of 5-hydroxytryotamine (5-HT) in serum and decreased the levels in the intestine. Due to its function of elevating the expression of tryptophan hydroxylase 1, this was reversed after Li01 treatment. Li01 also promoted the expressions of 5-HT receptor 3 and 4, indicating that the 5-HT signaling pathway may play a critical role in the mechanism by which Li01 alleviate constipation symptoms. Additionally, Li01 significantly altered the gut microbiota composition, by enhancing the ratio of Firmicutes/Bacteroidetes and increasing the abundance of Rikenellaceae_RC9 genera. Based on the above results, Li01 may have the potential to effectively alleviate constipation by regulating the 5-HT pathway and alteration of the gut microbiota.

7:55 Lonicera caerulea L. polyphenols alleviated oxidative stress induced intestinal environment imbalance and lipopolysaccharide translocation liver injury by regulating pathways of Nrf2/HO-1/NQO1 and MAPK in rats Zhen Cheng, czsyau@163.com, Bin Li, Yuehua Wang. Shenyang Agricultural U., Shenyang, China In the present study, the modulatory effects of Lonicera caerulea L. polyphenols (LCP) on intestinal environment and lipopolysaccharide (LPS) translocation liver injury in oxidative stress damage (OSD) rats by regulating Nrf2/HO-1/NQO1 and MAPK pathways were investigated. To examine the prebiotic properties of LCP, an OSD model induced by high fat diet in SD rats was constructed, over eight weeks. In colon, we found that LCP inhibit intestinal permeability (GLP-2 content and occludin protein increased and claudin-2 protein decreased), intestinal inflammation (proinflammatory cytokines such as TNF-α, IL-6, COX-2 and NF-κB p65 decreased) and intestinal OSD (the regulation of Nrf2/HO-1/NQO1 pathway). Moreover, in liver, LCP alleviated liver injury by suppressing LPS translocation-induced NF-κB p65 nuclear transcription level and mitogen activated protein kinase (MAPK) signaling pathway activation. In addition, we found that Bacilli, Lactobacillales, Lactobacillaceae, Lactobacillus, Akkermansia, Actinobacteria, Proteobacteria, Rothia and Blautia are the key intestinal microbiota that related to intestinal OSD and LPS translocation liver injury in rats. Taken together, our results suggest that LCP treatment can potentially modulate intestinal environment and liver injury by suppressing oxidative stress related pathways and intestinal microbiota. We constructs a high-fat diet-induced oxidative stress injury model to investigate the effect mechanism of Lonicera caerulea L. polyphenols on regulating intestinal environment and lipopolysaccharide translocation liver injury in rats by regulating Nrf2/HO-1/NQO1 and MAPK signaling pathways. Our findings will help develop microbiological engineering of functional foods and accelerate the application of Lonicera caerulea L. polyphenols in improving intestinal environment and liver injury induced by oxidative stress.

8:05 Effects of acute and chronic heat stress on rumen microbiome in dairy goats Min 1. Li, 12217030@zju.edu.cn, Lianbin Xu, Chen Zhang, Hongyun Liu. Zhejiang U., Hangzhou, China Our previous study found that heat stress (HS) significantly reduced the lactation performance and feed intake of dairy goats. However, the microbial regulatory mechanism remains unclear. In the study, the alterations of rumen microbiome in dairy goats with exposure to acute and chronic phases of HS were elucidated. The study included 12 dairy goats that were randomly assigned to two groups based on parity and milk protein, being housed in temperature-controlled chambers with duration of 28 days. The control group (CT) was kept at approximately 18°C -21°C and temperature-humidity index (THI) of 68 ± 4.5 condition, while the HS group was subjected to 37°C during the day, 30°C at night, and a THI of 85 ± 5.0. The study

collected data from two periods: 1 day (acute HS phase, CT1 and HS1) and 28 days (chronic HS phase, CT28 and HS28). Results showed that the concentrations of acetate and propionate significantly decreased in both HS phases compared to the controls, but there was no notable difference between acute and chronic HS groups. Despite no change of ruminal bacterial structure in two phases of HS-exposed dairy goats, there was a disruption in rumen microbiome at chronic phase HS, represented by an increase in the abundances of Prevotella, Prevotellaceae and Planococcaceae, and the upregulation of "Carbohydrate transport and metabolism". Additionally, with exposure to chronic HS, the abundance of Succinivibrionaceae that produces succinate was reduced, and the functional terms of "Intracellular trafficking, secretion and vesicular transport" and "Cytoskeleton" were downregulated. Collectively, chronic HS exerted more striking effects on changing ruminal microbial composition and their function compared to acute HS. This study provided a possibility to alleviate the damage of acute and chronic HS in dairy goats by regulating rumen microbes.

8:20 Sleep promoting effect and mechanism of goat milk Casein Hydrolysate on rat and Caenorhabditis elegans Zhuobin Li, lizhuobinnnnn@163.com, Qiuyi Zhu, Xingyu Liu, Yali Zhang, Zhian Zeng, Guo Liu, Yong Cao, Yunjiao Chen. College of Food Sci., South China Agricultural U., Guangzhou, Guangdong Background: The incidence rate of insomnia has been rising in recent years. Therefore, hypnotic and sedative drugs with higher safety and efficacy are urgently needed. Goat milk casein hydrolysate (GMCH), the polypeptide obtained from goat milk, has the biological activity of improving sleep and its main component's sequence is TQTPVVVPPFLQPEIM. However, the mechanism of improving sleep is still unclear. Therefore, the purpose of this study is to explore the sleep promoting effect of GMCH and the underlying mechanism. Result: GMCH significantly improved the body weight and alleviated the anxiety level of insomnia rat in the open field in the insomnia rat model. Meanwhile, the duration and frequency of sleep were significantly increased with GMCH treatment in the C. elegans model. Therefore, GMCH improved the sleep behavior in rat and C. elegans. Furthermore, GMCH treatment restored the levels of neurotransmitters like 5-HT and GABA, and increased significantly the levels of ATP and MMP both in two models. The expression of c-fos protein in the hypothalamus of rat was decreased significantly, and the damage of hypothalamus and hippocampus also was recovered. In addition, the damage degree of dopaminergic neurons and cholinergic neurons of C. elegans was significantly reduced, and the mitochondrial damage and amyloid β-protein deposition in the body wall muscle of the mutant were significantly reduced. Finally, the underlying mechanism was that GMCH restored beneficial bacteria levels of intestinal flora through the brain-gut axis and significantly increased the level of metabolite short chain fatty acids, which could reduce the level of inflammatory reaction after sleep deprivation and achieve sleep promoting effect. Conclusion: GMCH could improve sleep in rat and C. elegans, regulate the level of neurotransmitter, recover brain tissue damage, and improve neural and mitochondrial damage. The underlying sleep promoting mechanism was that GMCH modulated the composition of beneficial bacteria in the intestine through the brain-gut axis to increase metabolite short chain fatty acids, then further promoting the quality of sleep. These results provided the theories for the development of GMCH as an innovative health active substance for the improvement of sleep.

8:30 Study on the preparation, bacteriostatic mechanism and intestinal microecological regulation function of antimicrobial peptide AMP1043 Zihao Zhang, 369826213@qq.com, Ping Li, Xiaogu Zheng, Yingjie Huang. College of Food Sci. and Biotechnology, Zhejiang Gongshang U., Hangzhou, China

Antimicrobial peptides (AMPs) are one of the important metabolites of intestinal microorganisms, which can inhibit or kill pathogenic bacteria in the intestine. AMP1043 is a novel AMP derived from the human gut, with advantages of low toxicity, and high antibacterial activity, however, its mechanism of inhibiting Escherichia coli and regulatory effect on intestinal microecology have not been reported. After heterologous expression, purification, and digestion, AMP1043 with a molecular weight of 3817.67 kDa was obtained. Bacteriostatic and stability experiments indicated that AMP1043 had a MIC of 4 μM against E. coli, and it is stable under hot and acidic conditions and sensitive to pepsin and trypsin. The results of scanning electron microscopy and transmission electron microscopy showed that AMP1043 caused damage to the cell membrane and wall and the release of cell contents of E. coli O104: H4. Fluorescence probe and colorimetric results confirmed that AMP1043 caused an increase in cell membrane conductivity and intracellular ATP, intracellular proton electromotive force collapse, lactate dehydrogenase leakage, and enhanced uptake of n-phenylnaphthylamine in E. coli. Binding test had shown that lipopolysaccharide on the outer membrane of E. coli is the target of AMP1043. Transcriptome results showed that AMP1043 downregulated the quorum sensing system, ABC transport system, and the expression levels of virulence factors regulating genes stxA and stxB in the Shigellin synthesis pathway, in addition, AMP1043 also inhibited the biofilm formation pathway and flagella assembly pathway. Subsequently, in an in vitro model of intestinal flora disturbance caused by E. coli, it was found that AMP1043 treatment inhibited the abundance of Escherichia_ Shigella, restored the abundance of Bacteroides, and increased the abundance of Paraacteroides and Muriaculaceae. This study revealed the antibacterial mechanism of AMP1043 against E. coli O104: H4, and preliminarily explored its regulatory effect on intestinal microecology, providing a theoretical basis for its application.

8:40 Effect of the probiotic strain, Lactiplantibacillus plantarum P9, on chronic constipation: a randomized, double-blind, placebo-controlled study Teng Ma, 18447054019@163.com, Yalin Li, Heping Zhang. Inner Mongolia Key Laboratory of Dairy Biotechnology and Engineering, Inner Mongolia Agricultural U., Hohhot, , China, Inner Mongolia Agricultural U., Hohhot, China Chronic constipation (CC) is a common gastrointestinal condition associated with intestinal inflammation, and the condition considerably impairs patients' quality of life. We conducted a large-scale 42-day randomized, double-blind, placebo-controlled trial to investigate the effect of probiotics in alleviating CC. 163 patients diagnosed with CC (following Rome IV criteria) were randomly divided into probiotic and placebo groups. Ingesting P9 significantly improved the weekly mean frequency of complete spontaneous bowel movements (CSBMs) and spontaneous bowel movements (SBMs), while significantly reducing the level of worries and concerns (WO; $P < 0.05$). Comparing with the placebo group, P9 group was significantly enriched in potentially beneficial bacteria, while depriving of several bacterial and phage taxa. Interesting significant correlations were also observed between some clinical parameters and subjects' gut microbiome, including: negative correlation between Oscillospiraceae sp. and SBMs; positive correlation between WO and Oscillospiraceae sp., Lachnospiraceae sp. Additionally, P9 group had significantly more predicted gut microbial bioactive potential involved in the metabolism of amino acids, short-/medium-chain fatty acids. Furthermore, several metabolites related to the intestinal barrier and transit decreased significantly after P9 administration. In short, the constipation relief effect of P9 intervention was accompanied by desirable changes in the fecal metagenome and metabolome. Our findings support the notion of applying probiotics in managing CC.

8:50 Ultra-Deep metagenomic sequencing-based high-quality metagenome-assembled genomes reveal novel insights into the microbial genomic dark matter in the human gut Hao Jin, jinhao94@126.com, Zhihong Sun. Inner Mongolia Agricultural U., Hohhot, China A large number of microbial genomes have already been identified from the human gut microbiome, the uneven quality and reliability of existing genomes remain a challenge to be overcome, largely due to the short-read sequencing used in most studies, which leads to the inability to resolve the genome duplication and limits assembly continuity. This study integrated the 3.7Tbp Nanopore and 21.6Tbp Illumina high-quality metagenomic data from 180 human gut samples to reconstruct the metagenome assembly genomes (MAGs) that specified in the high-quality MIMAG standard. The combination use of the ultra-deep long and short sequencing data has substantially improved the accuracy and continuity of metagenomic assembly and generated 830 circular MAGs (CMAG) and 6729 high-quality MIMAG (NHMG), which were 6.2 and 1.7 times the number of available CMAG and NHMG, respectively. Of these CMAGs, 120 represented the first circular genome for their corresponding species. By comparing the NHMG with the available microbial repositories, we found the NHMG can boost the analysis performance in uncovering the dark matter in the microbial genome, including 16S ribosomal RNA copy number, secondary metabolite gene synthesis cluster, prophage region and insertion sequences.

MONDAY EVENING

AGFD Sci-Mix Live Session (see first 36 posters listed under Sunday Evening General Posters session)

AGFD Sci-Mix Virtual Session

8:00 Developing food preference behavior-based method to identify effectors of substance use disorder Aaron T. Kim, aaronkim@umass.edu, Yeonhwa Park. Food Sci., U. of Massachusetts Amherst Substance use disorder (SUD) affects over 20 million Americans aged 12 and over, and drug overdose is the leading cause of death among those under 45. Cannabis is the most widely used drug, while opioids are responsible for the most drug overdose deaths in 2022. Identifying novel molecules that contribute to SUD will be critical for developing efficient prevention and mitigation strategies. Considering the complexity of the actions and effects of these substances on human behavior, a high-throughput platform using a living organism is ideal. However, no screening methods have been developed using in vivo model organisms. Thus, we developed a quick and easy screening assay using Caenorhabditis elegans, which contains NPR-19, a homolog of cannabinoid receptor type 1 (CB1R), and NPR-17, a homolog of opioid receptors (OR). In this assay, C. elegans were given a choice between high-quality food (Escherichia coli HB101) and low-quality food (Bacillus megaterium). The food preference index was calculated from the number of worms in each food lawn divided by the total number of worms. C. elegans naturally prefers high-quality food, displaying the food preference index of ~0.2. The food preference index was increased by 73% after arachidonyl-2'-chloroethylamide (a CB1R agonist) and decreased by 84% with rimonabant (a CB1R inverse agonist), while these modulations disappeared in the npr-19 null mutant. Similarly, the food preference index was increased by 76% with loperamide (an OR agonist) and decreased by 91% after naloxone (an OR antagonist), while these alterations were absent in the npr-17 null mutant. These results suggest that cannabinoid and opioid systems participated in the changes in the food preference index, and one screening method can be used to examine two different systems. Our developed screening method can be applied to identify previously unknown effectors for the cannabinoid and opioid systems. (note - This poster also presented at Tuesday noon Virtual Poster session)

8:00 Determination of phytochemical content and antioxidant capacity of dried haskap berries (Lonicera caerulea L.) and its potential value-added products Yihan He1, yihan.he@mail.mcgill.ca, Kiren Singh2, kiren.singh@haskalife.ca, Xiaonan Lu1, xiaonan.lu@mcgill.ca. (1) Food Sci. and Agricultural Chemistry, McGill U., Montreal, Quebec, Canada(2) Haskalife Inc., Picture Butte, Alberta, Canada Haskap berries commonly refer to the fruits of Lonicera caerulea L and have higher anthocyanin content and antioxidant capacity than other berries known for their health promoting properties, such as blueberries. In this study, the effect of processing methods on the quality of dried haskap berries was investigated. Phytochemical content and antioxidant capacity were also evaluated in haskap juice under different sterilization process; and haskap agricultural wastes (i.e., leaves and branches). Haskap extracts were used for determination of total phenolic content, anthocyanin content, total flavonoids and antioxidant capacity. Haskap powders produced by vacuum microwave drying have similar phenolic content, anthocyanin, flavonoids, and antioxidant capacity to freeze-dried powders. Haskap juice under high pressure processing preserved a higher anthocyanin content compared to its counterpart under heat pasteurization. This study provided critical and insightful results for the development of innovative value-added haskap products to agri-food industry.

8:00 Protein Extraction from Spent Oil-Cakes D. Smit Kumar, dsmit.chemist@gmail.com, Hardi Makwana. School of Science, GSFC U., Vadodara, Gujarat, India The study will aim at development of a cheaper and more viable industrial process for protein extraction. Major objectives of the study will be: i) To explore the chemistry of chemicals and find the cheapest reagents for the extraction; ii) To investigate and establish the feasibility/viability of the method at industrial level. Groundnut cake is a by-product obtained after extraction of oil. The cake contains 45–60% protein, 22–30% carbohydrate, 3.8–7.5% crude fibre and 4–6% minerals. The extraction of protein from oil spent cake can be done by two methods, by alkaline isoelectric precipitation and physical separation procedures. We are going to extract the protein by alkaline isoelectric precipitation method. For this method, we have selected the cheapest reagents out there in the market while, maintaining the maximum yield and recovery of protein. We need 0.2 M NaOH and 1 N H2SO4 solution for the pH adjustment and precipitation of protein. The whole method comprises various steps like Stirring, Centrifuge, Filtration and Drying. Utilization of defatted meal/residue into food products could be an excellent way for boosting the utilization of groundnut protein in the diets of malnourished people in developing and poor countries. Application and Usage of defatted groundnut meal with mild processing treatment is becoming increasingly popular in many countries. So, the extraction of peanut protein will aid the little valued spent oil cakes and will reap financial reward to the peanut industry and will also be beneficial to various food manufacturing company.

8:00 Quality evaluation of artificially cultivated Atractylodes lancea (Thunb.) DC. from genuine producing areas Junming Chen, chenjm@cczu.edu.cn, Longyu Li, Ying Liu, Mengyi Huang, Cheli Wang. School of Pharmacy, Changzhou U., Jangsu, China Atractylodes is a medicinal and edible herb with the same origin. It is the dried root and rhizome of Atractylodes lancea (Thunb.) DC. or Atractylodes chinensis (DC.) Koidz. It has the effects of prolonging life, invigorating the spleen and nourishing the liver, and resisting viruses. It is one of the most frequently used Chinese medicinal materials for the treatment of COVID-19. Since the Ming and Qing Dynasties, Atractylodes has been produced in Maoshan and is known as genuine medicinal materials. However, in recent years, due to environmental factors and other reasons, wild resources of

Atractylodes lancea (Thunb.) DC. are scarce and have been listed as endangered medicinal plants in China. The chemical composition of Atractylodes is easily affected by climate, ecological environment, and other factors, and the quality of Atractylodes on the market varies greatly. Its quality evaluation only considers volatile oil components, ignoring the water-soluble components used in traditional Chinese medicine decoction. This article comprehensively evaluates the quality of artificially cultivated Atractylodes lancea (Thunb.) DC. in terms of its characteristics, surface texture, cross-sectional features, water-soluble components, and volatile oil components, providing a reference for the expansion and promotion of artificially cultivated Atractylodes lancea (Thunb.) DC. from genuine producing areas. The study found that artificially cultivated Atractylodes lancea (Thunb.) DC. from genuine producing areas has a nodular appearance, and its volatile oil content and water-soluble components are higher than those in other producing areas and in a certain proportion, which is consistent with the synergistic effect of multiple components in clinical efficacy of traditional Chinese medicine. Atractylolone is the main active ingredient of Atractylodes, and the content of Atractylolone from genuine producing areas is more than 20 times that from other producing areas, which can be used as a marker of the genuine producing areas of Atractylodes.

8:00 Impact of foliar and shade application on blackberry flavor and phenolics Tianyou Xu1, tianyou21@vt.edu, Jayesh Samtani2, Han Chen3, Yun Yin1. (1) Food Sci. and Tech., Virginia Polytechnic Inst. and State U., Blacksburg(2) Hampton Roads Agricultural Research and Extension Center, Virginia Polytechnic Inst. and State U., Virginia Beach(3) Dept. of Statistics, Virginia Polytechnic Inst. and State U., Blacksburg Blackberry is a popular fruit due to its delightful taste and notable health benefits. This study evaluated the influence of shade cloth and pre-harvest foliar treatments on production quality, aroma profiles and phenolics of two Virginia-grown blackberry cultivars. The study was conducted over two growing seasons (2021-2022) at Hampton Roads Agricultural Research and Extension Center in Virginia Beach, VA using a completely randomized design with three replicates per treatment. Each replicate includes three plants of Prime-Ark® Traveler or Prime-Ark® Freedom blackberry. Calcium (Ca), salicylic acid, shade cloth with 30% light reduction and one grower standard control were randomly assigned to each variety. Fruits harvested from July were used for further flavor and chemical analysis each year. The aroma-active compounds in blackberries were identified by use of headspace-solid-phase microextraction-gas chromatography-mass spectrometry-olfaction (HS-SPME-GC-MS-O). The total phenolic content and antioxidant activities (DPPH, ABTS) were measured by spectrophotometry. Normal berry production quality were observed with all treatments for two seasons. The same 16 aroma-active compounds were identified in both blackberry cultivars and across all treatments for two seasons. Three esters, 5 alcohols, 2 carboxylic acids, 2 aldehydes and 2 monoterpenes were identified; with ethyl butyrate (fruity), 2-heptanol (fresh, green), 1-octen-3-ol (cooked potato) and p-cymen-8-ol (floral) as key aroma compounds. However, all 16 aroma contents were found to be higher in blackberries from 2021 compared to 2022, likely due to climate variation (e.g., high heat and drought in 2022). Flavor profiles for two cultivars were distinct: PrimeArk® Freedom is characterized to be more “fruity” and “floral”, while PrimeArk® Traveler features more “green” and “fresh” notes. The foliar and shade application treatments, however, did not seem to significantly influence berry flavor and phenolics. This study first characterized the flavor profiles of above two VA blackberry cultivars. Regional berry growers should be more conservative when adopting foliar and shade applications because seasonal variations seemed to surpass the significance from applied agronomic treatments.

8:00 Molecular assessment of metabolome alterations in Lotus japonicus roots induced by arbuscular mycorrhiza Josef Ranner[1], josef-ranner@web.de, Michael Paries[3], Georg Stabl[2,3], Caroline Gutjahr[2,3], Timo D. Stark[1], Corinna Dawid[1]. (1)Chair of Food Chemistry and Molecular Sensory Science, Technische U. Munchen, Bayern, Germany(2) Max-Planck-Institut fur molekulare Pflanzenphysiologie, Potsdam, Brandenburg, Germany(3) Plant Genetics, Technische U. Munchen, Bayern, Germany Agricultural crop plants can experience enhanced growth, stress tolerance, and yield when engaging in an arbuscular mycorrhiza symbiosis with Glomeromycota fungi. This interaction involves the fungus absorbing mineral nutrients from the soil and exchanging them for hexoses and lipids from the plant through so-called arbuscules, which are tree-like fungal structures formed within root cortex cells. Arbuscule formation and degradation result in extensive cell reprogramming, which is well understood, but little is known about how arbuscular mycorrhiza affects the host root metabolome. To examine the impact of arbuscular mycorrhizal symbiosis on the root metabolome of the model legume Lotus japonicus, we employed an untargeted metabolomics approach. We analyzed methanolic extracts of mycorrhizal (myc) and non-mycorrhizal roots (mock) using ultra-high-performance liquid chromatography–electrospray ionization–time-of-flight–ion mobility–mass spectrometry (UPLC–ESI–ToF–IM–MS) and identified up-regulated marker metabolites through principal components analysis (PCA) and orthogonal partial least squares–discriminant analysis (OPLS–DA) highlighted as S-plots. We characterized these marker metabolites by co-chromatography with authentic standards or by isolation from L. japonicus roots using preparative HPLC and one- and two-dimensional nuclear magnetic resonance (NMR) spectroscopy experiments. We discovered three previously unknown mycorrhizal marker polyphenols in L. japonicus roots, including one coumaronochromone, one pterocarp-6a-ene, and one aryl benzofuran carbaldehyde. Moreover, we detected three further coumaronochromones, three flavonoids, three isoflavonoids, and one coumestan in mycorrhizal L. japonicus roots.

TUESDAY MORNING August 15
JAFC Best Paper and AGFD Young Scientists Awards Symposium

8:10 Sweet biotechnology: enzymatic production and digestibility screening of novel kojibiose and nigerose analogues Shari Dhaene1, shari.dhaene@gmail.com, Amar Van Laar2, Marc De Doncker1, Emma De Beul1, Koen Beerens1, Charlotte Grootaert2, Jurgen Caroen3, Johan Van Der Eycken3, John Van Camp2, Tom Desmet1. (1) Biotechnology, U. Gent Faculteit Bio-Ingenieurswetenschappen, Gent, Belgium(2) Food technology, Safety and Health, U. Gent Faculteit Bio-Ingenieurswetenschappen, Gent, Belgium(3) Organic and Macromolecular Chemistry, U. Gent Faculteit Wetenschappen, Gent, Belgium In view of the global pandemic of obesity and related metabolic diseases, there is an increased interest in alternative carbohydrates with promising physiochemical and health-related properties as a potential replacement for traditional sugars. However, our current knowledge is limited to only a small selection of carbohydrates, whereas the majority of alternative rare carbohydrates and especially their properties remain to be investigated. Unraveling their potential properties, like digestibility and glycemic content, could unlock their use in industrial applications. Here, we describe the enzymatic production and in vitro digestibility of three novel glycosides, namely, two kojibiose analogues (i.e., D-Glcp-α-1,2-D-Gal and D-Glcp-α-1,2-D-Rib) and one nigerose analogue (i.e., D-Glcp-α-1,3-L-Ara). These novel sugars were discovered after an intensive acceptor

screening with a sucrose phosphorylase originating from Bifidobacterium adolescentis (BaSP). Optimization and upscaling of this process led to roughly 100 g of these disaccharides. Digestibility, absorption, and caloric potential were assessed using brush border enzymes of rat origin and human intestinal Caco-2 cells. The rare disaccharides showed a reduced digestibility and a limited impact on energy metabolism, which was structure-dependent and even more pronounced for the three novel disaccharides in comparison to their respective glucobioses, translating to a low-caloric potential for these novel rare disaccharides.

9:05 Cracking the code of food quality and health: combating fraud and unlocking nutraceutical potential Zhuohong Xie, kyx@usp.org. The US Pharmacopeial Convention, Rockville, Maryland Food fraud is a serious problem that can have a negative impact on consumer wallets, company brand reputation, and consumer health. Standards that include test methods, specifications, and materials can help ensure food quality, safety, and integrity. A series of high-impact food standards on dietary proteins, oils, colorants, and non-targeted methods have been developed. State-of-the-art methods have also been utilized in detecting foreign addition of adulterants. In addition, a new material initiative at USP, the first in the industry, on authentic and genuine adulterated food authentication reference materials was created to support method development and standardization. Beyond quality, consuming foods containing nutraceuticals can build resilience. Studies on different foods have led to the discovery of bioactive molecules and extracts that have demonstrated promising biological effects in preclinical studies, such as antioxidant, anti-inflammatory, anti-cancer, hypolipidemic, anti-diabetic activities, and reducing the risks of COVID-19. The relationship between bioactives and biological activities has been investigated. Through chemistry, these studies combated food fraud by developing new methods to detect adulterants; unlock the nutraceutical potentials of foods by identifying and studying bioactives.

9:40 Importance influence of gums on promoting the fiber formation for soy proteins-based meat analogues by high moisture extrusion Xiaonan Sui, xiaonan.sui@neau.edu.cn. College of Food Sci., Northeast Agricultural U., Harbin, China Adding gums to protein matrices is a promising strategy for improving the fibrous structure of meat analogs by high moisture extrusion, mimicking the texture and sensory properties of real meat. In this study, the effects of three food gums (iota carrageenan, carboxymethylcellulose sodium, and sodium alginate) on promoting fiber formation in extrudates were investigated. Results showed that lamellar structures were formed at the cooling zone for samples containing 6% CMC and 6% SA, while the addition of 6% SA improved extrudate quality, including rehydration rate and digestion rate. The importance of molecular bonds in extrudate formation was also determined, with disulfide bonds being the most crucial, followed by hydrogen and hydrophobic interactions. This research has implications for the design of meat analogs with improved texture and provides insights into protein-protein interactions during extrusion.

ACS Microbiome Consortium Kick off Symposium

8:05 Bidirectional interactions between the small intestinal microbiota and bile acids in health and disease Gary D. Wu, gdwu@pennmedicine.upenn.edu. Division of Gastroenterology, U. of Pennsylvania Perelman School of Medicine, Philadelphia Bile acids play an important role, not only in the digestive process where they are critical for nutrient assimilation, but they can also act as hormones that regulate host physiology as ligands for various receptors. The composition of bile acids are regulated by bacteria through enzymatic reactions such as deconjugation and dihydroxylation. Conversely, bile acids can have an impact on the composition of the gut microbiota by inhibiting growth of specific taxa. By integrating gut microbiome analyses involving shotgun metagenomic sequencing with fecal and plasma quantitative metabolomics of bile acids in both human subjects and mice, I will provide evidence that bile acids regulate the composition of the small intestinal microbiota which, in turn may have an impact on bile acid function. The inhibition of endogenous bile acid synthesis via the activation of the farnesoid X receptor (FXR) by obetacholic acid (OCA) leads to a reversible induction of gram-positive bacteria that are found in the small intestine and are components of the diet and oral microbiota. These findings indicate that FXR activation alters the intestinal microbiota and could provide opportunities for microbiome biomarker discovery or new approaches to engineering the human microbiome. Conversely, by studying the composition of the gut microbiome and bile acids in children with short bowel syndrome (SBS) we provide evidence that dietary fiber is associated with bile acid deconjugation likely via an interaction between gut microbiota bile salt hydrolases and glycoside hydrolases in the small intestine, which may lead to whole food intolerance in patients with SBS. This mechanism not only has potential utility in clinical phenotyping and targeted therapeutics in SBS based on bile acid metabolism but may have relevance to other intestinal disease states such as irritable bowel syndrome.

8:50 Comprehensive metabolomics analyses of gut microbiome Chris Zhu[1,2], zhu.2484@osu.edu. (1) Human Sciences, The Ohio State U., Columbus(2) James Comprehensive Cancer Center, The Ohio State U., Columbus Mechanisms that link the gut microbiota with metabolic diseases emerged over the past decade through a powerful combination of ‘omics’ technologies and translational research. Previous research has found that metabolomics can be used to monitor the impact of host diet on gut microbiota functionality. Therefore, the goal of this talk is to share some of the recent development in mass spectrometry-based metabolomics approaches that allow systematically investigatation of the gut microbial metabolome and to accurately measure the metabolic responses of gut microbes to nutritional perturbations, both in vitro and in vivo.

9:10 Bridging preclinical and clinical gut microbiota research using the ex vivo SIFR® technology Pieter Van den Abbeele1, pieter.vandenabbeele@cryptobiotix.eu, Stef Deyaert1, Clémentine Thabuis2, Caroline Perreau2, Danica Bajic3, Eva Wintergerst3, Marie Joossens4, Jenni Firrman6, Dana Walsh5, Aurélien Baudot1. (1) Cryptobiotix SA, Ghent, Belgium(2) Roquette Freres, Lestrem, France(3) DSM Nutritional Products AG, Kaiseraugst, Aargau, Switzerland(4) U. Gent Faculteit Wetenschappen, Gent, Belgium(5) CosmosID, Germantown, Maryland(6) USDA, Agriculture Research Service, Eastern Regional Research Center, USDA, Wyndmoor, Pennsylvania While modulation of the human adult gut microbiota is a trending strategy to improve health, the underlying mechanisms are poorly understood. This study aimed to assess the predictive value of the ex vivo, reactor-based, high-throughput SIFR® (Systemic Intestinal Fermentation Research) technology for clinical findings using three structurally different prebiotics (inulin (IN), resistant dextrin (RD) and 2’-fucosyllactose (2’FL)). The key finding was that data obtained within 1-2 days were predictive for clinical findings upon repeated prebiotic intake over weeks: amongst hundreds of microbes, IN stimulated Bifidobacteriaceae, RD boosted Parabacteroides distasonis, while 2’FL specifically increased Bifidobacterium adolescentis and Anaerobutyricum hallii. In line with metabolic capabilities of these taxa, specific SCFA were produced thus providing insights that cannot be obtained in vivo where such metabolites are rapidly absorbed. Further, in contrast to using single or pooled fecal microbiota (approaches used to

circumvent low throughput of conventional models), working with 6 individual fecal microbiota enabled correlations that support mechanistic insights. Moreover, quantitative sequencing removed the noise caused by markedly increased cell densities upon prebiotic treatment, thus allowing to even rectify conclusions of previous clinical trials related to the tentative selectivity by which prebiotics modulate the gut microbiota. Counterintuitively, not the high but rather the low selectivity of IN caused only a limited number of taxa to be significantly affected. Finally, while a mucosal microbiota (enriched with Lachnospiraceae) can be integrated, other technical aspects of the SIFR® technology are a high technical reproducibility, and most importantly, a sustained similarity between the ex vivo and original in vivo microbiota. By accurately predicting in vivo results within days, the SIFR® technology can help bridge the so-called Valley of Death between preclinical and clinical research. Facilitating development of test products with better understanding of their mode of action could dramatically increase the success rate of microbiome modulating clinical trials.

9:30 Bioenergy homeostasis: Major node in holobiont's stress response model Nabarun Chakraborty, nabarun.chakraborty2.civ@health.mil, Alexander B. Lawrence, Allison Hoke, Aarti Gautam, Rasha Hammamieh. MRSB, Walter Reed Army Inst. of Research, Silver Spring, Maryland The bi-directional relationship/association between the host and its resident microbiome could be defined as the holobiont that regulates a wide range of host's health, fitness and performance. Our current understanding is that essentially, any stress challenges this relationship; and therefore, the microbiota's composition and diversity of these commensal shifts, which ultimately influences the host's psycho-physiological health. In this context, metabolites, the typical end products of any biological function within human and microbial cells alike hold key information regarding their crosstalk. Our hypothesis is that the systems analysis of the metabolite profile is linked to host and microbiome, respectively. Towards this objective, we studied both rodent and human microbiome challenged by several stressors, such as traumatic brain injury (TBI), post-traumatic stress disorder (PTSD), and radiation. Functional analysis underlined that host and microbiome synergistically fostered certain biofunctions irrespective of the stress types. For instance, existing literature found immune response as one such functional node; holistic communication between innate and adaptive immune cells and the intestinal microbiota potentially maintains the balance between immune tolerance and host inflammation. In support, our studies with PTSD and TBI models reported elevated inflammation in host's blood and brain tissues, and a concerted shift in the abundances of those fecal commensals, which were typically associated with inflammation. In addition, our studies of multiple stress models identified energy homeostasis as a key node fostered by host-microbiome crosstalk. In a rat TBI model, an energy deprived condition was accompanied by elevated abundance of Deferribacteres phylum, an anaerobic bacterium in fecal samples. In conclusion, energy homeostasis or its disruption emerged as a common theme in the stress response of functional microbiome. Restoring this functional node could be a fitting purpose of next generation therapeutic strategy.

10:05 Reference-free and ecology-based discovery of microbiome biomarkers for disease monitoring and therapeutics development Liping Zhao, liping.zhao@rutgers.edu. Biochemistry and Microbiology, Rutgers The State U. of New Jersey, New Brunswick The gut microbiome is not simply the "ome of all microbial genes" but rather the "biome of all microbes" living in the human gut. As a microbial ecosystem, the microbiome is a complex adaptive system in which strains, as the most basic building blocks, organize themselves into higher-level structures called guilds. Guilds are functional units comprising strains with diverse taxonomic backgrounds that work together to contribute to community-level emergent functions relevant to human health. Co-abundance analysis of amplicon sequence variants (ASVs) of the 16S rRNA gene or high-quality draft genomes assembled from metagenomic datasets (MAGs) can help identify key guilds whose ecological behavior correlates with host phenotypes. Distinct from taxon-based and gene-centric approaches, this strategy does not require any prior databases and can discover ecologically robust microbiome biomarkers for disease monitoring and therapeutics development.

10:50 Quantitative analysis of bile acids in complex biological matrices by UHPLC-MS/MS for the assessment of microbiome alterations Michael Gigl1, michael.gigl@tum.de, Sinah Reiter1, Andreas Dunkel2, Dirk Haller1, Corinna Dawid1, Thomas Hofmann1. (1) Technische U. Munchen, Freising, Bayern, Germany(2) Leibniz Inst. for Food Systems Biology, Freising, Germany Bile acids are steroidal end products of cholesterol metabolism that serve a central role in lipid metabolism through the formation of micelles that facilitate the absorption of lipids, lipid-soluble vitamins, and steroids. In recent years, bile acids have become increasingly associated with various diseases, including inflammatory bowel disease (IBD), cholestasis, obesity, type 2 diabetes, and cancer. Since modern bile acid quantitation methods usually only include a small number of bile acids and need elaborate sample preparation, a robust and fast high-throughput method was developed to quantify 45 bile acids simultaneously: 2 human primary, 2 murine primary, 26 secondary unconjugated, 8 taurine-conjugated and 7 glycine-conjugated bile acids. For this purpose, ultra-high performance liquid chromatography in combination with tandem mass spectrometry (UHPLC-MS/MS) was used to quantify 45 bile acids and 5 internal standards within a runtime of 22 minutes. Method validation was carried out considering the parameter recovery rate (70–112 %), intraday-, interday variation (<12 %), linearity, selectivity as well as the limit of detection (0.0012–0.3785 nmol/g), and limit of quantitation (0.0044–0.7569 nmol/g) The quantitation method was further validated successfully within an international ring trial. Application to biological matrices, such as different animal tissues, compartments of the enterohepatic and systemic circulation, showed distinct bile acid profiles. The developed method was further used in a study with Crohn's disease patients to examine the bile acid profile of patients after receiving a hematopoietic stem cell transplantation, as well as to generate bile acid profiles of germ-free IL-10-/- mice, used as a humanized model after receiving a stool transplant from IBD-patients. Quantitative analysis of comprehensive bile acid profiles with the herein described method proved to be a versatile tool to examine microbiome alterations caused by a multitude of diseases.

11:10 Bifidogenic effect of tomato seed extract on the gut microbiota demonstrates new potential for valorization of tomato waste Jenni Firrman1, jenni.firrman@ars.usda.gov, Adrienne Narrowe1, Lin Liu1, Karley Mahalak1, Johanna M. Lemons1, Pieter Van den Abbeele2, Aurélien Baudot2, Stef Deyaert2, Margaret Slavin3, Liangli Yu3, Brian Fanelli4. (1) USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania(2) Cryptobiotix SA, Ghent, Belgium(3) U. of Maryland at College Park(4) CosmosID, Germantown, Maryland Tomatoes are a popular and commonly used food globally. They are often processed to make tomato-based products, generating food waste largely comprised of skins and seeds. The current effort to valorize waste byproducts to increase sustainability and reduce agricultural loss has stimulated interest in the potential utilization of waste components as dietary, health-promoting supplements. In particular, tomato seeds contain an array of phenolic compounds that are known to have biological activity, functioning as anti-inflammatories,

antioxidants, and displaying anti-proliferative effects against cancer cells. Importantly, phenolic compounds have also been found to exert health benefits through modulation of the gut microbiota within the colon. In this study, we set out to determine how tomato seed phenolic extracts obtained from tomato waste may impact the gut microbiota of adults ex vivo over the course of 48 hours. Data obtained from six healthy individuals were compiled to identify donor-independent changes that occurred in the gut microbial community structure and short-chain fatty acid production. The results found that tomato seed phenolic extracts significantly impacted alpha diversity and increased levels of the beneficial taxa Bifidobacteriaceae. These community changes corresponded with a significant increase in total short chain fatty acids (SCFAs), specifically acetate and propionate. These results demonstrate that tomato seed phenolic extracts influence the gut microbiota in a healthy manner, which can have an overall effect on human health. The potential to incorporate these extracted compounds in supplements or to form functional foods that promote health is an innovative way to further valorize tomato waste products.

11:30 Analysis of human, soil, and wildlife microbiomes in forensic science Kelly M. Elkins, kellymelkins@hotmail.com, Jillian Malbrough, Jmalbrough@towson.edu, Constance Onyinye Ihearahu. Chemistry, Towson U., Maryland Microbial genetics and next generation sequencing (NGS) are being applied in forensic science. NGS enables analysis of samples without culture steps and its ability to perform whole genome and targeted sequencing has enabled its application to analysis of microbiomes and bacterial communities. Human, soil, and wildlife microbiomes are of interest in forensic science for connecting suspects to victims and crime scenes. The soil microbiome has been demonstrated for use in forensic analysis for geolocation. Analysis of the human microbiome from skin has been used to associate cohabiting partners. Microbiome analysis is also applied in wildlife forensics for characterizing habitats and disturbances. Forensic applications of microbiome analysis will be the focus of this talk.

Nutraceutical Lipids, Proteins and Biopeptides

8:05 Bioactive lipids and their conjugates Fereidoon Shahidi, fshahidi@mun.ca. Biochemistry, Memorial U. of Newfoundland Faculty of Science, St. John's, Newfoundland, Canada Bioactive lipids are most often highly unsaturated, especially those of the omega-3 family, and as such are also prone to oxidation. In order to extend the shelf-life of such oils and products thereof, it is important to consider the structural features as well as the minor constituents present to devise strategies for their quality preservation. In this connection, the role of minor constituents such as tocopherols, carotenoids and chlorophylls in the oils is essential. Furthermore, addition of phenolic and polyphenolic compounds has commonly been practiced to enhance oxidative stability of fats and oils. However, low lipophilicity of naturally occurring phenolics and polyphenolics may require their lipophilization to allow their use in bulk oils. Thus, their esterification to achieve this goal was attempted using a number of phenolic and polyphenolic compounds. The resultant products performed well in oxidation control and some of them exhibited unique properties and health benefits. In addition, the release of such lipophilized compounds was tested under in-vitro conditions that indicated its dependence on the fatty acids involved as well as the degree of esterification of phenolics used.

8:25 Functional lipids from food processing byproducts Boyan Gao1, raphaelgao1985@gmail.com, Hanshu Zhu1, Yinghua Luo2, Liangli Yu3, lyu5@umd.edu. (1) Shanghai Jiao Tong U., China(2) China Agricultural U., Beijing(3) U. of Maryland at College Park The triacylglycerol (TAG) compositions of blackberry, red raspberry, black raspberry, blueberry and cranberry seed oils were examined using ultra-performance convergence chromatography-quadrupole time-of-flight mass spectrometry (UPC2-QTOF MS). A total of 52, 53, 52, 59 and 58 TAGs were detected and tentatively identified from the blackberry, red raspberry, black raspberry, blueberry and cranberry seed oils, respectively, according to their accurate molecular weight in MS1 and fragment ion profiles in MS2. OLL was the most abundant TAG in the blackberry, red raspberry and black raspberry seed oils. Furthermore, the fatty acid compositions of the five berry seed oils were directly determined by GC-MS. In addition, the seed oils had the total phenolic contents ranging from 13.68-177.06 μmol GAE (gallic acid equivalent)/L oil, and significant scavenging capacities against DPPH, peroxyl, and ABTS+ radicals. These results indicated that the combination of UPC2 and QTOF MS could effectively identify and semi-quantify the TAGs compositions of the berry seed oils with sn-position information for the fatty acids. Understanding the TAGs compositions of these berry seed oils could improve the utilization of these potential high nutritional value oils for human health.

8:45 Comparison of nutritional quality of fourteen wild Linum species based on fatty acid composition, lipid health indices, and chemometric approaches revealing their nutraceutical potential Navdeep Singh Plaha1, plahanavdeep@gmail.com, Nutan Kaushik1, Sumegha Awasthi1, Mamta Singh2, Vikender Kaur2, Sapna Langyan2, Ashok Kumar2, Sanjay Kalia3. (1) Amity Food and Agriculture Foundation, Amity U., Noida, Uttar Pradesh, India(2) Indian Council of Agricultural Research- National Bureau of Plant Genetic Resources, New Delhi(3) Dept. of Biotechnology, Government of India, New Delhi Fatty acid profiles of 14 Linum species was determined by GC-MS analysis to study the nutritional quality of Linum species based on fatty acid composition, lipid health indices, and chemometric approaches. L. lewisii and L. marginale found to have the highest content of ALA i.e., 65.38% and 62.79%, respectively. However, L. tenuifolium recorded the highest linoleic acid content (69.69%), while, L. catharticum recorded highest oleic acid (27.03%). The lipid profile of Linum species could be well distinguished by two principal components (PC1 and PC2) determined by Principal Component Analysis (PCA). First principal component was composed of PA, SA, OA, SFA, MUFA and PUFA with an eigen value of 4.18, contributing to 52.27% variance. The second principal component was composed of LA and ALA with an eigen value of 2.24, accounting for 28% variance. Lipid health indices including polyunsaturated fatty acids/ saturated fatty acids, omega 6/ omega 3 fatty acids; desirable fatty acids, atherogenicity, thrombogenicity, oxididability, oxidative, hypocholesterolemic/hypercholesterolemic fatty acids, peroxidisability of wild Linum species were studied on the basis of their fatty acid profiles. Most of the Linum species recorded lipid health/nutritional indices in accordance with the recommended values. L. lewisii was identified as the superior Linum species exhibiting high pro-health values due to excellent lipid health indices. The fatty acid profiles and lipid health indices results can be used to facilitate the selection of Linum species for further nutraceutical applications with high economic value. Interestingly, L. hudsonioides was found to have lipid profile similar to sunflower oil, which may be a key finding of this study and require further research on its thermal stability, shelf life and possible applications in cooking.

9:05 Lipids as a source of flavors Keith R. Cadwallader, cadwlldr@illinois.edu. Food Sci. and Human Nutrition, U. of Illinois Urbana-Champaign Flavor is the main determinant of food quality and acceptance. Lipids play an important role in flavor development and in sensory perception through flavor modulation. Triglycerides and their constituent fatty acids can degrade to form a range of flavor active substances via lipolysis, autoxidation and

thermal degradation. This discussion will focus on the reactions responsible for the formation of potent odorants from lipid components. Emphasis will be placed on the sensory-directed analytical approaches used for the identification and quantitation of some common and less common lipid derived potent odorants.

9:45 Extraction and measurement of total lipids in fresh royal jelly samples: Comparison of several methods Weiqiang Zhang, weiqiang.zhang@usda.gov, Amy Ray, Giovanni Tundo, Pierre Lau, Yu-Cheng Zhu. Pollinator Health in Southern Crop Ecosystem Research Unit, USDA-ARS Southeast Area, Stoneville, Mississippi Royal Jelly (RJ) is a honey bee dietary secretion for developing bees and has exceptional biological properties used in many industries. Several methods have been reported to extract total lipids from RJ; however, no standardized method is available. This study investigated the extraction efficiency of several solvent combinations, including chloroform/methanol (C/M: 1:1, 2:1, 1:2, v/v%) and diethyl ether followed by methanol, and measured the purity of resulting lipid fractions using Folch and sulfo-phospho-vanillin (SPV) methods. We also tested the possibility of using SPV to measure total lipids content in RJ directly. Our data showed that (1) RJ samples were difficult to mix with diethyl ether. C/M combinations mixed well with RJ. (2) Increasing methanol levels in C/M combinations produced lipid fractions with higher yield but less purity. Total lipids levels were 11±0.65%, 16.8±0.19%, and 17.5±0.14% using C/M 2:1, 1:1, and 1:2, respectively (n =3), and, by the inclusion of a purification step with water washing, the levels were 4.2±0.8% and 1.7±0.6% using C/M 1:1 and 1:2, respectively (n =3). It was difficult to separate layers when C/M 2:1 was used. (3) SPV direct measurement of RJ using olive oil as the standard gave total lipids level of 1.42% (±0.21, n=4), which seemed to under-estimate total lipids levels and indicated a need to identify more suitable standards which closely mimic the lipid compositions of RJ. Our study could help prepare samples for lipidomics studies of RJ and other biological samples and develop simpler methods to determine total lipids content in biological samples.

10:05 Quantification of Chemical compounds of Linseed and their health benefits Sumegha Awasthi, awasthisumegha24@gmail.com, Nutan Kaushik, Navdeep Singh Plaha. Amity Food and Agriculture Foundation, Amity U., Noida, Uttar Pradesh, India Different geographical areas of the globe cultivate oilseed crops that are used for their edible oils. Given the rising global population and diminishing supply of fossil fuels, these edible oils have significant uses as biofuels and commercial bio products. Linseed being one of the major oilseed crops has been used as a high-value-added raw material for commercial and food applications. Due to its ability to prevent non-communicable diseases and the cooperative actions of its bioactive molecules, linseed has attracted more notice as a significant functional food. Linseed has been reported to have 28% of dietary fibres, 6% of carbs, 1% lignans, 21-23% of proteins, and 4% of ash. Due to its extremely high oil concentration (30–45%), both edible and non-edible industrial oils can be produced from it. Numerous health advantages are attributable to the significant physiologically active components of linseed, including ALA, dietary fiber, and phenolic compounds like lignan-Secoisolariciresinol diglycoside (SDG). Linseed has been reported as a significant source of compounds for human anticancer and anti-atherosclerosis prophylaxis and an alternative antibiotic against pathogenic microbes. Thus, we conducted a study on 10 different Indian linseed varieties to analyse these compounds such as fatty acid, lignan, and amino acids. Varieties with highest (53.61%) and lowest (1.69%) ALA content was recorded.

10:25 Sensoproteomics discovery of taste-active and DPP-IV inhibitory peptides in quinoa Magdalena Holzer1, magdalena.holzer@tum.de, Verena K. Mittermeier1, Tabea Kröber2, Roland Kerpes2, Thomas Becker2, Corinna Dawid1. (1) Chair of Food Chemistry and Molecular Sensory Science, Technische Universitat Munchen, Munich, Germany(2) Chair of Brewing and Beverage Technology, Technische Universitat Munchen, Munich, Germany Diabetes mellitus is one of the most widespread diseases in the 21st century. According to the International Diabetes Federation, diabetes currently affects 537 million people and is expected to increase to 783 million patients worldwide by 2045. Several studies have shown that selective peptides from different (pseudo-)cereals inhibit the enzyme dipeptidyl peptidase IV (DPP-IV). DPP-IV cleaves and subsequently inactivates incretins such as glucose-dependent insulinotropic polypeptide (GIP) and glucagon-like peptide-1 (GLP-1), thereby decreasing insulin secretion by pancreatic beta cells. Hence, DPP IV inhibition is essential for insulin secretion in the human body, especially for patients of type 2 diabetes. Absorption of these inhibitory peptides occurs in the small intestine, and their inhibitory potential depends on both protein hydrolysis and gastrointestinal digestion. This study aimed to isolate and identify naturally occurring DPP-IV inhibitory peptides in quinoa hydrolysates using a bioactivity-guided approach. Moreover, the influence of DPP-IV inhibitory peptides on the overall taste was investigated to develop a food with antidiabetic properties in future. Quinoa exhibited DPP-IV inhibition activity upon treatment by enzymatic hydrolysis. Fractionation of the quinoa hydrolysate by ultrafiltration and preparative HPLC combined with DPP-IV inhibition and human sensory experiments led to the identification of several unknown DPP-IV inhibitory and taste-active peptides. Subsequently, a robust, rapid, and selective UHPLC-MS/MS method was developed to quantify these peptides in various foods. In addition, the antidiabetic potential of the bioactive peptides and their corresponding IC50 were measured using a DPP-IV inhibition assay. Based on these results, cereal processing and breeding strategies may be further optimized to enhance the levels of DPP-IV inhibitory peptides and to modify the taste to design a food with antidiabetic properties for the treatment of type 2 diabetes mellitus in future.

10:45 Selection of qPCR reference gene for human colon cancer cells in cottonseed bioactive research Heping Cao, heping.cao@usda.gov, Kandan Sethumadhavan. Southern Regional Research Center, USDA Agricultural Research Service, New Orleans, Louisiana Cottonseed value can be increased by providing high-value bioactive molecules such as polyphenols for improving nutrition and health. However, there was little molecular evidence for cottonseed bioactivity in mammalian cells. Quantitative real-time-PCR (qPCR) is one widely used method for bioactivity study of natural products. It is a crucial task of qPCR data analysis using stably expressed internal reference genes. The hypothesis for reference gene selection is that a lower standard deviation of the cycle of threshold (Cq) among the treatments indicates a more stable expression of the gene. The objective of this study was to select reference genes in human colon cancer cells (COLO 205) treated with gossypol and bioactive extracts from cottonseed along with bacterial endotoxin lipopolysaccharides (LPS). SYBR Green qPCR analyzed a wide range of biomarkers at the mRNA levels involved in glucose transport, lipid biosynthesis, inflammatory response, and cancer development. 10,560 Cq values were generated from qPCR assay from 55 genes analyzed from 64 treatments with triplicate per treatment for each gene. The qPCR data showed that B-cell lymphoma 2 (Bcl2) mRNA was the most stable expressed gene among the 55 mRNAs analyzed in the human colon cancer cells. The commonly used glyceraldehyde 3 phosphate dehydrogenase (Gapdh) and ribosome protein L32 (Rpl32) mRNAs were not good qPCR references for the cells. These observations were consistent

regardless of the treatment comparison between gossypol and LPS, glanded and glandless seed extracts, seed coat and kernel extracts, or treatment for 8 and 24 h. The results suggest that Bcl2 is a preferable reference gene for qPCR assays in human colon cancer cells treated with cottonseed-derived gossypol and bioactive extracts as well as LPS. The qPCR results strongly support the conclusion that the Bcl2 gene is stably expressed at the mRNA level in the human colon cancer cells regardless of the treatment, suggesting that Bcl2 gene expression is not regulated at the mRNA level but at the post-transcriptional level. These results should facilitate studies designated to evaluate bioactivity on gene expression regulation by cottonseed molecules and other natural and synthetic molecules for nutrition and health uses.

Virtual Session - Bioproducts from Biomass

10:05 Hydrophobic modification of arabinoxylan for improving emulsifying properties Brajendra Sharma1, Brajendra.Sharma@usda.gov, Madhav P. Yadav1, Atanu Biswas2, H.N. Cheng3. (1) USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania(2) USDA-ARS National Center for Agricultural Utilization Research, Peoria, Illinois(3) USDA-ARS Southern Regional Research Center, New Orleans, Louisiana, US Arabinoxylans isolated from corn bran were modified using two different succinic anhydride derivatives to impart hydrophobicity to their structures. The optimum reaction conditions (time, pH, ratio of reactants) for reacting arabinoxylans with octenyl succinic anhydride were established. The reaction products were purified through dialysis, lyophilized, and characterized using FTIR, NMR, and TGA. FT-IR spectra of the reaction product showed the characteristic absorption peak at 1722-1728 cm-1 for the ester carbonyl groups. The NMR spectra of the reaction product confirm the reaction. The titration method was used to determine the degree of substitution on various products. Some of the products with varying degrees of substitution were evaluated for their emulsification properties. The stabilization of oil-in-water emulsions was investigated by preparing the emulsions with a high-pressure homogenizer and measuring the particle size distribution using a laser diffraction particle size analyzer as a function of time. The emulsions prepared using modified arabinoxylan showed superior emulsifying abilities, such as smaller particle size compared to the unmodified one. These findings should benefit beverage industries in producing a high-quality emulsifier from the low-value byproducts of corn grain milling.

10:25 Evaluation of sugar yields from biomass pretreated with alkaline solution from absorption of recovered CO2 Valerie Garcia-Negron, valerie.garcianegron@usda.gov, Matthew J. Toht. SBCP, USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania The continuing need for fuels and climate concerns require fossil fuel alternatives that are sustainable and energy-efficient. Therefore, optimizing the conversion of biomass into biofuels is key towards achieving this goal. This work evaluates the effects of chemical pretreatments and the conversion of lignocellulosic biomass into fermentable sugars for potential conversion into biofuels or value-added products. Corn stover, an agricultural waste residue, was pretreated with 2.2 M Na2CO3 produced from CO2 captured via absorption of a 5 M NaOH solution. Composition analysis of pretreated corn stover exhibited high cellulose content (40.96%) and less lignin (16.50%) compared to the untreated counterpart. The sugar release from hydrolysis was evaluated with 2:1 and 3:1 CTec2-to-HTec2 enzyme ratios and at interval times up to 72 h. The pretreated biomass produced higher and more stable glucose yields than the untreated samples, reaching 90% yields after 24 h with the cellulase-rich enzyme solution. FTIR-ATR detected changes in the chemical structure due to the presence of cellulose and lignin-related absorption bands. These results clearly indicate pretreatments promoted biomass conversion and improved the performance of enzyme digestibility.

10:45 Assay-guided isolation, structural elucidation, and action mechanisms of anti-inflammatory compounds in papaya leaves Yujia Cao1, yujia.cao@u.nus.edu, Xiang Wang1, Dejian Huang1,2. (1) Food Sci. and Tech., National U. of Singapore(2) Food Sci. and Tech., NUS Suzhou Research Inst., Jiangsu, China Carica papaya leaves have long been used as vegetable and folk herbal tea for effective treatment of dengue fever, a tropical inflammatory condition caused by virus infection via mosquitoes, but the scientific principle was not clear. To fill the research gap, we utilized cell-based assay as guide in rapid fractionation and identification of the anti-inflammatory phytochemicals. Fresh papaya leaves juice was extracted with hexane, diethyl ether, ethyl acetate, n-butanol sequentially and tested their nitrite oxide (NO) inhibitory effects on lipopolysaccharides (LPS)-stimulated murine macrophage RAW 264.7 cell line. Compound identification was carried out using analytical techniques including liquid chromatography hybrid quadrupole time-of-flight mass spectrometry (LC-qToF-MS) and nuclear magnetic resonance (NMR). Some flavonoids and alkaloids unique to papaya leaves were identified in papaya leaves. Biochanin A which is an isoflavone was found as the main compounds in the final active fractions and were likely to be responsible for the anti-inflammatory effects of papaya leaves. The action mechanisms of the biochanin A and its structural analogue acacetin were comparatively investigated by transcriptome analysis. Molecular biology methods such as Western blotting and reverse transcription polymerase chain reaction (RT-PCR) were employed for pathway confirmation. Our work help paving the molecular foundation of papaya leaves as potential functional food for controlling inflammation caused by dengue fever virus.

11:05 Counteracting roles of lipidic aldehydes and isoflavone antioxidants on soy protein oxidation revealed by chemometric survey of solvent and mechanically extracted soybean meals Junwei Zhang1, zhan8011@umn.edu, Pedro E. Urriola2, Seth L. Naeve3, Gerald C. Shurson2, Chi Chen1,2. (1) Food Sci. and Nutrition, U. of Minnesota Twin Cities, Minneapolis(2) Animal Science, U. of Minnesota Twin Cities, Minneapolis(3) Agronomy and Plant Genetics, U. of Minnesota Twin Cities, Minneapolis Soybean meal (SBM) is a premier source of protein for feeding production animals. Protein oxidation negatively affects the nutritional value of SBM, but its causative associations with soybean oil extraction methods and non-protein components in SBM were not well examined. In the current study, 40 solvent extracted SBMs (SSBM) and 8 mechanically extracted SBMs (MSBM) collected from different commercial producers and geographic locations were profiled by chemometric analysis. The results showed that the extraction methods led to diverse differences between SSBM and MSBM. In gross composition, SSBM had greater crude protein, ash, moisture, and water activity while MSBM had greater crude fat and crude fiber. In protein oxidation, MSBM had greater protein carbonyl contents than SSBM (9.2 vs 5.2 mmol/kg protein, $p<0.0001$). In lipid oxidation, MSBM also had greater p-anisidine values than SSBM (1.25 vs 0.48, $p<0.001$), and more lipidic aldehydes, including 2-hexenal, 2-heptenal, 2,4-heptadienal, octanal, 2-octenal, 2-decenal, and nonanal. In antioxidant status, SSBM had greater Trolox equivalent antioxidant capacity (TEAC) than MSBM (25.0 vs 23.6 μmol/g, $p<0.0001$), which was in consistent with the total phenolics content (1.17 vs 0.86 mg caffeic acid equivalent/g, $p<0.0001$) and the total content of isoflavones, including genistin, genistein, daidzin, and daidzein (2147.0 vs 1481.8 μg/g, $p<0.0001$). Interestingly, MSBM had greater contents of tocopherols, including α- and g-tocopherol, than MSBM due to higher residual oil content. Pearson correlation

analysis showed that protein carbonyl content was positively correlated with the p-anisidine value and total aldehydes, but inversely correlated with the TEAC value. Among antioxidants, total phenolics and isoflavones contents had inverse correlations with protein carbonyl content, total aldehydes, and p-anisidine value, respectively. Overall, extraction methods significantly affected gross composition, oxidation, and antioxidant status of SBMs. Lipidic aldehydes and phenolic antioxidants play counteracting roles in the oxidation of soy protein.

11:35 Biochemical analysis of polysaccharides from Indian ginseng, Withania somnifera Syed Badshah, sbadshah@asu.edu. Chemistry, Islamia College Peshawar, Khyber Pakhtunkhwa, Pakistan Withania somnifera is an important medicinal herb in the Ayurvedic system. Many secondary metabolites extracted from the plant showed pharmacological properties. In the present work, polysaccharides were extracted from the roots and seeds of W. somnifera, via hot water extraction and ethanol precipitation. These water-soluble polysaccharides had major typical functional groups when characterized by FTIR, including hydroxyl (OH), methylene (CH) and, carboxylic (COOH) groups, as well as pyranose. NMR data of the seeds revealed mannose and glucose residues in the backbone and the side chains, showing that it is glucomannan. The roots showed GalpA and Rhap in the backbone, while Galp and Arabf residues were present in sidechains, suggesting pectin-like RG-1 polysaccharides. Scanning electron microscopy (SEM) revealed that root and seed polysaccharides had different surface topologies at various magnifications. XRD data revealed that the polysaccharides are semi-crystalline. The polysaccharides did not show antibacterial and anticancer activity, as there were no zone of inhibition and less percent inhibition of U87 cancer cells. Further future bioassays will help in revealing their medicinal potential.

11:55 Green synthesized trimetallic (Cu/Ni/Co) oxide nanoparticles used to enhance rice straw and pressmud based vermimanure quality: Growth performance of Abelmoschus esculentus Shalu Yadav, shalooyadav777@gmail.com, Praveen K. Srivastava, Abhay K. Choubey. Sciences and Humanities, Rajiv Gandhi Inst. of Petroleum Technology, Jais, Uttar Pradesh, India Vermimanure composed of trimetallic (Cu/Ni/Co) oxide nanoparticles (TmONs) synthesized using Moringa oleifera leaves extract is utilized as eco-friendly soil additive for increasing crop yields. The research was conducted in producing rice straw and pressmud based vermimanure and sustainable nanovermimanure (NV) employing TmONs as a catalyst to evaluate the growth performance of A. esculentus. Characterization of the material was performed using various analytical tools like FTIR, XRD, XPS, FESEM-EDX and TEM. The nitrogen, phosphorous and potassium content in blended vermimanures were found significantly ($P < 0.05$) increased by 26%, 20% and 72% respectively over the initial raw materials used as feedstock. Synergetic approach of synthesized vermimanure remarkably ($P < 0.05$) increased seed germination, co-efficient velocity, and vigour index by 167%, 67% and 95% respectively while mean germination time was decreased by 41% as compared to untreated vermimanure. Agri based NVs shown positive effects and no toxic impact on seed germination.

TUESDAY AFTERNOON

Award for the Advancement of Application of Agricultural and Food Chemistry in honor of Liangli (Lucy) Yu

2:05 Decoding chemosensory systems for flavor innovations Thomas Hofmann, thomas.hofmann@wzw.tum.de. Technische U. Munchen, Bayern, Germany The presentation will a review on recent developments on deciphering the complex chemical signatures of food taste.

2:35 Factors affecting the formation of process contaminants and transfer of toxic elements to food and beverages Lauren Jackson, Lauren.Jackson@fda.hhs.gov. Division of Food Processing Science & Technology, U.S. FDA, Bedford Park, Illinois Although processing generally improves the quality and safety of foods, it can decrease nutrient levels and bioavailability and produce chemical and physical changes that result in the formation or transfer of toxic compounds to food. Process-induced toxic compounds such as acrylamide, furan, 3-monochloropropane-1,2-diol (MCPD), and glycidyl esters and have gained international media attention over the past several decades. In addition, there has been concern over the presence of elevated levels of toxic elements (arsenic, lead, cadmium) in food and beverages, and efforts are currently underway to identify ways to reduce dietary exposure to these contaminants to as low as possible especially in infants and young children. Acrylamide and furan are formed during thermal processing of carbohydrate-rich foods, while MCPD and glycidyl esters are chemical contaminants found in refined edible vegetable oils and processed foods containing these oils. Juices, wine and beer can contain elevated levels of toxic elements due transfer of these contaminants from filtering aids used to clarify these beverages. This presentation will summarize key research studies conducted by FDA to evaluate the factors and conditions resulting in the formation of process contaminants in food and transfer of toxic elements to beverages. Understanding the chemical transformations and transfers that occur during food processing will lead to strategies for minimizing the presence of chemical contaminants in foods and beverages.

3:05 Nutraceutical properties of soybeans Margaret Slavin1,2, mms@umd.edu. (1) Nutri. and Food Sci., U. of Maryland at College Park(2) Nutri. and Food Studies, George Mason U., Fairfax, Virginia Soybeans are an important agricultural crop globally with manifold applications in foods and diverse influences on health. This talk will review the awardee's contributions to the field through advancing knowledge of soy nutraceutical properties, ranging from phytochemicals to traditional nutrients and oils. Discussion of the impact of the work will be oriented in the context of public health resulting from deepened chemical understanding of a staple crop.

3:55 Food, food function and human health Thomas Wang, tom.wang@usda.gov, Quynhchi Pham. Diet, Genomics and Immunology Lab., USDA-ARS Beltsville Human Nutrition Research Center, Beltsville, Maryland Diet plays an important role in the human health. However, it remains unclear what in the food that's good for you, when is good for you, how or why is good for you as well as who is good for. We targeted the questions of what's in the food that's good for you and how or why food is good for you. We also tackled issues such as effects of growing condition on bioactive composition in the food. The following describe some examples of our recent efforts. Using rodent diet-induced obesity model, we demonstrated that cooked rice with different resistant starch level modulate obesity related risk factors and modulate the gut microbiome. Employing a rodent model of Citrobacter rodentium infection, a pathogenic E coli-like infection, we identified cruciferous vegetables-derived indoles may be protective against infection. The indoles appeared to act through prevention of bacterial attachment as well as modulating host immune responses. Additionally, we also identified growing condition may impact bioactive components profiles in brassica microgreens. Overall, the research efforts contribute to 1) the understanding of how food may influence physiology, disease prevention. 2) elucidate the mechanisms of action; as well as 3) what environment can do to the composition of a food.

4:25 Bioactive food factors, and their health beneficial and toxic

effects Liangli Yu, lyu5@umd.edu. Dept. of Nutri. and Food Sci., U. of Maryland at College Park Bioactive food factors including nutraceuticals and food processing-induced toxicants play a critical role in human health. Our recent research showed that clove and cinnamon are rich in nutraceuticals which may suppress the binding of SARS-CoV-2 virus spike protein to angiotensin-converting enzyme 2 (ACE2) on host cells, reduce the ACE2 availability and decrease the oxidative stress and possibly the inflammation to possibly reduce the risk of SARS-CoV-2 virus infection and the development of severe COVID-19 symptoms. Our research also showed that wheat grain, soybean, spices, edible oil seeds and edible botanicals are rich in health beneficial components, and may reduce the risk of several aging associated health problems such as obesity and cardiovascular diseases. In addition, our research discovered the chemical mechanisms involved in the processing-induced formation of food toxins such as 3-MCPD fatty acid esters, as well as their toxicology.

Sustainable Agriceuticals

2:03 Capsinoids enriched extract from Capsicum sp. fruit and its associated pharmacological activities Charles L. Cantrell1, charles.cantrell@usda.gov, Robert L. Jarret2, Hee-Sung Chae3, Alexander Andersohn4, Sean P. Marrelli4, Shabana Khan3. (1) USDA-ARS Natural Products Utilization Research Unit, U., Mississippi(2) USDA-ARS Plant Genetic Resources Conservation Unit, Griffin, Georgia(3) National Center for Natural Products Research, U., Mississippi(4) Dept. of Neurology, The U. of Texas Health Science Center at Houston John P and Katherine G McGovern Medical School Capsinoids, the nonpungent analogs of capsaicinoids, are present in the fruit of many Capsicum species and genotypes - typically at low concentrations. Recently, a method to efficiently extract and purify capsinoids from Capsicum annuum fruit has been published and patented. A critical step in this process is the unique liquid/liquid extraction procedure that utilizes a pentane crude extract, and acetonitrile as the extraction solvent, to provide capsinoids of 45.7 % (wt/wt) purity. A >90 % capsinoids-enriched product can also be accomplished in bulk using an hp20ss resin system. A series of pharmacological studies utilizing these enriched capsinoid extracts and pure capsiate have been completed and used to investigate the effects of capsinoids on nuclear factor erythroid 2–related factor 2 (NRF2), peroxisome proliferator-activated receptors alpha and gamma (PPARα and PPARγ), liver X receptor (LXR), glucose uptake, and lipid accumulation in relevant cellular models. This study revealed the multiple nuclear receptors agonistic action and glucose uptake-enhancing properties of capsiate, and also its antiadipogenic effect, indicating its potential in preventing the undesired adipogenic effects of full PPARγ agonists such as the glitazone class of antidiabetic drugs. In a related study, it was hypothesized that capsinoids – non-pungent agonists of the transient receptor potential vanilloid 1 (TRPV1) channel – would activate vagal afferents, triggering thermoregulatory regions of the brain to induce mechanisms of whole-body cooling, protecting the brain, and preventing injury progression after a stroke. This study demonstrated that capsinoid extract delivered to TRPV1-containing visceral afferents promoted reversible mild hypothermia in freely moving conscious mice. These and other pharmacological studies utilizing enriched capsinoid extracts will be discussed.

2:33 Effects of high hydrostatic pressure pretreatments of orange peel on pectin extraction, structural and functional properties of the extracted pectin Wei Zhao1, wei.zhao@usda.gov, Yixiang Xu2, Christina Dorado1, Hoa K. Chau3, Arland T. Hotchkiss3, Randall G. Cameron1. (1) USDA-ARS, US Horticultural Research Laboratory, Fort Pierce, Florida(2) USDA-ARS, Western Regional Research Center, Albany, California(3) USDA-ARS, Eastern Regional Research Center, Wyndmoor, Pennsylvania Orange peel is rich in pectin, a complex polysaccharide widely used in the food and pharmaceutical industries due to its gelling, thickening, and stabilizing properties. Pectin functionalities can be tailored by modifying its structure through various processing techniques. High hydrostatic pressure (HHP) technology, a non-thermal food processing technique, has been successfully used for shelf-life extension and structural modifications. This study explored the use of HHP to aid pectin extraction and modify the structure of pectin. Juice-extracted orange peel from a local commercial juice plant was treated with HHP at different pressures and durations, followed by pectin extraction. The effects of HHP treatments on pectin yield, structure, and functional properties of the extracted pectin were examined. HHP treatments were found to increase pectin yield by 41%. The molecular weight of the extracted pectins ranged from 362 kDa to 443 kDa, which is ideal for a commercial pectin. Compared to the controls (pectin extracted mimicking the commercial process), the HHP-treated samples had a higher degree of blockiness, galacturonic acid content, and pectin backbone linearity; but a lower degree of methyl-esterification, neutral sugar content and degree of branching, and smaller particle size. The results of functionality analyses showed that pectins extracted from HHP-treated peel generated stronger, more stable, and more elastic calcium gels than the control pectins. HHP treatment also increased pectin water solubility and water holding capacity at certain pressure and duration conditions. The study indicates HHP treatment of orange peel is a promising approach to increasing pectin yield and improving functional properties of the extracted pectin.

2:53 Evaluation of grape marc from different varieties as potential sustainable agriceuticals Xueqi Li, spsli@ucdavis.edu, Selina Wang. Food Sci. and Tech., U. of California Davis Sustainable agriceuticals enable the idea of incorporating bioactive-compound-rich byproducts from the agriculture sector into food system to obtain desirable sensory attributes in foodstuffs and enhance human health. As California produces nearly 4 million tons of world-class wine annually, the byproduct grape marc generated during the production is substantial. Despite the progress on new environmental policies and strategies to drive more sustainable byproduct management in the food and agriculture sector, the wine industry is still relying heavily on conventional composting and animal feed for byproduct utilization. Our study indicated red and white grape marc are rich sources of phenolic compounds. Specifically, grape marc from white varieties chardonnay and sauvignon blanc and red varieties pinot noir and merlot from the Los Carneros AVA in California showed promising values in antioxidant capacity analyses DPPH and FRAP as well as high concentrations in 1) flavan-3-ols (+)-catechin and (-)-epicatechin; 2) phenolic acids gallic acid and vanillic acid; 3) flavonols rutin and myricetin; and 4) quercetin-3-glucoside and kaempferol-3-glucoside. In addition, extractable proanthocyanidins (EPA) that are immediately available for absorption by human body, and non-extractable proanthocyanidins (NEPA) that are bound to fibers but can reach the colon for bacterial metabolism which has been shown to be beneficial to gut health, are presented in high levels in grape marc ranging from 88 to 141 mg/g for EPA and 33 to 46 mg/g for NEPA, respectively. Dietary recommendations have promoted the inclusion of plant-based natural products that grape marc could potentially play an important role in which not only adds more economic values to an underutilized byproduct but also helps push the forefront of sustainable agriceuticals.

3:13 Wine grape seed waste improves brain health of mice on high-fat diets Hanna Lee1, Christina Tam2, Priscila Alves1, Barbara Shukitt-Hale3, Wallace H. Yokoyama1, wally.yokoyama@ars.usda.gov. (1) Healthy Processed Foods Research, USDA, Washington, California(2) Foodborne Toxin

Detection and Prevention, USDA, Albany, California(3) HNRCA, USDA, Boston, Massachusetts Agricultural waste presents significant challenges to the environment and economy worldwide, with up to 43% of[HL1] fruits, vegetables, and fish lost as waste in the US and other countries. Middle-aged mice were fed high-fat diets supplemented with grape seed extract or grape seed flour. Our results demonstrated that supplementation could attenuate high-fat induced metabolic dysregulation, including insulin resistance and hypercholesterolemia. Additionally, we observed significant cognitive improvements in the Morris Water Maze test, where mice supplemented with grape seed extract on a high-fat diet took significantly less time and swimming distance to reach the target zone, indicating improved hippocampal-dependent spatial learning and memory. Furthermore, the Novel Object Recognition test showed an increased discrimination index, which is a measure of recognition memory involving the perirhinal cortex and hippocampus. To gain insight into the molecular mechanisms underlying these improvements, we explored global RNA expression profiles in the hippocampus and adipose tissues. Our findings suggest that upcycling grape seed waste holds great promise for improving metabolic and brain health.

3:43 Hesperetin modulates gut microbiota, and attenuates bleomycin-induced pulmonary fibrosis Ping Li, ping-biology@outlook.com, Xia Meng, Zihao Zhang, Yingjie Huang. College of Food Sci. and Biotechnology, Zhejiang Gongshang U., Hangzhou, China Hesperetin is a dietary flavonoid widely found in plants with various physiological activities, however, whether it can regulate gut microbiota is not well understood. By a simulated human intestinal model, hesperetin was found to have a positive effect on human intestinal microecology, as evidenced by a significant increase in the relative abundance of Lactobacillus and the Lachnospiraceae-ND3007-group, and production of butyrate and acetate in the fermentation system. To investigate the potential of hesperitin to alleviate bleomycin induced pulmonary fibrosis by regulating intestinal microbiota. In vivo, the bleomycin induced overexpression of inflammatory cytokines (α-sma and collagen I) and weakening of pulmonary motility (MMEF and VT) in the lung of mice. We found that the degree of pulmonary fibrosis gradually decreased with increasing hesperitin dose. Meanwhile, hesperitin dietary interventions can significantly inhibit the proliferation of Staphylococcus, and promote the growth of Clostridia UCG-014. Our study delineated the regulatory effects of hesperetin on the gut microbiota, and provide scientific evidence to support the development of hesperitin as a dietary supplement for inhibit pulmonary fibrosis.

4:13 Dietary macronutrients determine the pathological process of alcoholic liver disease Songtao Li, lisongtao@zcmu.edu.cn, Jiaomei Li, Rui Guo, Qinchao Ding, Jiannan Qiu. College of Public Health, Zhejiang Chinese Medical U., Hangzhou, Zhejiang Excessive alcohol consumption is widely recognized as a major social and health problem worldwide, which leads to about 5.9% of all deaths worldwide annually, and is positively associated with multiple disorders and diseases, among which, alcoholic liver disease (ALD) has become one of the most serious health issues globally, accounting for 47.9% of all liver cirrhosis deaths and 30% of all hepatocellular carcinoma deaths. The spectrum of ALD ranges from steatosis, steatohepatitis, characterized with hepatocyte cell death and immune cell activation and infiltration, to fibrosis/cirrhosis, even HCC. Malnutrition caused by excessive alcohol intake is one of the pathological mechanisms of ALD; on the other hand, dietary nutrients are highly associated with the pathological development of ALD. Here, we observed that high protein diet significantly attenuated chronic alcohol consumption induced hepatic steatosis and liver injury in mice. Interestingly, although high fat diet has been shown to induce hepatic steatosis in mice, it significantly reduced liver damage in our ALD mouse model. Low-carbohydrate diet prevented liver injury in ALD model. Additionally, dietary lipid components are also closely related to ALD. Our result showed that monounsaturated fatty acid-enriched olive oil and camellia oil exacerbated chronic alcohol-induced hepatic steatosis when compared with that in polyunsaturated fatty acid-enriched corn oil-fed mice liver. While saturated fatty acid-enriched palm oil protected ALD when compared to corn oil. These results indicated that dietary macronutrients determine the pathological process of ALD. Reasonable dietary choices among drinkers may have a positive effect on the prevention and treatment of alcoholic liver disease.

4:33 Improved anti-colitis activity of Faecalibactrium prausnitzii by incorprated in a riboflavin conjugated alginate based delivery system Mingfei Yao, mingfei@zju.edu.cn, Bo Qiu, Lanjuan Li. Zhejiang U., Hangzhou, China Next generation probiotics (NGPs) are potential live biotherapeutics to treat various diseases. Faecalibactrium prausnitzii is one of the most important butyrate-producing NGPs and have been proved to ameliorate colonic inflammation diseases. However, NGPs are strictly anaerobic and susceptible to harsh conditions, which limit their further applications. In this study, we developed a layer-by-layer delivery system to incorporate F. prausnitzii ATCC27766 cells with glycol chitosan and riboflavin conjugated alginate as wall materials, where riboflavin is an antioxidant for F. prausnitzii. The results showed that the resistance of F. prausnitzii to oxygen was prolonged. Moreover, the viability of the cells in the simulated gastric acid and bile acids also enhanced, and significant more cells adhered to the intestinal monolayer through an in vitro Caco-2 and HT29-MTX monolayer model. The encapsulated F. prausnitzii colonized in the colon of germ-free model faster and more sustainable than the non-encapsulated ones. The study also showed that encapsulated F. prausnitzii obviously reduced colonic histological injury and alleviated inflammation in DSS induced colitis mouse model, with a higher ratio of Firmicutes/ Bacteroidates compared to the disease model group, which should attribute to the increased colonization of F. prausnitzii in the colon, since significant higher level of butyrate level was identified in the colonic content. In addition, we found higher abundance of F. prausnitzii was associated with increased secondary bile acids in DSS induced colitis mice. This study of encapsulating F. prausnitzii by riboflavin conjugated materials provided important strategy for further application of F. prausnitzii in clinic.

4:53 Extracting bioactive phytochemicals and macronutrients from agriculture waste and food processing side streams: Simple solutions to complex global problems on food security, aging population, and sustainability Dejian Huang, fsthdj@nus.edu.sg, Joanne y. Toy, Xin Yang, Bernice Hui Yi Neo, Yi Lin. National U. of Singapore Sustainable development, nutritional insecurity, and aging are three of the many challenges of human society. In this talk I will illustate, by using hree research projects we have been working on, that effective and scalable methods to reclaim phytochemicals and macronutrients such as proteins and fibre from side-stream of agri-food industry could provide simple solution to these problems. Firstly, spent grains in brewing industry and bioethanol industry are depleted with startch yet rich in proteins and fiber. We utilized a simple protess to reclaim the proteins and fiber from spent barley grains (generated in beer brewing process) for making starchless noodle as functional foods for controlling blood glucose level after meal. Moreover, zein was isolated from dried distillers' grains with solubles (DDGS) and applied as ink materials for 3D printing of high precision scaffolds for 3D cell and meat culture use. Furthermore, phytochemicals such as luteolin and resin glycosides

extracted from peanut shell and sweet potato stems and leaves could be developed into bioactive constituents that have potential for nutraceutical use in combating diabetes and obesity.

5:13 Rapid photocrosslinking α-LAMA hydrogels biomaterial to facilitate wound healing Yaqing Huang, 1024927323@qq.com, Qinchao Zhu, Davi Ren. Zhejiang U. Inst. of Dairy Science, Hangzhou, Zhejiang, China As the skin is the largest organ in the human body, skin damages have always been considered as one of the most common physical injuries. Accelerating wound healing and improving its rate is an urgent issue requiring a solution. Due to its suitable characteristics, hydrogels are widely utilized for this purpose. In this study, we present a mile-derived α-lactalbumin (α-LA) as a new kind of natural protein-based biomaterial. The α-LA was methacrylated to generate a photocrosslinkable material. The physicochemical properties of α-LAMA hydrogels were investigated by morphology, swelling properties, degradability, cytocompatibility and toxicity properties. This photomediated system rapidly crosslinked α-LAMA (<1 min), allowing 3D printing of constructs with high resolution features, in the range of 50-100 μm. In vivo evaluation of the α-LAMA hydrogels showed promising biocompatibility. Finally, the therapeutic function of α-LAMA hydrogels was evaluated in the full-thickness dermal wound in a mice model. Our results indicated that α-LAMA hydrogels had better wound closure than the control group. In a word, this study shows photomediated system to produce α-LAMA hydrogels, and this material can be used to treat skin injuries in humans.

ACS Microbiome Consortium Kick off Symposium

2:05 Stress and the gut-brain axis in military health Rasha Hammamieh, rasha.hammamieh1.civ@health.mil, Aarti Gautam, Nabarun Chakraborty. Walter Reed Army Inst. of Research, Silver Spring, Maryland The gut-brain axis is a bidirectional communication pathway between the gut and the brain that plays an important role in regulating many physiological and psychological processes, including stress. Stress can affect the gut microbiome, which can in turn affect the gut-brain axis. Stress can disrupt the balance of the gut microbiome, leading to a decrease in beneficial bacteria and an increase in harmful bacteria. This disruption can lead to increased intestinal permeability, which can allow harmful bacteria and toxins to enter the bloodstream and potentially affect brain function. The gut microbiome communicates with the brain through several mechanisms including the production of neurotransmitters and other signaling molecules that can cross the blood-brain barrier and affect brain function, including stress and anxiety levels. For example, the gut provides approximately 95% of total body serotonin, the neurotransmitter which is important for central nervous system development and function. Alterations of the composition of the gut microbiome are potentially associated with pathophysiology of diseased states, including autism, anxiety, stress, major depressive disorder, irritable bowel syndrome, and bipolar disorder. In addition, specific classes of microbiota-derived metabolites, have been implicated in the pathogenesis of multiple disorders. We have been assessing the gut-brain axis in response to battlefield like stressors including psychological and physiological stress such as post-traumatic stress, sleep restriction, traumatic brain injury and exposure to austere conditions. Our studies show the essential role the gut microbiome plays in the host response to the different stressors, and interventions aimed at promoting a healthy gut microbiome may have the potential to improve stress resilience and reduce the risk of stress-related disorders. Interventions aimed at promoting a healthy gut microbiome, such as probiotics and prebiotics, have been shown to improve stress resilience and reduce stress-related symptoms in animal and human studies. These interventions may work by restoring the balance of the gut microbiome, reducing intestinal permeability, and modulating immune function and neurotransmitter production. Overall, the gut-brain axis plays an important role in the stress response, and interventions aimed at promoting a healthy gut microbiome may have the potential to improve stress resilience and reduce the risk of stress-related disorders.

2:50 SRS-FISH: A high-throughput platform linking microbiome metabolism to identity at the single cell level
Ji-Xin Cheng, jxcheng@bu.edu. Boston U., Massachusetts One of the biggest challenges in microbiome research is to better understand functional properties of microbial community members at a single cell level. Single cell isotope probing has become a key tool for this purpose, but the current detection methods for determination of isotope incorporation into single cells do not allow high-throughput analyses. Here, we report on the development of an imaging-based approach termed stimulated Raman scattering - two-photon fluorescence in situ hybridization (SRS-FISH) for high-throughput function-identity analysis of microbial communities with single cell resolution. SRS-FISH offers an imaging speed of 10 to 100 milliseconds per cell, which is two to three orders of magnitude faster than achievable by state-of-the-art methods. Using this technique, we delineated metabolic responses of thirty thousand individual cells to various mucosal sugars in the human gut microbiome via incorporation of deuterium from heavy water as an activity marker. Application of SRS-FISH to investigate the utilization of host-derived nutrients by two major human gut microbiome taxa revealed that response to mucosal sugars tends to be dominated by Bacteroidales, with an unexpected finding that Clostridia can outperform Bacteroidales at foraging fucose.

3:10 Differential modulatory effects of kale microgreen and mature kale on the gut microbiome Thomas Wang1, tom.wang@usda.gov, Adrienne Narrowe4, Quynhchi Pham1, Jiawei Wan2, Liangli Yu2, Yaguang Luo3, Tianbao Yang3, Lin Liu4. (1) Diet, Genomics and Immunology lab., USDA-ARS Beltsville Human Nutrition Research Center, Beltsville, Maryland(2) Dept. of Nutri. and Food Sci., U. of Maryland at College Park(3) Food Quality Lab, USDA Agricultural Research Service, Beltsville, Maryland(4) ERRC, USDA Agricultural Research Service, Wyndmoor, Pennsylvania Interest in healthy living lifestyles has promoted the emergence of many new purported healthy foods, such as microgreens, in the market. Microgreens are young vegetables, different from baby greens and sprouts, harvested ~7-21 days after the cotyledon leaves appeared. However, relatively less is known of the health benefit of microgreens and this warrants further elucidation. Recent advances also indicate modulation of the gut microbiome may contribute to health effects in human. The literature on the effects of kale microgreen as well as mature kale on the gut microbiome remain scarce. In this study, the effects of kale (Darkibor variety) microgreen and its mature counterpart on the gut microbiome were examined to provide science-based information for the emerging new food. Using a mouse model of diet-induced obesity, animals (C57BL mice) were fed with diets contain low fat (10%, LF)) or high fat (45%, HF), supplemented with or without Kale microgreen (KMG) or mature kale (MK) in the perspective diet matrix for 8 weeks. After feeding, cecal content was harvested and subject to 16S rRNA amplicon sequencing followed by bioinformatic analysis. Consumption of KMG and KG significantly attenuated HF diet induced weight gain in mice. Consumption of KMG or MK leads to changes of alpha and beta-diversity in the gut microbiome. However, MK was less effective in modulating the alpha diversity in a low fat matrix. Further analysis also identified as a potential biomarker, an unidentified Ruminococcus species, to be correlated with KMG and MK consumption in both low fat and high matrix. Overall, our results support modulatory effect of consuming kale microgreen on the gut microbiome which appeared to be different

from the effects exerted by MK; and diet matrix may also influence manifestation of an effect exerted by vegetables.

3:30 Microbiome assessment of diet and stress effects in rodent models of brain insults Aarti Gautam1, aarti.gautam.civ@health.mil, James DeMar1, Nabarun Chakraborty1, Matthew Rusling1, Allison Hoke1, Franco Rossetti2, Donna Wilder2, Joseph Long2, Marti Jett3, Rasha Hammamieh1. (1) Medical Readiness Systems Biology, Walter Reed Army Inst. of Research, Silver Spring, Maryland(2) Blast-Induced Neurotrauma Branch, Walter Reed Army Inst. of Research, Silver Spring, Maryland(3) Headquarters, Walter Reed Army Inst. of Research, Silver Spring, Maryland Traumatic neurological insults, such as traumatic brain injury (TBI) or post-traumatic stress disorder (PTSD), can occur in combat operations as well as in training, are multifactorial in nature, and can be major career limiting factors for US Soldiers. Although studies have examined the association of these disorders both by themselves and together with sociodemographic features, as well as psychiatric and medical comorbidities, the impact of these disorders by real-world dietary practices has not been thoroughly characterized. Thus, we are exploring the possibility that an omega-3 polyunsaturated fatty acid poor diet increases the vulnerability to TBI and PTSD, as this nutrient is essential for proper neuronal cell function. Likewise, we recognize that nutritional countermeasures will be potentially a safe and readily translatable approach to alleviating TBI and PTSD-related debilitations. Adult male rats were anesthetized and subjected to a closed-head TBI model and in parallel, another group was subjected to an acute model for instigating the early stages of PTSD development consisting of a single exposure to an underwater trauma (UWT) psychological stressor. Prior to trauma, animals were maintained on either a standard house chow diet or a customized one that was deficient in omega-3s and increased in pro-inflammatory omega-6 content. Microbiome evaluations were completed using 16S ribosomal RNA sequencing on fecal samples. Our findings showed that TBI exposure, within 14 days, produced significant neurobehavioral impairments that are associated with neuropathological changes. Likewise, UWT exposure produced aberrant behaviors, brain neuronal cell alterations and systemic endocrine imbalances. Diet played a significant role in microbiome composition irrespective of the trauma. Omega-3 deficiency predisposes the rats to significant decreases in microbiome diversity following both TBI and UWT. The taxonomic phylogenetic profiles linked to TBI and UWT exposure were distinct from their corresponding shams. Correlation analysis of taxa individually on behavioral and pathophysiological outcomes was also performed. Overall, our findings suggest that poor dietary conditions can markedly influence the vulnerability or resilience of the Warfighter to TBI and PTSD. Of great interest, it is known from the work of others that microbiome imbalances similar to what we observed can disrupt the normal hormone communications between the gut and healthy brain.

4:00 Relationship between functional components of agricultural products and the gut microbiome in several human intervention studies Masuko Kobori, kobori@affrc.go.jp. Inst. of Food Research, National Agriculture and Food Research Organization, Tsukuba, Ibaraki, Japan Recent prospective cohort studies have shown a positive relationship between the Japanese-style diet and health in Japan. We have conducted a systematic literature review and showed that the Japanese-style diet or the characteristic Japanese food reduces cardiovascular disease mortality. The result also showed that increasing the intake of vegetables and fruits and complementary ingestion of soy products, and so on, is essential for further reducing the cardiovascular disease mortality risk for Japanese. Moreover, the health function of vegetables and soy products can be adopted to a healthy personalized diet. We conducted human intervention trials and showed that poly-gamma-glutamic acid of the Japanese fermented soy product Natto suppressed the elevation of postprandial blood glucose levels and quercetin of onions suppressed age-related cognitive decline. These food components are known to affect gut microbiomes. The relationship between the intake of these food components and the gut microbiome is under investigation.

4:20 Taking a closer look: What we can learn by incorporating food type into analyses of fiber-microbe relationships Mary Kable1,2, mary.kable@usda.gov. (1) Immunity and Disease Prevention, USDA, Agricultural Research Service, Davis, California(2) Nutrition, U. of California Davis Some characteristics of the foods we eat, which are important influences on gut microbiota, are unmeasured or left unreported in standard dietary databases. This presentation will focus on a recently published analysis, conducted to capture relationships between gut microbiota composition and unmeasured aspects of food. Dietary data collected from 343 healthy adults in Automated Self-Administered 24hr recall questionnaires were edited to a tree format. The tree structure was annotated with the average total grams of dry weight, fat, protein, carbohydrate, or fiber from each food item reported and the UniFrac distance metric was used to understand the relatedness of individual diet patterns. Diversity measurements, calculated using the tree structure, were analyzed relative to the microbial community diversity, determined by a Quantitative Insights Into Microbial Ecology (QIIME) 2 analysis of the bacterial 16S ribosomal RNA V4 region, sequenced from stool samples. Hypotheses that were generated by identifying diet-microbe relationships in this study are currently being investigated using in vitro fermentations.

4:40 Impact of three traditional Chinese herbal extracts on the human gut microbiome Johanna M. Lemons[1], johanna.lemons@usda.gov, Adrienne Narrowe[1], Lin Liu[1], Jenni Firrman[1], Karley Mahalak[1], Pieter Van den Abbeele[2], Aurélien Baudot[2], Stef Deyaert[2], Margaret Slavin[3], Liangli Yu[3]. (1) Dairy and Functional Foods, USDA Agricultural Research Service, Wyndmoor, Pennsylvania(2) Cryptobiotix SA, Ghent, Belgium(3) Dept. of Nutri. and Food Sci., U. of Maryland at College Park There is a long history of utilizing plants for their medicinal properties. In traditional Chinese medicine, the root of Atractylodes macrocephala Koidz (Baizhu), the leaves of Isatis indigotica Fort. (Daqingye) and the bark of Albizia julibrissin Durazz (Hehuan) are prized for their palliative effects. While these plants have been used for centuries, modern researchers are still exploring the biological and chemical mechanisms responsible for their effects. Much of this research has described the impact of purified chemicals or mixed extracts from these plants on cells in tissue culture or in rodent models, but few have explored the effect on the human gut microbiome. In this study, we assessed the individual effects of carbohydrate-free ethanol extracts of Baizhu, Daquingye and Hehuan on the human gut microbiome via short-term incubation in Systemic Intestinal Fermentation Research (SIFR®) bioreactors, which enable ex vivo fermentation of extracts by donor fecal samples (n=6). Fermentation markers including pH, gases, and short chain fatty acids (SCFAs) were measured throughout the 48-hour incubation and flow cytometry was used to quantify bacterial cell counts. Bacterial community structure and functional potential was characterized using shotgun metagenomic sequencing after incubation with each of the extracts and compared to a no substrate control. Each of these medicinal extracts elicited very different responses from the bacterial community. Baizhu resulted in a bloom of several Bifidobacteriaceae which is consistent with the observed increase in SCFAs, increase in overall bacterial cell counts and slightly lowered alpha diversity. Daquingye showed limited effect

on bacterial community compared to no treatment but still promoted microbial fermentation as measured by pH and SCFA production. Hehuan resulted in slightly lower cell counts, but overall large changes in the functional potential of the bacterial community. While all orally consumed medicinal plants are processed through the human digestive tract their effects on the gut microbiome are unique. Further investigation into the interactions between these extracts and the gut microbiome may yield a better understanding of how they exert their varied effects on circulation, digestive health, mood, immunity, and metabolism.

5:00 Broad-spectrum antimicrobial triclosan and the gut microbiome Karley Mahalak1, karley.mahalak@usda.gov, Lin Liu1, Jenni Firrman1, Adrienne Narrowe1, Lillian Chau2, Elliot S. Friedman2, Lindsay Herman2, Gary D. Wu2. (1) Dairy and Functional Foods RU, US Dept. of Agriculture, Wyndmoor, Pennsylvania(2) Division of Gastroenterology, U. of Pennsylvania Perelman School of Medicine, Philadelphia Triclosan is an antimicrobial agent that was in widespread use for decades until its ban in 2016 for use in consumer soaps due to concerns about its impact on the environment and human health. More recently, it has also been reported that triclosan can exacerbate colonic disease in mouse models, with speculation this is due to its effect on the gut microbiota, in part because inflammation was not found to occur with TCS treatment in germ-free mice. To understand the impact of triclosan on the gut microbiota, we performed a study using a TripleSHIME® in vitro model of the human gut microbiota, with 2, 1-week cycles of triclosan treatment, followed by a washout period. Using metagenomics and targeted metabolomics, we determined that while treatment with triclosan significantly decreased the gut microbial community in terms of population levels, diversity, and metabolite production, a 2-week recovery period allowed these effects to be reversed, indicating that removal of triclosan could result in a reversal of its harmful effects. Following this finding, we performed an experiment using healthy mice, treated them with triclosan for 4 weeks, followed by 4 weeks of washout. Colonic tissue histology and 16S tagged sequencing analysis of the gut microbiome from the fecal samples, showed that treatment of mice with 80ppm triclosan did not induce an inflammatory response in the colonic tissue in contrast to previous reports, nor did this treatment significantly change the composition of the gut microbiota. This finding indicates that the in vitro modeling of triclosan's effects on the gut microbiota does not reproduce the effects observed in mice where no significant effect on fecal microbiota composition was observed. Additionally, since there was no effect on gut health of mice, our results do not support that triclosan is harmful to gut health.

5:20 Degradation of food-grade λ-carrageenan by human gut microbiota: Potential adverse effect Xiaojing Guo, xiaojingguo0131@gmail.com, Yanhui Han, Zhenjun Zhu, Pongpol Thanuphol, Hang Xiao. Food Sci., U. of Massachusetts Amherst Carrageenans (CGN) are large linear sulfated polysaccharides extracted from seaweeds and have been widely applied in the food industry as a emulsifier, stabilizer and thicker. However, there is a controversy over CGN safety as the field is re-evaluating if CGN can be degraded in vivo, especially the potential degradation by gut microbiota. To resolve this controversy, selected culture medium with food grade CGN as the sole carbon source was used to screen CGN-degrading bacteria (from human fecal samples) under anerobic circumstance. Our results showed the degradation of food grade CGN by purified bacteria colony, as indicated by the significant decrease of pH and total carbohydrate, and the increase of SCFA. Thin layer chromatography and HPLC data suggested the presence of degrade-CGN in culture medium. Moreover, the bacteria was identified as Bacteroides xylanisolvens, via 16s rDNA sequencing and whole genome sequencing. Furthermore, cell culture study suggested the proinflammatory effect of degrade-CGN, as the fermentation supernatants promoted the production of nitric oxide and the pro-inflammatory cytokines. In summary, food-grade CGN can be broken down into degrade-CGN by gut microbiota, e.g. Bacteroides xylanisolvens, and its potential risks to human health are deserved further investigation.

5:40 Identification of a human gut bacterial strain with anti-inflammatory potential in gastrointestinal tract Yukun Sun, yukunsun@umass.edu, Min Gu, Hang Xiao. Food Sci., U. of Massachusetts Amherst The human body is an ecosystem that hosts a variety of microorganisms and a majority of those are colonized in the human gastrointestinal tract (GIT). Some of these microbes are considered probiotics, showing beneficial health effects. We isolated a strain of probiotics from the feces of healthy male adults which was identified as Bifidobacterium pseudocatenulatum UMA14 based on the whole genome sequencing. To determine the potential health effects, the bacterial secretion of the strain was subjected to cell culture models to establish the potential anti-inflammatory effect. The results showed that the bacterial secretion inhibited inflammatory response in lipopolysaccharide (LPS)-stimulated RAW 264.7 macrophages. Moreover, oral administration of Bifidobacterium pseudocatenulatum UMA14 alleviated the severity of colonic inflammation in dextran sulfate sodium (DSS)-treated CD-1 mice, which was evidenced by decreased disease activity index (DAI), enhanced structural integrity of colon, and improved organ index. The histological analysis illustrated that the abundance of pro-inflammatory immune cells in colonic mucosa were reduced, accompanied with the modulated mRNA levels and the suppression overproduction of pro-inflammatory cytokines such as interferon-gamma (IFN)-γ, tumor necrosis factor (TNF)-α, interleukin (IL)-1β, and IL-6. Overall, our results demonstrated the potential anti-inflammatory effects of Bifidobacterium pseudocatenulatum UMA14 in both in vitro and in vivo models, which provided a foundation for further development of a novel anti-inflammatory probiotic.

Virtual Session - Nutraceutical Lipids, Proteins and Biopeptides

3:05 Structure-function of the Plant-specific insert: A natural antimicrobial domain Rickey Yada1, rickey.yada@gmail.com, Lennie K. Cheung1, Brian C. Bryksa7, John H. Dupuis1, Jenny J. Tian1, Prasenjit Baumik5, Alexander Wlodawer6, Xiaoli Zhao4, Ruxi Qi8, Xiaomin Ma8, Shenlin Wang2,3. (1) Land and Food Systems, The U. of British Columbia, Vancouver, Canada(2) East China U. of Science and Tech., Shanghai, China(3) Peking U., Beijing, China(4) Shandong Polytechnic, Jinan, China(5) Indian Inst. of Technology Bombay, Mumbai, Maharashtra(6) National Cancer Inst. Center for Cancer Research, Bethesda, Maryland(7) U. of Guelph, Ontario, Canada(8) Southern U. of Science and Tech., Shenzhen, Guangdong, China Many plant aspartic proteases contain an additional sequence of approximately 100 amino acids termed the plant-specific insert which is involved in host defense and vacuolar targeting. The mode of action of action is thought to function via protein-membrane interactions, however, the specific nature of plant-specific insert (PSI) mediated membrane disruption has remained relatively elusive. In attempts to elucidate the mechanism, our laboratory has utilized various biophysical techniques ranging from NMR to fluorescence all aided by molecular modeling. The crystal structure of the PSI domain from a potato aspartic protease at a resolution of 1.9 Angstroms, and it was observed that dimerization and adoption of an open, active conformation at acidic pH were prerequisites of potent fusogenic and vesicle leakage activity. Comparison of recombinant PSI domains from different crops revealed remarkably different structural features and protein-membrane bilayer interactions, despite sharing high sequence similarity. In particular, the potato

PSI exhibited five times higher membrane leakage activity and distinct fusogenic activity. The helical domains of the potato PSI reached at most 4% of that of the complete PSI, highlighting that the overall PSI structure is essential for native functionality. The integral roles of positively-charged and hydrophobic residues for initial membrane contact and subsequent membrane anchoring, respectively, were subsequently characterized using in silico site-directed mutagenesis, the insights of which were used to rationally design PSI with adjustable fusogenic activity.The presentation will discuss an overview of our results obtained to date. Such results will aid in the development of successful strategies regarding microbial attack of plant material, and possibly human maladies such as cancer.

3:25 Quantitative structure-activity relationship modelling of penta- and hexapeptide inhibitors of islet amyloid polypeptide fibrillation Raliat Abioye1, rabio069@uottawa.ca, Judith Oballa2, Monica Delgado Martinez2, Rotimi Aluko3, Chibuike Udenigwe2,1. (1) Dept. of Chemistry and Biomolecular Sciences, U. of Ottawa Faculty of Science, Ontario, Canada(2) School of Nutrition Sciences, U. of Ottawa Faculty of Health Sciences, Ontario, Canada(3) Dept. of Food and Human Nutritional Sciences, U. of Manitoba Faculty of Agricultural and Food Sci, Winnipeg, Canada Bioactive peptides have demonstrated promising anti-islet amyloid polypeptide (IAPP) fibrillation activities via diverse mechanisms. However, their structure-activity relationship is only speculated and not well understood. Furthermore, ambiguity still exists regarding the importance of non-covalent interactions, such as π-π and hydrophobic interactions, in IAPP self-assembly and thus in the anti-fibrillation activity of peptides. In this study, multivariate data analysis of peptides was performed using partial least squares (PLS) regression modeling to understand the structural requirements of food peptides for anti-fibrillation activity. A random library of peptides (n = 30) derived from yellow pea protein was evaluated for in vitro anti-fibrillation activity, which was taken to be the Y-matrix. Then, 16 different descriptors were used to develop the X-matrix of the peptides that showed anti-fibrillation activity. PLS models were then validated via cross-validation and the most significance was observed when the parent list was subdivided by peptide chain length into penta- and hexapeptides. The 3-z scale, Kidera Factors, FASGAI, and VSW descriptors returned significant models with high R2 (0.95-0.997) and Q2 values (0.134-0.892), hence their selection for further analysis. Extraction of the variable importance for the projection (VIP) and coefficients plot identified position-based features that contributed to or diminished anti-fibrillation activity. Furthermore, comparison between features of significance revealed the effect of peptide chain length on bioactivity. For example, α-helical preference and hydrophobicity of internal amino acid residues (n3 and n4) of pentapeptides positively contributed to anti-fibrillation activity. Moreover, the β-structure preference of C-terminal amino acids (n6) positively contributed to the activity of hexapeptides, but bend structure preference at n2 influenced this activity negatively. Additionally, the n4 and n2 positions largely contributed to the activity of pentapeptides and hexapeptides, respectively. Taken together, these findings provide a novel perspective on anti-fibrillation inhibitors and the interplay between amino acid features and position within the peptides on the bioactivity. Findings can be used to promote rational development of novel anti-diabetic peptides with anti-fibrillation mechanism.

3:45 Structure, assembly and applications of peanut oil body proteins Yijun Pan, Qingrong Huang, qhuang@sebs.rutgers.edu. Food Sci., Rutgers The State U. of New Jersey, New Brunswick Oil bodies (OBs), which are found mainly in the seeds or nuts of oleaginous plants, are spherical droplets with a triacylglycerol core covered by a phospholipid-protein layer. Oil body protein extracts (OBPEs), mainly oleosins, contribute to the unique physicochemical stability of OBs. The application of OBPEs in an aqueous environment has been greatly limited by their highly hydrophobic structures. In this study, OBPEs were successfully extracted from peanut seeds, and their profiles were characterized by LC-MS/MS. OBPEs nanoparticles were successfully assembled in an aqueous environment for the first time using the antisolvent precipitation method. The mean diameter of OBPEs nanoparticles was 215.6 ± 1.8 nm with a polydispersity index of 0.238 ± 0.005. The morphology of these colloidal particles was found to be roughly spherical shape as confirmed by transmission electron microscopy (TEM). Oil-in-water (O/W) Pickering emulsions with good stability against coalescence could be formed at protein concentrations as low as 0.1 mg/mL. Cryo-scanning electron microscopy (cryo-SEM) confirmed that spherical nanoparticles were packed at the oil–water interface. Oil body proteins were also used to prepare Pickering emulsions loaded with nobiletin, one of the major components in orange peels. The TNO dynamic gastrointestinal model-1 (TIM-1) results indicated that nobiletin had a higher in vitro bioaccessibility in oil body protein nanoparticles -stabilized Pickering than in oil suspension. This research will greatly expand the applications of OBPEs in structuring the interfaces and developing novel formulations in the food and pharmaceutical fields.

4:05 Structure-function properties of peptides with dual inhibitory activity against acetylcholinesterase and butyrylcholinesterase Rotimi Aluko1, rotimi.aluko@umanitoba.ca, Nancy Asen1, Chibuike Udenigwe2. (1) Food and Human Nutritional Sciences, U. of Manitoba, Winnipeg, Canada(2) U. of Ottawa, Ontario, Canada Acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) are two critical enzymes involved in the onset and progression of neurodegenerative diseases, especially Alzheimer's and other types of dementia. In this work, we determined the quantitative structure-activity relationships of tetrapeptides with dual inhibition of AChE and BuChE activities based on a dataset consisting of 19 tetrapeptides and pentapeptides identified from the enzymatic digests of yellow field pea protein. Using partial least square regression (PLS) analysis and amino acid 5-z scores, a 9-component model was created from 16 pentapeptides for AChE-inhibitory peptides (Q2 = 67.2%, R2 = 0.9974) while three datasets were prepared for BuChE inhibitory peptides to improve quality of the models (Q2 = 26.7 – 46.4%, R2 = 0.9577 – 0.9958). Using the AChE and BuChE PLS models, 1231 and 483 new peptides were predicted, respectively. The models showed that the most potent peptides were dominated by polar, slightly polar, and neutral amino acids (i.e., valine, proline, aspartic acid, threonine, alanine, arginine, and leucine). The predicted cholinesterase-inhibitory peptides with lower IC50 values than the training sets have amino acid residues threonine, leucine, alanine, and valine at the N-terminal, asparagine, histidine, proline, and arginine at the second position, aspartic acid, and serine at the third and arginine at the C-terminal. Cross validation of the models showed validity and robustness while experimental validation of the most active predicted peptides revealed low prediction errors. We conclude that availability of these new and highly potent AChE and BuChE inhibitory amino acid sequences could facilitate the development of peptide tools suitable for therapeutic management of Alzheimer's disease and related neurodegenerative disorders.

4:45 Food proteins in the prevention of osteoporosis Jianping Wu, jwu3@ualberta.ca. U. of Alberta, Edmonton, Canada Osteoporosis is a skeletal disorder characterized by a systemic impairment of bone mass, strength, and microarchitecture, resulting in increased bone fragility and risk of facture, particularly of the hip, spine, wrist and shoulder. Osteoporotic fracture contributes significantly to functional decline, increased morbidity and mortality, and increased

healthcare spending. Osteoporotic fracture affects at least one in three women and one in five men during their lifetime, costing annually to the Canadian healthcare over $2.3 billion. Dietary proteins are key nutrients for bone health, and in the prevention of osteoporosis. Dietary proteins contain bioactive proteins such as milk basic proteins, lactoferrin etc that can suppress bone resorption and promote bone formation, thus improving bone health and preventing osteoporosis. Our recent study reported that ovotransferrin, an iron-binding glycoprotein from egg white, significantly stimulated osteoblast differentiation and osteoprotegerin (OPG), while inhibited the level of receptor activator of nuclear factor kappa-B (RANKL), indicating its potential role on regulating osteoclast. Using ovariectomized (OVX) rats, a widely used model to mimic menopausal-induced osteoporosis, oral administration for 12-week at 1% (w/w, ovotransferrin/diet) significantly preserved OVX-induced loss of bone mineral density and deterioration of trabecular micro-architecture. Additionally, ovotransferrin administration suppressed the overactive bone remodeling by inhibiting osteoclastogenesis and osteoclastic bone resorption, while exerting considerable positive influence in bone formation. Ovotransferrin also inhibited marrow adipogenesis, modulated immune function (both systemic and local), and enhanced the formation of short-chain fatty acids in the gut. This study demonstrated the potential of ovotransferrin as a function food ingredient in the prevention of osteoporosis.

5:05 Bioactive peptides with antioxidant and DPP-IV inhibitory activity extracted from bones by-products Gisela Carrera-Alvarado, Leticia Mora, Fidel Toldra, ftoldra@iata.csic.es. Instituto de Agroquímica y Tecnología de Alimentos (CSIC), Paterna, Valencia, Spain Animal bones constitute an interesting protein source for the sustainable production of bioactive compounds. Depending on the type of peptidases used for hydrolysis, bones may experience a more or less intense hydrolysis of collagen with the release of large amounts of diverse bioactive peptides with different lengths. The purpose of this work was to determine the potential generation of bioactive peptides from bones by-products having antioxidant and DPP IV inhibitory activity with potential benefits for health. Bones were defatted and crushed to powder and then pretreated during 3 h with pepsin (PEP) at 37°C and pH 3.6 to improve the further accessibility of peptidases to target sites. Then, pretreated bones were sequentially hydrolyzed for 2 h with Alcalase (PA) at 65°C and pH 8.0, and Alcalase and Protana Prime (PAPP) for 12 h at 60°C and pH 6.8. Antioxidant activity was assayed using DPPH radical scavenging activity, Ferric reducing antioxidant power and ABTS radical scavenging assay, and the hypoglycemic activity was assayed measuring DPP-IV inhibitory activity. Peptides were analyzed using a nanoESI qQTOF 6600 plus TripleTOF mass spectrometer (ABSCIEX), where peptides were ionized in a Nano Optiflow by applying 3.0 kV to the spray emitter at 200 °C. The obtained degrees of hydrolysis were 23.41%, 35.36% and 68.38% for PEP, PA, and PAPP, respectively. The amount of released free amino acids was also progressively increased, reaching 54.62, 88.12, and 668.46 mg/100 mL hydrolyzate, respectively. The generated peptides were identified by LC-MS/MS resulting in a total of 550 peptides identified in PEP, 1087 in PA, and 1124 in PAPP. The highest antioxidant and DPP-IV inhibitory activities were obtained with the PAPP hydrolyzate while the AP hydrolyzate gave intermediate values. In summary, the results confirm that pepsin pretreatment followed by further hydrolysis with peptidases like Alcalase and Protana Prime can constitute an effective method for the sustainable use of bone sources in the production of antioxidant and hypoglycemic bioactive peptides.

5:25 Valorisation of surimi processing by-products and formulation of value-added product (Ready to cook protein enriched soup mix) Asha Kumari1, kumariasha9019@gmail.com, Nutan Kaushik1, Rasa Slizyte2, Khushboo .1. (1) Amity Food and Agricultural Foundation, Amity U., Noida, Uttar Pradesh, India(2) SINTEF, Trondheim, Norway In this modern era convenient food products are emerging objective of food processing industries. These food products include ready to cook and ready to eat/drink products. Soup is one of such value-added food products that is made by blending ingredient such as meat, vegetables with various other ingredients. Fish are important source of animal protein and Omega-3-polyunsaturated fatty acids (EPA –eicosapentanoeic acids and DHA-decosahexanoic acids) which has many health benefits. In this study Pink Perch (Nemipterus japonicus) head & viscera which are generated as by-products during surimi processing are used for extraction of protein hydrolysates through enzymatic hydrolysis. The Pink Perch head & viscera protein hydrolysates are having moderate antioxidant activity (24.8%) and high essential amino acids content (35%) are further microencapsulated by using different wall material (maltodextrin, gum arabic, sodium alginates and carboxyl methyl cellulose) to lower the fishy odour and bitter taste of protein hydrolysates. The microencapsulated protein hydrolysates were used for preparation of Ready to Cook protein rich soup powder. The Ready to Cook protein rich soup powder was prepared by blending microencapsulated protein hydrolysates with vegetables (beans & carrot), starch, milk solid, species and salt. The Physio-chemical and sensory analysis of Ready to Cook soup powder was conducted and observed that microencapsulated soup powder contains approximately high amount of protein content (approximately 15%) with acceptable aroma and taste. These Ready to Cook soup powder can be potential alternative food for the protein deficient peoples.

5:45 Optimizing gelatin from pink perch skin and bones and its application in development of ready-to-cook chicken meatballs Khushboo .1, khushboo14@s.amity.edu, Nutan Kaushik1, Kristina Widell2, Rasa Slizyte2, Asha Kumari1. (1) Amity Food and Agriculture Foundation, Amity U., Noida, Uttar Pradesh, India(2) Fisheries and New Biomarine Industry, SINTEF Ocean, Trondheim, Norway Rapid growth of fish processing has resulted in increasing quantities of waste. It is estimated that fish processing waste after filleting accounts for approximately 75% of the total fish weight. Global fish waste is estimated to be approximately 100 mMT, and more than 4 mMT in India. These wastes are dumped, buried, used for landfilling, or incinerated, increasing environmental hazards, pollution, and threat to public health and increasing greenhouse gas emissions. These wastes are inexpensive sources of amino acids and protein, underlining their potential to be used as food, animal feed and fertilizer. The objective of this work was to extract gelatin from industrial sample of pink perch skin and bones, and further, optimize of gelatin extraction process by Response Surface Methodology (RSM) to maximize yield along with quality. Yield and L-hydroxyproline content obtained at optimal conditions were 16.2% and 41.62 mg/g respectively. The gelatin exhibited thermo-reversible properties, with gel strength of 251 g. The extracted gelatin was used to develop low-fat ready-to-cook (RTC) chicken meatballs. Meatballs were prepared with different concentrations of fish gelatin (3%, 4%, 5%, and 6%). The effect of fish gelatin content on the physicochemical, cooking, textural, and sensory properties of meatballs was investigated. Furthermore, the shelf-life of meatballs was also been studied. Compared to control and brand-name meatballs, adding fish gelatin to meatballs reduced fat content by 67.2% and79.7%, and protein content increased by 20.1% and66.4%, respectively. Compared to control meatballs, adding fish gelatin also reduced hardness by 26.4% and increased yield and moisture retention in RTC meat balls by 15.4% and 20.9%, respectively. Sensory analysis suggests that adding 5% fish gelatin in meatballs has the highest acceptance among all tested treatments.

The storage study indicated that the addition of fish gelatin to RTC meatballs delayed lipid oxidation both in refrigeration and in freezing storage. The results indicate that pink perch gelatin can be used as a fat substitute in chicken meatballs and potentially increase their shelf life.

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5:35 Development of method for simultaneously determining 11 triterpene alcohols and analysis of their characteristics in camellia oil Yonglin Li, 807144819@qq.com, Yaoyao Dong, Yuan Gao, Qi Li, Xiuzhu Yu. Engineering Research Center of Grain and Oil Functionalized Processing U. of Shaanxi Province, College of Food Sci. and Eng., Northwest A&F U., Yangling, Shaanxi, China Triterpene alcohol with a series of bioactivities is an important minor compound in camellia oil. Thus, determination and characterization of triterpene alcohol in camellia oil are essential to develop bioactivity of camellia oil. Herein, a method that simultaneously determines 11 triterpene alcohols was developed and validated; samples of different production areas and oil processing methods were determined, and the storage and thermal stability of triterpene alcohol were characterized. Results showed that the proposed method had good sensitivity, accuracy, precision, and robustness, with linearity, LOD, LOQ, spike recovery, and RSD of 0.9964–0.9989, 0.14–5.53 mg/kg, 0.45–18.44 mg/kg, 82.90%–108.51%, and 4.38%–12.69%, respectively. Oils processed with low press flux, cold press, and aqueous extraction had high triterpene alcohol contents. As for stability, although triterpene alcohol would fluctuate like sterol, they were stable during storage and degraded during heating. Our study can be used as reference for triterpene alcohol determination and development of functional oil containing triterpene alcohol.

5:45 Dynamics of composition, structure, and metabolism of three energy substances in flaxseed (Linum usitatissimum L.) during germination Yaoyao Dong, yaoyaodong@nwafu.edu.cn, Qi Li, Yuan Gao, Xiuzhu Yu. Northwest A&F U., Yangling, Shaanxi, China The composition and structure changes of three energy substances (protein, lipid, and sugar) and minerals during flaxseed germination were investigated. Na, Ca, Fe, and total free amino acids fluctuating increased and peaked at 7 d. Oil and linolenic acid contents increased initially and reached the maximal increment by 14.8% and 1.4% ($p < 0.05$) at 2 d, after which it declined. Soluble sugar mainly consisted of sucrose (50.47%–72.77%), glucose, and fructose during germination. Semi-cylindrical depression was enhanced on flaxseed granule surface, and oil bodies distribution from relatively uniform toward cell wall during 0–2 d. Protein order and stability were varied firstly, then grew steadily at 4–7 d and peaked at 7 d. Metabolic sequence (sugar, protein, and lipid) and related tricarboxylic acid pathway were proposed. Conclusively, germinated flaxseed at 2 and 4 d had higher physicochemical and structural properties, which could serve as high-quality resources for lipid and protein processing respectively.

5:55 SlRBP1 promotes translational efficiency via SleIF4A2 to maintain chloroplast function in tomato Liqun Ma, lqma@cau.edu.cn, Hongliang Zhu. The College of Food Sci. and Nutritional Eng., China Agricultural U., Beijing Many glycine-rich RNA-binding proteins (GR-RBPs) have critical functions in RNA processing and metabolism. Here, we describe a role for the tomato (Solanum lycopersicum) GR-RBP SlRBP1 in regulating mRNA translation. We found that SlRBP1 knockdown mutants (slrbp1) displayed reduced accumulation of total chlorophyll and impaired chloroplast ultrastructure. These phenotypes were accompanied by deregulation of the levels of numerous key transcripts associated with chloroplast functions in slrbp1. Furthermore, native RNA immunoprecipitation-sequencing (nRIP-seq) recovered 61 SlRBP1-associated RNAs, most of which are involved in photosynthesis. SlRBP1 binding to selected target RNAs was validated by nRIP-qPCR. Intriguingly, the accumulation of proteins encoded by SlRBP1-bound transcripts, but not the mRNAs themselves, was reduced in slrbp1 mutants. Polysome profiling followed by RT-qPCR assays indicated that the polysome occupancy of target RNAs was lower in slrbp1 plants than in wild-type. Furthermore, SlRBP1 interacted with the eukaryotic translation initiation factor SleIF4A2. Silencing of SlRBP1 significantly reduced SleIF4A2 binding to SlRBP1-target RNAs. Taking these observations together, we propose that SlRBP1 binds to and channels RNAs onto the SleIF4A2 translation initiation complex and promotes the translation of its target RNAs to regulate chloroplast functions.

6:10 Recent advances on the stability of anthocyanins regarding the interaction with food proteins and polysaccharides Zhihuan Zang, 302810541@qq.com, Bin Li. Shenyang Agricultural U., China The health benefits of anthocyanins are compromised by their chemical instability and susceptibility to external stress. Researchers found that the interaction between anthocyanins and macromolecular components such as proteins and polysaccharides substantially determined the stability of anthocyanins during food processing and storage. The topic thus has attracted much attention in recent years. This report underlines the new insights gained in our current study of physical and chemical properties and functional properties in complex food systems. It examines the interaction between anthocyanins and food proteins or polysaccharides by focusing on the “structure–stability” relationship. Furthermore, multispectral and molecular computing simulations are used as the chief instruments to explore the interaction’s mechanism. During processing and storage, the stability of anthocyanins is generally influenced by the adverse characteristics of food and beverage, including temperature, light, oxygen, enzymes, pH. While the action modes and types between protein/polysaccharide and anthocyanins mainly depend on their structures, the noncovalent interaction between them is the key intermolecular force that increases the stability of anthocyanins. Our goal is to provide the latest understanding of the stability of anthocyanins under food processing conditions and further improve their utilization in food industries.

6:20 Effects of soybean isoflavone aglycone on osteoporosis in ovariectomized rats Lulu Li, lilulushunliyitain@163.com, Na Zhang, Yang Yang, Chun-Min Ma, Xiao-Mei Li, Xin Bian, Likun Ren. Harbin U. of Commerce, Harbin, Heilongjiang, China In this study, the effect of different doses of soybeans isoflavone aglycone on the ovariectomized female osteoporosis rat model was evaluated by oral gavage. The rats were divided into seven experimental groups including SHAM, OVX, EE, SIHP, AFDP-L, AFDP-M, and AFDP-H, which was administered for 60 days from 30 days after ovariectomy. We collected blood from the abdominal aorta of rats on the 30th, 60th and 90th days respectively, analyzed its serum biochemistry, and took out the femur for micro-CT imaging and bone microstructure parameter analysis. Results showed that the intervention effect of AFDP-H group on osteoporosis rats at 60 and 90 days was similar to that of EE group, and superior to the OVX group, SIHP group, AFDP-L group, AFDP-M group. The AFDP-H group inhibited the decrease in serum bone markers, bone density, trabeculae quantity, trabeculae thickness, and bone volume fraction, and increased the trabecular separation caused by ovariectomy, thereby significantly improving bone microstructure. It also prevented continuous weight gain and increased cholesterol levels in female rats. In conclusion, the study showed that soybeans isoflavone aglycone could effectively inhibit and improve osteoporosis symptoms in ovariectomized rats.

6:30 Effect and mechanism of thermostable β-glucosidase on aroma enhancement of instant Oolong tea at high temperature Qi Lin, 994808865@qq.com. Jimei U., Xiamen, Fujian, China β-glucosidase is promising for a wide range of applications in increasing the aroma quality of tea. However, the inactivation and instability of enzyme activity under high temperature is a limitation for the application of β-glucosidase in tea aroma enhancement. Hence, thermostable β-glucosidase (TPG) enhanced the aroma quality of instant Oolong tea was reported in this study. Quantitative descriptive analysis showed that TPG could enhance floral and grassy notes of instant Oolong tea, while reduced the roasted, caramel and woody notes under 90 degrees Celsius. The results were obtained by GC-MS, OAV and aroma reconstruction and omission tests assayed benzyl alcohol, geraniol, (Z)-3-hexen-1-ol, benzaldehyde and 1-hexanol were the key glycosidic aroma compounds to enhance the aroma of instant oolong tea. The affinity of geranyl-β-D-glucoside hydrolyzed by TPG was lower than that of hexyl-β-D-glucoside, and the catalytic efficiency was higher than that of hexyl-β-D-glucoside hydrolyzed by TPG, and belonged to mixed competitive inhibition when both substrates were present. Homology modeling and molecular docking resulted that TPG belonged to the GH1 family, the nucleophile and acid-base residue were Glu166 and Glu351. Glu405, Glu166, Asn165 and Glu351 were essential amino acids for hydrolyzing glycosidic aroma compounds to release aroma. It was the first report that thermostable β-glucosidase could enhance the aroma quality of instant Oolong tea and continuously released the aroma at high temperature, and it provided theoretical guidance for the development of enzymatic technology to improve aroma quality of tea and opened up a new way for the development and utilization of thermostable β-glucosidase.

6:45 Structural characterization and hypoglycemic activity of glycoproteins extracted from Porphyra haitanensis by different extraction methods Ou Yujia, oyjfst@163.com, Baodong Zheng. Fujian Agriculture and Forestry U., Fuzhou, China In this study, two glycoproteins were extracted from porphyra haitanensis by ammonium sulfate and ethanol extraction methods, and their differences in structure and hypoglycemic activity were compared. The results showed that the protein, amino acid, and galactose contents of the glycoprotein (PG) extracted using an ammonium sulfate method were higher than those of glycoprotein (PP) extracted from ethanol. PG inhibited both α-amylase and α-glucosidase, substantially reduced in vivo hyperglycemia, regulated the intestinal production of beneficial bacteria (Lachnospiraceae, Odoribacter, and Lactobacillus), and increased the abundance of commensal microbial metabolites (e.g., taurine and hypotaurine) via the activation of taurine and hypotaurine, butanoate metabolism, and insulin secretion pathways. PP was superior in regulating lipid metabolism through the AMPK and fatty acid degradation pathways, which was positively correlated with its increased polysaccharide fragment, Lactobacillus and Rikenellaceae_RC9_ gut_group. Our findings shed light on the potential of Porphyra haitanensis glycoproteins as novel natural antidiabetic compounds.

6:55 Effects of non-covalent interactions between pectin and volatile compounds on the flavor release of tomato paste Xuejie Li, lxj13105161752@163.com, Jian Li. Beijing Technology and Business U. School of Food and Health, China Breaking methods have been shown to affect the sensory attributes of tomato paste, including volatile compounds and pectin content. This study aimed to explore the roles of interactions between pectin and aroma active compounds in the flavor release of tomato paste. Based on our results, phenethyl alcohol (PA) was one of the representative aroma active compounds and showed highly negative correlation with pectin content in tomato paste. According to ultraviolet-visible, fluorescence emission spectra and DLS analysis, PA could interact with pectin through hydrophobic and electrostatic interactions. The IGM analysis showed that van der Waals forces played a dominant role in the formation of PA-pectin complexes, which was further confirmed by ^{1}H NMR spectra and MD simulation. Overall, the non-covalent interaction of volatile compounds with pectin remarkably affected their release in tomato paste. These findings provide some insights into methods for improving the sensory quality of tomato paste.

7:05 Investigation of the anti-aging activity of the R-phycocyanin of Porphyra haitanensis Yanyu Feng, fengyanyu1221@163.com, Yi Zhang. Fujian Agriculture and Forestry U., Fuzhou, China Aging has become a global public health challenge. Many studies have revealed that the excessive generation of ROS and oxidative stress could be the major causative factors contributing to aging. In this study, R-phycocyanin (R-PC) was isolated from Porphyra haitanensis, and its anti-aging ability was explored by natural aging Drosophila melanogaster and H2O2 -induced HUVEC cells as the aging model. Results showed that R-PC α and β subunits expressed have antioxidant activity and can inhibit the generation of radicals, exhibiting a protective effect against H2O2 -induced apoptotic HUVEC cells death. R-PC prevented the H2O2 -induced HUVEC cell cycle phase arrest by regulating cell cycle-related protein. Furthermore, R-PC prevented the H2O2 -induced HUVEC cell cycle phase arrest by regulating cell-cycle-related protein expression. In vivo study also indicated that R-PC significantly increased the survival time and alleviated the oxidative stress of Drosophila melanogaster. Moreover, R-PC notably decreased levels of ROS in natural aging flies and inhibited lipid peroxidation by enhancing the expressions of the endogenous stress marker genes (SOD1, SOD2, CAT of Drosophila melanogaster). Taken together, a study on the antioxidation extract from Porphyra haitanensis, such as R-PC, may open a new window for the prevention of anti-aging.

7:20 Effects of genes required for exopolysaccharides biosynthesis in Lacticaseibacillus paracasei S-NB on cell surface characteristics and probiotic properties Luyao Xiao, 1798292124@qq.com, Wei Li. Nanjing Agricultural U., Nanjing, Jiangsu, China The cell surface of lactic acid bacteria (LAB) plays an essential role in cell-cell and cell-host interactions. Exopolysaccharides (EPSs) are produced on the cell surface of LAB or in the surrounding medium and are considered to be in favor of the specific probiotic surface characteristics. In our study, the structure features of EPS from Lacticaseibacillus paracasei S-NB were analyzed preliminarily, the putative eps gene cluster of L. paracasei S-NB was sequenced and 19 genes related to EPS biosynthesis was annotated through bioinformatic analysis. To analyze the relationship between EPS biosynthesis and phenotypic characteristics of S-NB, four knockout mutants of different functional genes in EPS biosynthesis were constructed. Analysis of TEM suggested that the S-NBΔ2176 (deletion of gene responsible for EPS polymerization) and S-NBΔ2175 (deletion of gene responsible for CpsD/CapB family tyrosine-protein kinase) had thinner cell wall thickness than wild-type S-NB. Meanwhile, both of the two mutants showed reduced biofilm formation, more hydrophilic surface, reduced auto-aggregation and decreased negative surface charge. Moreover, the deletion of genes involved in EPS synthesis may negatively affect the adherence of L. paracasei S-NB to the host cells (Caco-2), but the presence of these genes does not contribute to survival under simulating gastrointestinal tract environments. Two EPS fractions (BEPS1 and BEPS2) could inhibit the transcriptional level of TNF-α, IL-1β, INOS and COX-2 in RAW 264.7 cells induced by LPS, and enhance host immune tolerance via suppressing NF-kB and MAPK signaling. Furthermore, the S-NBΔ7576 mutant supplied with the BEPS1/BEPS2 exhibited more significant inhibition of

cytokines production and the phosphorylation of p65 and JNK in LPS-stimulated cells compared with the S-NB△7576 mutant alone. Taken together, results indicated the importance of genes associated with EPS biosynthesis in L. paracasei S-NB as a determinant in strain surface characteristics and cell-host interaction.

7:30 Novel viscous hydrophilic colloidal polysaccharide produced by Lactiplantibacillus plantarum T1: structural characterization, rheological behavior and biological activity Zhang Xueliang, 2017808124@njau.edu.cn. Nanjing Agricultural U., Nanjing, Jiangsu Lactic acid bacteria exopolysaccharide (EPS) with viscosity and biological activities has huge potential applications in functional fermented foods. In this study, an EPS (EPS-T1) with high molecular weight (1.41×10^6 Da) was isolated and purified from the Lactiplantibacillus plantarum T1, which was composed of glucose, galactose at a molar ratio of 1.21: 1.00. Through the size-exclusion chromatography and multi-angle laser light scattering (SEC-MALLS) analysis, the intrinsic viscosity [η] and hydrodynamic radius (Rh) of EPS-T1 were calculated to be 458.1 mL/g and 45.4 nm, respectively, which showed a flexible chain conformation. Rheological properties showed that EPS-T1 was a typical pseudoplastic fluid with high viscosity and weak gel performance, and which can be adjusted by the conditions of temperature, pH value and saline ions. Meanwhile, the in vitro immunomodulatory assays presented that it could induced the secretion of nitrous oxide, cytokines (IL-1β, TNF-α, IL-6 and IL-10) and significantly enhanced the pinocytic and phagocytic activities of macrophages. This work provides some basis for the functional applications of EPS-T1 from the Lactiplantibacillus plantarum T1.

7:40 Small molecules interaction-mediated steady system for the construction and mechanism Xiaojuan Chen, xiaojuanfood@webmail.hzau.edu.cn, hongshan Liang. Huazhong Agricultural U., Wuhan, Hubei, China How to improve the solubility or loading capacity of hydrophobic dietary bioactive compounds, achieve accurate nutrition delivery and obtain biological efficacy maximally has attracted immense scientific interest in the field of food nutrition. Herein, we proposed an innovative strategy of small molecules interfacial assembly, which availed the special structure and interfacial properties of plant polyphenol molecules to assemble and deposit onto the surface of critical nanoaggregates formed by antisolvent for hydrophobic polymethoxyflavone (PMFs), and further regulate the crystallization transition process of PMFs. On the basis of clarifying the crystallization thermodynamics and kinetics of PMFs, this study demonstrated detailedly the effect of interfacial deposition of small molecules on the phase transition of critical nanoaggregates, and decrypted the main forces driving this phenomenon. The results revealed that such assembled nanoparticles compared to pure hydrophobic nanoparticles, could exhibit considerable differences in crystal size and morphology. And then PMFs crystallization transition process could be further affected by the supersaturation, temperature, and pH, important factors regulating the interaction. Besides, to elucidate the assembly mechanism, we described the assembly process between polyphenol and PMFs nanoparticles by ultraviolet-visual spectral scanning spectrum (UV-Vis), molecular docking, nuclear magnetic resonance (NMR) and isothermal titration calorimetry (ITC). Taken together, these findings unlocked a new perspective for exploring the construction of the steady system based on the interaction of small molecules.

7:55 Physicochemical stability and in vitro digestibility of goat milk affected by freeze-thaw cycles Yue Ma, Myue09418@neau.edu.cn, juncai hou. Northeast Agricultural U., Harbin, China As the nutritional value of goat milk is gradually reflected, the demand for raw milk in the goat milk industry is gradually enhanced. However, its production has problems such as strong seasonality, short lactation period, and low milk yield and the year-round sustainable supply of goat milk is facing challenges. Because the supply of goat milk is limited, raw milk must be collected, and reasonable storage techniques used to ensure continuity of production in dairy factories. A common solution is to freeze goat's milk quickly to reduce enzyme activity and microbial growth rate, thus prolonging the storage life of raw milk. At present, plenty of reports have investigated the effects of freezing or thawing on physicochemical properties, structural characteristics, and processability of milk. Nevertheless, the influences of the repeated freeze-thaw cycles on goat milk in vitro digestibility during the whole processing process are rarely reported. In virtue of this, we demonstrated the influences of freeze-thaw cycles on the basic composition, protein structure, particle size distribution, and microstructure of goat milk. And the relationship between physicochemical properties and in vitro digestibility of goat milk was also elucidated. Experimental results showed that repeated freeze-thaw cycles led to the increase of acidity and medium-short chain free fatty acids of goat milk, and the significant decrease of fat and apparent viscosity. Furthermore, the degree of protein oxidation was enhanced, and the secondary structure changed to random coil. The particle size distribution and microstructure all showed the aggregation of goat milk droplets, resulting in the decrease of physical stability. Nevertheless, repeated freeze-thaw cycles could enhance the simulated in vitro digestibility and antioxidant capacity of digested products. These results are helpful to evaluate the quality characteristics of raw goat milk and provide theoretical reference for the industrial production of goat milk products.

8:05 Digestive properties of meat and plant-based meat analogue and their effects on gastrointestinal digestion function in mice Yunting Xie, 2019208024@njau.edu.cn, Chunbao Li. Nanjing Agricultural U., Jiangsu, China In order to evaluate the differences in nutritional function between meat and plant-based meat analogue, the protein digestion characteristics of pork, beef, plant-based pork and beef analogue as well as their effects on the gastrointestinal digestion function were systematically explored. In vitro simulated digestion showed that the digestibility of pork was higher than that of the plant-based pork analogue, while the value of beef was lower than that of the plant-based beef analogue in the gastric phase. The digestibility of meat proteins was significantly higher than that of the corresponding plant-based meat analogue in the intestinal phase. Both particle size and protein profiles showed similar results. A greater number of small molecular peptides and potential bioactive peptides were released from meat after gastrointestinal digestion. Further exploration found that meat has a particular charge state and lower apparent viscosity in the digestive system. Additionally, the meat protein had higher surface hydrophobicity and less β-sheet content. These make it simpler for digestive enzymes to access the active site of the protein and, as a result, easier be digested when compared to plant-based meat analogue. In mice, the long-term intake of meat significantly increased the number of gastric parietal cells, the levels of gastrin/CCKBR, acetylcholine/AchR, Ca2+, CAMK II, PKC and PKA, the activity of H+, K+-ATPase and pepsin, as well as duodenal villi height and the ratio of villi height to crypt depth compared with the plant-based meat analogue. Simultaneously, meat intake upregulated the expression of nitrogen sensors (GPR92, GPRC6A, T1R1, T1R2 or T1R3) in the gastrointestinal tract. These results indicated that meat protein had better digestion performance than plant-based meat analogue. After long-term ingestion, more peptides and amino acids released from meat enhanced the gastrointestinal digestion function of mice by upregulating the expression of nitrogen sensors.

8:15 Surface modifications of Pediococcus pentosaceus Li05 for improved adhesion and function against Citrobacter rodentium infection Shengyi Han, 21918241@zju.edu.cn. Zhejiang U. School of Medicine, Hangzhou, China Probiotics have been widely used as an adjuvant therapy to treat various diseases. However, therapeutic effect is usually contingent on the ability of the probiotic cells to adhere to and colonize the gastrointestinal tract. Pediococcus pentosaceus Li05 has previously been shown an anti-inflammatory effect, however, the mucoadhesive ability of the strain needs to be improved for further application. In this study, MUC2 polyclonal antibody was used as an adhesin and conjugated to the surface of Li05 to improve the adhesion ability of the probiotic. The results showed that the growth and survival rate of Li05 were not affected after the modification, whereas the adhesion rate was significantly improved in a Caco-2 cell monolayer cell model. Moreover, in vivo competitive adhesion experiments in mice demonstrated that Li05 outcompeted Citrobacter rodentium; an effect even more pronounced with aMUC2-targeted Li05. The study also showed that aMUC2-targeted Li05 significantly reduced colonic histological injury, alleviated inflammation and decreased C. rodentium colonization in the C. rodentium-infection colitis mouse model. The relative abundance of Lactobacillus, and concentrations of short-chain fatty acids, were significantly higher in colon of the mice after treatment of modified Li05. In summary, the results presented in this study demonstrated that aMUC2-targeted Li05 showed promise for future application as a therapeutic strategy for infectious colitis.

8:30 Hypoxia impairs lactation in bovine mammary epithelial cells Yanshan Jin, cedarjys@gmail.com, Hongyun Liu. Zhejiang U., Hangzhou, China Heat stress (HS, namely hyperthermia) is one of the most important environmental factors causing a huge negative impact on milk production in dairy mammals. Studies revealed that hyperthermia can induce hypoxia occurrence in the mammary glands of lactating animals. To determine whether and how hypoxia exerts a negative effect on lactation in dairy cows under HS, bovine mammary epithelial cells (BMECs) were exposed to normoxia (control), HS, and hypoxia conditions within different duration time. Results uncovered that the protein expression of HIF-1α was significantly upregulated under HS in a time-dependent manner in line with the corresponding elevation of HSP90 expression compared to the controls, protein expression of β-casein and κ-casein were significantly decreased while no reductions were observed of the triglyceride content and lipid droplet synthesis in BMECs under hypoxia. Moreover, hypoxia significantly decreased the phosphorylation of mTOR/P70S6K/4EBP1 and increased the expression of FASN and PPAR-γ regulating milk fat synthesis in BMECs. Aside, transcriptomics data revealed that hypoxia mainly disrupted the metabolism to produce milk synthesis precursors and impaired energy generation through mitochondria dysfunction, ROS accumulation, and ATP production reduction in BMECs. Furthermore, we found that hypoxia-induced reduction in casein was independent of HIF-1α, in contrast to the elevation of milk fat synthesis partially depending on HIF-1α. Overall, these novel findings provide more understanding of the molecular mechanisms underlying hypoxia triggering the impaired lactation in BMECs.

8:40 Construction of EGCG loaded in the edible complex delivery system: Masking bitterness and control release Chenlu Ma, ncuspymachenlu@163.com, Kui Zhang, Ying Liu, Yingying Zhou, Xiong Ye, Liqiang Zou. Nanchang U., Jiangxi, China (-)-Epigallocatechin gallate (EGCG) has a strong bitter taste and low bioacceptability, making it difficult to apply in food systems. To overcome the application limitations, this article successfully masked the bitter taste of EGCG by constructing an edible complex system to stabilize the encapsulated EGCG. The electronic tongue and sensory evaluation showed excellent bitterness masking effect, transmission electron microscopy (TEM) showed a clear vesicle structure, and the encapsulation efficiency reached 94.6%. Fourier transform infrared spectroscopy (FTIR) and Quartz Crystal Microbalance with Dissipation (QCM-D) demonstrated the existence of interaction forces in this system, which could form a tight complex structure. Meanwhile, the encapsulated EGCG in this system also showed relatively good slow-release performance: the in vitro release ratio at 4h was 8.67%, while the release of unencapsulated EGCG at the same concentration was 84.9%. After the simulated in vitro simulated digestion, the digested solution of encapsulated EGCG and unencapsulated one showed obvious color differences, reasonably inferring that this system can effectively protect EGCG from degradation in gastrointestinal digestion. This study is beneficial to expand the wide application of EGCG in functional foods.

8:50 Endogenous enzymes-based fermentation simulation reactions reveal metabolic pathways of key aroma compounds in fermented sea bass (Lateolabrax japonicus) Xialei Liu, 1613416864@qq.com. Jimei U., Xiamen, Fujian, China Improving fish quality during storage after postharvest could increase demand, but fish quality has complex characteristics requiring a deep understanding the change law of aroma in order to find metabolic pathways that can improve the sensory quality of the fermented fish. Here, geraniol, vanillin, β-caryophyllene, indole, and octanal was identified as the key aroma compounds in fermented sea bass by molecular sensory science analysis. Through endogenous enzyme fermentation simulation experiments, it was clarified that the metabolic pathways of key aroma compounds in fermented sea bass were from geranyl pyrophosphate metabolism pathway, tyrosine metabolism pathway, farnesyl diphosphate metabolism pathway, tryptophan metabolism pathway, and linolenic and linolenic acid pathway, respectively. The degradation pathway of geraniol, the conversion between vanillin and eugenol, and the conversion of octanal to unsaturated aldehyde, and then cyclization to 2-pentylfuran were first demonstrated. It provides a theoretical reference for the control of flavor precursors and key enzymes in the fermentation process to regulate sensory quality.

9:00 Proteins from different sources in a high-fat food matrix influence lipid hydrolysis through bolus coalescence and interactions with bile salts Mengzhen Ding, mengzhending@foxmail.com. Nanjing Agricultural U., Jiangsu, China Bile salts (BS), as an important biosurfactant, play a vital physiological role in lipid digestion and transport. However, nutrient intake is often not uniform, and the protein-BS interaction may affect the interfacial process of lipolysis and reduce hydrolysis. In this study, an in vitro digestion model was used to explore the digestion behaviours of high-fat and high-protein diets prepared with different protein sources (pork, chicken, casein and soy protein). Interestingly, the final degree of hydrolysis of the same type and level of fat differed in the following order: casein > soy protein > pork protein > chicken protein. This difference was attributed to the findings that the salt-soluble proteins in pork and chicken effectively bound BS during intestinal digestion, reducing its efficiency in participating in fat digestion. Fluorescence spectra demonstrated that myofibrillar proteins of pork and chicken exhibited a strong binding capacity to BS. The addition of BS increased the proportion of random coils in the protein, and hydrophobic interactions played an essential role in the degree of binding. In addition, the rheological characteristics and microstructure of diets differed by protein source. Meat protein diets exhibited stronger aggregation, resulting in a smaller interface area for reaction. This in vitro study could provide a potential mechanism explaining the inhibition of fat digestion by different protein diets and provide more reasonable dietary guidance for obese people.

Virtual Session - General Posters

12:00 Insights into effects of simultaneous uptake, controlled release and antioxidant activity of β carotene and curcumin by Octenylsuccinated gastrodia elata starch micelles Zhen Wu, wuzhen985@126.com. Chongqing Academy of Chinese Materia Medica, Chongqing, China Gastrodia elata Bl. f. glauca S. chow is a high-value homology of medicine and food in China, and the starch amounts to about 70% of its dry weight. Gastrodia elata starch shows high amylopectin amount, small size, high swelling ability and low gelatinization temperature, which indicated that Gastrodia elata starch can be applied as a novel starch resource for food and pharmaceutical industries. Improving the properties of starch by octenylsuccination and preparing octenylsuccinated starch materials are common to broaden its functionality and meet application requirements. Simultaneous encapsulation of hydrophobic bioactive compounds by nanocarriers has been widely used to improve their loading capacity, bioactivities, and stability. This study aimed at fabricating a novel co-delivery system to encapsulate and protect β-carotene and curcumin. Possibility and mechanisms behind the micellizations of octenylsuccinated Gastrodia elata starch micelles and relevant loading and controlled-releasing were probed using multi structural characterization approaches. Results showed that octenylsuccinated Gastrodia elata starch molecules could spontaneously self-assemble to form spherical nanomicelles with various hydrophilic shell and hydrophobic cores. For simultaneous uptake, the obviously enhanced solubilities of β-carotene and curcumin were due to favorable interactions. β-carotene and curcumin molecules were located at the interior and periphery of hydrophobic cores of octenylsuccinated Gastrodia elata starch micelles, respectively, and they did not exist in isolation, and always linked together. The interactions of β-carotene and curcumin retarded their release due to both the interactional strength and structural compactness. Additionally, combination of β-carotene and curcumin via loading by micelles improved their antioxidant activities. Therefore, data support development and fabrication of functional food matrix encompassing both β-carotene and curcumin by using new Gastrodia elata starch.

12:00 Determination of phytochemical content and antioxidant capacity of dried haskap berries (Lonicera caerulea L.) and its potential value-added products Yihan He1, yihan.he@mail.mcgill.ca, Kiren Singh2, kiren.singh@haskalife.ca, Xiaonan Lu1, xiaonan.lu@mcgill.ca. (1) Food Sci. and Agricultural Chemistry, McGill U., Montreal, Quebec, Canada(2) Haskalife Inc., Picture Butte, Alberta, Canada Haskap berries commonly refer to the fruits of Lonicera caerulea L and have higher anthocyanin content and antioxidant capacity than other berries known for their health promoting properties, such as blueberries. In this study, the effect of processing methods on the quality of dried haskap berries was investigated. Phytochemical content and antioxidant capacity were also evaluated in haskap juice under different sterilization process; and haskap agricultural wastes (i.e., leaves and branches). Haskap extracts were used for determination of total phenolic content, anthocyanin content, total flavonoids and antioxidant capacity. Haskap powders produced by vacuum microwave drying have similar phenolic content, anthocyanin, flavonoids, and antioxidant capacity to freeze-dried powders. Haskap juice under high pressure processing preserved a higher anthocyanin content compared to its counterpart under heat pasteurization. This study provided critical and insightful results for the development of innovative value-added haskap products to agri-food industry.

12:00 Protein Extraction from Spent Oil-Cakes D. Smit Kumar, dsmit.chemist@gmail.com, Hardi Makwana. School of Science, GSFC U., Vadodara, Gujarat, India The study will aim at development of a cheaper and more viable industrial process for protein extraction. Major objectives of the study will be: i) To explore the chemistry of chemicals and find the cheapest reagents for the extraction; ii) To investigate and establish the feasibility/viability of the method at industrial level. Groundnut cake is a by-product obtained after extraction of oil. The cake contains 45–60% protein, 22–30% carbohydrate, 3.8–7.5% crude fibre and 4–6% minerals. The extraction of protein from oil spent cake can be done by two methods, by alkaline isoelectric precipitation and physical separation procedures. We are going to extract the protein by alkaline isoelectric precipitation method. For this method, we have selected the cheapest reagents out there in the market while, maintaining the maximum yield and recovery of protein. We need 0.2 M NaOH and 1 N H2SO4 solution for the pH adjustment and precipitation of protein. The whole method comprises various steps like Stirring, Centrifuge, Filtration and Drying. Utilization of defatted meal/residue into food products could be an excellent way for boosting the utilization of groundnut protein in the diets of malnourished people in developing and poor countries. Application and Usage of defatted groundnut meal with mild processing treatment is becoming increasingly popular in many countries. So, the extraction of peanut protein will aid the little valued spent oil cakes and will reap financial reward to the peanut industry and will also be beneficial to various food manufacturing company.

12:00 Towards the structure elucidation of an antibiotic adjuvant alkaloid Corozine A from corozo palm (Attalea cohune) applying experimental and computational tools Lucia Nitsch Velasquez1,2,3, escucha_al_viento@yahoo.com. (1) Instituto de Investigaciones Centro U. de Zacapa, U. de San Carlos de Guatemala(2) Research and Development, Proyectos Educativos Regionales de Autoayuda, Guatemala(3) Chemical and Food Engineering, U. Rafael Landivar, Guatemala Corozo palm-CP forests were cultivated by Mayan peoples in México and Central America. Its coconut oil is commercialized for cosmetic and gourmet markets with a limited expansion due to the seed hardness. Natural products research on CP is scarce and needed to seek further sustainable exploitation of rainforest products. CP male inflorescences were targeted for extract analysis, they may be a more tractable raw material. Inflorescences were macerated and boiled in ethanol. Supernatant was collected, evaporated and resuspended in ethanol. The product purity was analyzed by LC-MS and spectroscopic methods and tested for exchangeable protons by HR-MS/MS . The structural analysis was based on an initial structural candidates exploration with 1H-NMR at empirical level with Chemdraw(R). 1H-NMR, IR and optical activity for the best match candidate were further analyzed with a basic computational modeling with DFT at DZ/LDA//DZ/LDA level of theory, in gas phase. Antibiotic adjuvant activity was determined by checkerboard method (aminoglycosides, MRSA-USA300). A compound was isolated with 95% purity, 0.03% extraction yield, molar mass of 325.22742Da-C21H28N2O±3.1mDa. Exchangeable protons and aromatic hydrogens were not detected by any of the applied techniques. No compound was found to match its features. Several structural candidates were considered. Computational modeling of the main structural candidate yielded a good coincidence between modeled and experimental spectroscopic findings, including the sign of molar rotation. Compound reduced to 1/16MIC-gentamicin at 10mg/mL. The isolated compound is a bioactive new chemical entity called Corozine A, which proposed structure includes oxazonine, pyrrole and pyridone cycles. Further investigation is ongoing.

12:00 Nutraceutical potential of industrial hemp (Cannabis sativa L.) extracts: physicochemical stability and bioaccessibility of cannabigerol (CBG) nanoemulsions Huijuan Zheng1,2, huijuanzheng87@gmail.com, Bingcan Chen1, Jiajia Rao1. (1) North Dakota State U., Fargo(2) Tongji U., Shanghai, China Cannabigerol (CBG) is a bioactive compound that mainly comes from industrial hemp (Cannabis sativa L.) with various beneficial health effects. However, the lipophilic nature of CBG impedes its application in aqueous-based systems and potentially hinders its bioavailability. Moreover, research on the stability and utilization of CBG in food-related systems is very limited until now. Herein, nanoemulsions were prepared from edible oils to deliver CBG and increase its solubility, stability, and bioaccessibility. Encouragingly, formulations with excellent physical stability (particle size between 160- 250 nm depending on the emulsifier type) were obtained under various conditions (pH 3.5 and 7.0, 25 and 37 °C, light exposure) during long-term storage (4 weeks). Quantitative analysis of CBG during storage using HPLC revealed excellent chemical stability of CBG in the nanoemulsions under the tested pH and temperature under dark conditions, whereas light caused chemical degradation of CBG in nanoemulsions. Therefore, antioxidants with various polarities were applied to test their efficacy in enhancing the chemical stability of CBG in nanoemulsions. The degradation of CBG decreased for all antioxidants (β-carotene, quercetin, and EGCG) inclusion samples except those with α-tocopherol. And hydrophilic antioxidant EGCG proved to be the most effective one for the tested samples followed by amphiphilic quercetin. In addition, quillaja saponin (QS) based nanoemulsions were found to better maintain CBG chemical stability than the modified starch ones. Furthermore, an in vitro digestion model was applied to elucidate the digestion kinetics of the nanoemulsions and the bioaccessibility of CBG encapsulated. Improved bioaccessibility of CBG was realized by the long-chain triacylglycerides-based nanoemulsions. The results from the current study provide effective ways to encapsulate and protect CBG using nanoemulsions. More importantly, the results may stimulate more food-related studies on CBG and cannabinoids, therefore facilitating the application of CBG and industrial hemp extracts as potential functional food ingredients.

12:00 Quality evaluation of artificially cultivated Atractylodes lancea (Thunb.) DC. from genuine producing areas Junming Chen, chenjm@cczu.edu.cn, Longyu Li, Ying Liu, Mengyi Huang, Cheli Wang. School of Pharmacy, Changzhou U., Jangsu, China Atractylodes is a medicinal and edible herb with the same origin. It is the dried root and rhizome of Atractylodes lancea (Thunb.) DC. or Atractylodes chinensis (DC.) Koidz. It has the effects of prolonging life, invigorating the spleen and nourishing the liver, and resisting viruses. It is one of the most frequently used Chinese medicinal materials for the treatment of COVID-19. Since the Ming and Qing Dynasties, Atractylodes has been produced in Maoshan and is known as genuine medicinal materials. However, in recent years, due to environmental factors and other reasons, wild resources of Atractylodes lancea (Thunb.) DC. are scarce and have been listed as endangered medicinal plants in China. The chemical composition of Atractylodes is easily affected by climate, ecological environment, and other factors, and the quality of Atractylodes on the market varies greatly. Its quality evaluation only considers volatile oil components, ignoring the water-soluble components used in traditional Chinese medicine decoction. This article comprehensively evaluates the quality of artificially cultivated Atractylodes lancea (Thunb.) DC. in terms of its characteristics, surface texture, cross-sectional features, water-soluble components, and volatile oil components, providing a reference for the expansion and promotion of artificially cultivated Atractylodes lancea (Thunb.) DC. from genuine producing areas. The study found that artificially cultivated Atractylodes lancea (Thunb.) DC. from genuine producing areas has a nodular appearance, and its volatile oil content and water-soluble components are higher than those in other producing areas and in a certain proportion, which is consistent with the synergistic effect of multiple components in clinical efficacy of traditional Chinese medicine. Atractylolone is the main active ingredient of Atractylodes, and the content of Atractylolone from genuine producing areas is more than 20 times that from other producing areas, which can be used as a marker of the genuine producing areas of Atractylodes.

12:00 Exploration of conditions for high-concentration leaching of aromatic components by surface treatment of oak wood using pulsed arc discharge Mei Iitomi, 236d8752@st.kumamoto-u.ac.jp, Mitsuru Sasaki, Ippei Yamashina. Kumamoto Daigaku, Japan Lignin and tannin, the main constituents of wood, can be converted into low molecular weight aromatic compounds with functional properties by thermal decomposition at high temperatures. This is used in whiskey production to produce a unique aroma and color. Conventionally, the char treatment of inner surfaces of woody barrels has been conventionally utilized. In this method, the inner walls of wooden barrels are burned with a flamethrower at around 800-900oC for several minutes to cause the decomposition of lignin and tannins. However, this method not only consumes a lot of thermal energy, but also produces a large amount of carbon monoxide and carbon dioxide, which cause environmental impacts, when burned. In this study, the pulsed arc discharge method was applied to the surface treatment of oak wood and investigate the elution behavior and elution rate of aromatic compounds, and also compared with conventional char treatment in order to evaluate the superiority of this method. American white oak (AWO) wood chips were used as raw material, and the repetition frequency and discharge duration were tuned at 100 and 150 pps, and 30~60 s, respectively. After treated, the wood chips were immersed in a 63% ethanol aqueous solution for 20 days, and the aromatic components were quantitatively analyzed using HPLC. Untreated wood chips, flame charred, and toasted wood chips were also used for comparison. The relationship between the amount of vanillin, vanillic acid, and syringaldehyde eluted and soaking time was examined. For all components, leaching was higher in the toast- and discharge-treated pieces than in the char-treated pieces using the conventional method. Specifically, for vanillin, toast and discharge treatments were about 4 times higher than char treatment; for vanillic acid, discharge treatment was about 5 times higher and toast treatment 3 times higher; and for syringaldehyde, discharge treatment was about 5 times higher and toast treatment was about 9 times higher. As for the effect of the different frequency of discharge treatment on the results, 100 pps was more eluted for vanillin, while the other two components were eluted at similar levels.

12:00 Impact of foliar and shade application on blackberry flavor and phenolics Tianyou Xu1, tianyou21@vt.edu, Jayesh Samtani2, Han Chen3, Yun Yin1. (1) Food Sci. and Tech., Virginia Polytechnic Inst. and State U., Blacksburg(2) Hampton Roads Agricultural Research and Extension Center, Virginia Polytechnic Inst. and State U., Virginia Beach(3) Dept. of Statistics, Virginia Polytechnic Inst. and State U., Blacksburg Blackberry is a popular fruit due to its delightful taste and notable health benefits. This study evaluated the influence of shade cloth and pre-harvest foliar treatments on production quality, aroma profiles and phenolics of two Virginia-grown blackberry cultivars. The study was conducted over two growing seasons (2021-2022) at Hampton Roads Agricultural Research and Extension Center in Virginia Beach, VA using a completely randomized design with three replicates per treatment. Each replicate includes three plants of Prime-Ark® Traveler or Prime-Ark® Freedom blackberry. Calcium (Ca), salicylic acid, shade cloth with 30% light reduction and one grower

standard control were randomly assigned to each variety. Fruits harvested from July were used for further flavor and chemical analysis each year. The aroma-active compounds in blackberries were identified by use of headspace-solid-phase microextraction-gas chromatography-mass spectrometry-olfaction (HS-SPME-GC-MS-O). The total phenolic content and antioxidant activities (DPPH, ABTS) were measured by spectrophotometry. Normal berry production quality were observed with all treatments for two seasons. The same 16 aroma-active compounds were identified in both blackberry cultivars and across all treatments for two seasons. Three esters, 5 alcohols, 2 carboxylic acids, 2 aldehydes and 2 monoterpenes were identified; with ethyl butyrate (fruity), 2-heptanol (fresh, green), 1-octen-3-ol (cooked potato) and p-cymen-8-ol (floral) as key aroma compounds. However, all 16 aroma contents were found to be higher in blackberries from 2021 compared to 2022, likely due to climate variation (e.g., high heat and drought in 2022). Flavor profiles for two cultivars were distinct: PrimeArk® Freedom is characterized to be more “fruity” and “floral”, while PrimeArk® Traveler features more “green” and “fresh” notes. The foliar and shade application treatments, however, did not seem to significantly influence berry flavor and phenolics. This study first characterized the flavor profiles of above two VA blackberry cultivars. Regional berry growers should be more conservative when adopting foliar and shade applications because seasonal variations seemed to surpass the significance from applied agronomic treatments.

12:00 β-Cyclodextrin encapsulated garlic oil and diallyl disulfide for sclerotium cepivorum sclerotia germination to control allium crop white rot disease YanPing L. Qian1,2, yan.ping.qian@oregonstate.edu, gia K. Hua3, Jeremiah K. Dung3, Michael C. Qian2. (1) Crop and Soil Science, Oregon State U. College of Agricultural Sciences, Corvallis(2) Food Sci. and Tech., Oregon State U., Corvallis(3) Horticulture, Oregon State U. College of Agricultural Sciences, Corvallis White rot, caused by Sclerotium cepivorum, is a devastating disease of onion, garlic, and other Allium crops. The pathogen reproduces and survives by forming sclerotia, which can survive in field soils for decades. The pathogen is host-specific to Allium spp., and sclerotia germinate in response to sulfur compounds produced by Allium roots. Sulfur-containing compounds such as diallyl disulfide (DADS) and garlic oil can stimulate sclerotia germination without host plants and effectively reduce pathogen populations before planting an Allium crop. However, garlic oil and DADS are highly volatile and challenging to handle and apply in the field. In addition, laboratory soil incubation experiments have demonstrated the strong interaction of DADS and garlic oil with soils and reduced efficiency. Therefore, this study was conducted to encapsulate DADS and garlic oil with β-cyclodextrin (β-CD) to protect sulfur volatiles from interactions with soil and against oxidation, degradation, and evaporation. Microcapsule extract analysis showed that garlic oil and DADS were successfully encapsulated with greater than 90% powder recovery. In addition, the micro-encapsulation process did not change the chemical structure, but the chemical composition was altered. Furthermore, lab and growth chamber incubation experiments revealed that DADS and DAS could be slowly released into the soil from microcapsules and worked effectively for white rot sclerotia germination. Compared to the mock-treated control, liquid DADS treatment, the microcapsules of DADS and microcapsules of garlic oil reduced sclerotia populations by between 73.7 and 82.3%, depending on the treatment. Compared to liquid DADS and liquid garlic oil, the encapsulated DADS and garlic oil are equally effective but easier to handle, providing more flexibility regarding timing, placement, and machine applications.

12:00 Effect of simulated gastrointestinal digestion on composition of anthocyanins and catechins and antioxidant properties of purple tea Elsayed M. Abdelaal1, elsayed.abdelaal@canada.ca, Iwona Rabalski1, Ishan Rai2. (1) Guelph RD Centre, Agriculture and Agri-Food Canada, Guelph, Ontario(2) 2Asilia Inc., Mississauga, Ontario, Canada Our previous research has shown that purple tea is a good source of anthocyanin and catechin compounds showing great potential as a heathy beverage and ingredient. In the current study, purple tea leaves were brewed and freeze dried to investigate the effect of simulated gastrointestinal digestion on composition of anthocyanins and catechins and antioxidant properties. Anthocyanin and catechin compounds were separated and quantified on UPLC and their identity was confirmed based on authentic standards and UV and MS properties. The antioxidant activity was assessed based on three assays including DPPH (2, 2-diphenyl-1-picrylhydrazyl) radical, ABTS (2, 2azino-bis (3-ethylbenzthiazoline-6-sulfonic acid) stable radical and ORAC (oxygen radical absorbance capacity). The purple tea freeze-dried powder contained on average 4.4% moisture, 15.1% total minerals, 45.0% protein and 1.5 mg/g total anthocyanin content measured spectrophotometry. The 10 major anthocyanin pigments present in purple tea were released in the aqueous phase following the 3-step simulated gastrointestinal digestion. Delphinidin-coumaroyl-hexoside was the dominant followed by delphinidin-3-galactoside and cyanidin-coumaroyl-hexoside. Additionally, 6 catechins and 2 alkaloids were found in the aqueous phase following the in vitro digestion with epigallocatenin gallate (EGCG), epicatechin gallate (ECG) and epigallocatechin (EGC) being the dominant. The purple tea powder showed improved scavenging capacities against DPPH, ABTS and peroxyl radicals. The initial data suggest that anthocyanins and catechins in purple tea can be metabolized which could enhance the oxidative status and health condition of humans.

12:00 Computer-aided design and synthesis of novel flavanone derivatives for use as potential inhibitors of the COVID-19 papain-like protease Anna Sigmon1, ajs8621@psu.edu, Neela Yennawar2, Eleanora Margulis1, Julia Fecko2, Hamzah Al-Quaid1. (1) Penn State Brandywine, Media, Pennsylvania (2) The Pennsylvania State U. Huck Inst.s of the Life Sciences, U. Park A series of novel derivatives of plant-based flavanones were designed using in silico docking against the papain-like protease of COVID-19. Initial docking results were obtained using a free and publicly available COVID-19 docking web server that utilizes AutoDock Vina as the docking engine. Those initial results were further evaluated using PRODIGY, a web server that evaluates the binding affinities of protein-ligand complexes. The docking results revealed that the most promising targets should comprise a naphthalenyl moiety linked to a flavanone core via a 4 or 5 atom linker. The most direct route to synthesize these compounds involved linking the naphthalenyl moiety to the flavanone core via a hydrazone functional group. The parent flavanones included naringenin, hesperetin, 7-hydroxyflavanone, 6-hydroxyflavanone, 4'-hydroxyflavanone and 6-methoxyflavanone. Hesperetin and naringenin are both found in citrus fruits, 6-hydroxyflavanone is present in
Crocus flowering plants, 7-hydroxyflavanone is derived from the stems of Spatholobus suberectus, 4’-hydroxyflavanoe is present in Dianthus caryophyllus and 6-methoxyflavanone is a synthetic derivative of 6-hydroxyflavanone. All compounds were made as racemic mixtures. The characterization and synthetic procedures for all compounds are described, along with the crystal structure of one of the naringenin-based compounds which illustrates that the E configuration of the hydrazone double bond, which is stabilized by a hydrogen bond between the imino nitrogen of the hydrazone group and the neighboring hydroxy group: (E)-N'-(5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-ylidene)-2-(naphthalen-1-

yl)acetohydrazide. Initial binding studies using circular dichroism are also reported.

12:00 Developing food preference behavior-based method to identify effectors of substance use disorder Aaron T. Kim, aaronkim@umass.edu, Yeonhwa Park. Food Sci., U. of Massachusetts Amherst (note - Abstract for this poster is the first abstract listed under Monday Sci-Mix 8:00 Virtual Session)

12:00 Promoting food and nutritional security through value added products of under-utilized Hibiscus sabdariffa calyces Sengnolotha A. Marak1, msengno@gmail.com, Nutan Kaushik1, Alexander Dikiy2, Eva Falch2, Elena Shumilina2. (1) Amity Food and Agriculture Foundation, Amity U., Noida, Uttar Pradesh, India(2) Dept. of Biotechnology, Norges teknisk-naturvitenskapelige universitet, Trondheim, Trøndelag, Norway Roselle (Hibiscus sabdariffa) belonging to Malvaceae family is under-utilized crop in India. Only few indigenous tribes of North East India grow for household consumption but generally, lack national recognition and appreciation. Usually, it is grown as fibre crop. Roselle, which is at present under-utilized have an important role to play in satisfying the demand for nutritious, delicately flavoured and attractive natural foods of high therapeutic value. They are in general rich in bioactive compounds such as ascorbic acid, anthocyanins, phenolic content, antioxidant activity, hibiscus acid and GABA. The experiment conducted with roselle calyx to prepare different beverages using different spices and fruit blends aim to standardized and optimized the beverage formulation, to obtained consumer acceptability and to analyse the phytochemical characteristics of the beverage. The standardization and optimization were carried out using Response Surface Methodology (RSM). Using sensory parameters, the consumer acceptance was assessed and the product analysis include the biologically active component that is total phenols, total anthocyanins, antioxidant and ascorbic acid. The result showed a successful optimization and consumer acceptance with desirability of 0.9. The optimum beverage is found rich in Vitamin C, phenolic, anthocyanins and antioxidant. Hence, this under-utilised Hibiscus sabdariffa has a promising scope in promoting food and nutritional security, enhancing small farmers' income and contributing to sustainable rural development.

12:00 Tuning the amphiphilicity of β-Cyclodextrin and L-Tryptophan nanoparticles in the development of ultrastable and eco-sustainable Pickering emulsions Junyi Wang, jw2554@cornell.edu, Younas Dadmohammadi, Alireza Abbaspourrad. Food Sci., Cornell U., Ithaca, New York Pickering emulsions are “surfactant-free” emulsions since they are stabilized by solid particles instead of surfactant adsorb onto the surface of the interface. However, Pickering emulsion tends to be thermodynamically unstable and causes phase separation, and constitutes a severe appearance defect in most food emulsions. The present study developed a novel β-Cyclodextrin (β-CD) and L-Tryptophan (Trp) complex colloidal particle by using a simple antisolvent approach. β-CD is an enzymatic derivative of starch and forms a host−guest inclusion complex or used as an emulsion stabilizer. Trp is an essential amino acid that is used in the induction of sleep, appetite, mood, and sensory perception. The complex was formed through antisolvent methodology and characterized by SEM, FTIR, XRD and molecular simulation. The SEM showed the morphology of the complex was different from the pure β-CD and Trp, suggesting the formation of the complex. Molecular simulation indicated the hydrogen bonds and hydrophobic interactions were the main driving force of β-CD and Trp interaction. According to XRD, compared to pure β-CD exhibited cage-like structure at the O/W interface, upon complexation with Trp, the morphology of the complex changed to channel-like structure. The wettability of the solid particles was also measured, and the result showed that the addition of Trp increased the hydrophobicity of the solid particles. Pickering emulsions were fabricated under different ratios of β-CD to Trp (1:0, 1:0.1, 1:0.25, 1:0.5, 1:1), and pHs (3, 5, 7, 9). The results showed that when the β-CD to Trp ratio was 1 to 0.1 under pH 9, the Pickering emulsion had the smallest particle size, lowest surface charge, and the highest storage stability (60 days at room temperature). The present study demonstrated the potential of using an eco-friendly and health-promoting emulsifier, β-CD/Trp nanoparticles in emulsions, which would help to promote natural surfactants in more food applications.

12:00 Development of a method to separate toxic compounds from fungal pathogens in hemp Isabelle A. Kagan, isabelle.kagan@usda.gov, Nicole Gauthier. Forage-Animal Production Research Unit, USDA Agricultural Research Service, Lexington, Kentucky Among the fungal pathogens being identified on hemp are Fusarium graminearum, known to produce mycotoxins on grains. Mycotoxins produced include deoxynivalenol (DON). Because DON can be harmful to both humans and livestock, and tight regulations exist on allowable amounts in the food supply, the detection and quantification of mycotoxins are essential tools to keep consumers safe. Existing mycotoxin extraction and separation methods are optimized for contaminated grain and flour, and new methods may be needed for hemp. Using commercially available standards, four mycotoxins were separated by high-performance liquid chromatography (HPLC), and these were well separated from several cannabinoids. Disease-free hemp seeds were extracted by ultrasonication and solid-phase extraction. When the mycotoxin standards were added to an extract of disease-free hemp seeds, separation of all four mycotoxins from hemp seed components was eventually achieved, indicating the potential to identify mycotoxins in diseased seeds. Future work will involve separating mycotoxins from the components of floral and leaf tissue and developing a method to quantify the separated mycotoxins.

WEDNESDAY MORNING August 16
Chemical Intervention Technology to Improve Microbial Stability of Food

8:05 Active polymers containing silver nanoparticles combined with active formulations based on essential oils: Quality effect on cereals and dairy products Monique Lacroix, monique.lacroix@iaf.inrs.ca. Armand Frappier Health Biotechnology, Institut national de la recherche scientifique, Laval, Quebec, Canada Several bioactive nanocomposite films containing plant essential oils (EOs) and silver nanoparticles (AgNPs) were tested against food-borne pathogens and spoilage organisms in packaged foods. The films were based on chitosan (CH), poly (butylene adipate-co-terephthalate) (PBAT) or polylactic acid (PLA) and contained cellulose nanocrystals (CNCs). Results showed that Bioactive CH-, PBAT-based nanocomposite films have strong antibacterial, and antifungal properties against Escherichia coli O157:H7, Salmonella Typhimurium, Aspergillus niger, Penicillium chrysogenum, Mucor circinelloides. PLA-based films showed less antibacterial, and antifungal properties. Challenge tests were conducted with packaged rice and yogurt. Rice was treated with bioactive CH- and PBAT-based films with and without γ-irradiation treatment (750 Gy) for 8 weeks at 28°C to control fungi and bacterial growth, while the yogurt was treated with bioactive PBAT- and PLA-based films for 8 weeks at 4°C. Bioactive PLA and PBAT-based nanocomposite films significantly reduced the growth of pathogenic bacteria and spoilage fungi in stored yogurt after 8 weeks at 4°C.

8:30 Development of antimicrobial food packaging materials with electrospinning technology Tony Jin, tony.jin@usda.gov, Lin Liu. Eastern Regional Research Center, USDA Agricultural Research Service, Wyndmoor, Pennsylvania Allyl isothiocyanate (AIT) is

one of plant essential oils and a potentially useful antimicrobial compound for food applications. Previous studies demonstrated that AIT coated onto biodegradable composite films exhibited strong antimicrobial activities against foodborne pathogens in various foods. However, its use in the food industry is limited by its volatility and pungency. These limitations could be effectively overcome by physically entrapping AIT molecules within an inert biopolymer matrix, then slowly release to food surface. This presentation will demonstrate an approach to developing antimicrobial packaging films with AIT. In this study, AIT was encapsulated in poly(lactic acid) (PLA) fibers of submicron sizes by electrospinning the mixture of PLA and AIT to a thin PLA film. The results revealed that the release of AIT from the fibers depends on its initial concentration in PLA electrospinning solution, film samples with more AIT incorporated showed a higher release rate and had less microbial cells grown on the culture plates. Populations of E. coli O157:H7 cells on grape without AIT/PLA film treatment increased to 3.5 log CFU/g after 40 h storage at 22°C while the grape sample with AIT/PLA film only had 1.5 log CFU/g. During the same storage period, populations of E. coli cells on deli meat without AIT/PLA film treatment increased to 4.8 log CFU/g, but the samples with AIT/PLA film only had 2.8 log CFU/g. Similarly, AIT films significantly inhibited the growth of Listeria monocytogenes in grape and meat samples, as compared 4.0 log CFU/g with 1.8 log CFU/g for grape and 5.0 log CFU/g with 2.9 log CFU/g for meat, respectively. These data indicate that the AIT/PLA grafted packaging materials can deliver effective antimicrobials to food products and be used in food packaging.

8:55 Fabrication of antimicrobial packaging materials using natural polymers by coaxial-electrospray Zicheng Yi1, zyi@tnstate.edu, Ying Wu1, ywu@tnstate.edu, Richard Mu1, Tony Jin2. (1) Tennessee State U., Nashville(2) USDA Agricultural Research Service, Washington, DC The development of packaging materials with antimicrobial properties is of great importance to extend product shelf-life and reduce the risk of foodborne illness. In the current study, coaxial-electrospray technique was used to encapsulate nanoparticles using natural polymers, namely potato starch and water-soluble yellow mustard mucilage (WSM). Emulsions were prepared as the core material by mixing essential oils (thhymol: carvacrol at the ratio of 1:1), starch and WSM solution, and starch-WSM solution was prepared as the shell material. The core-shell structured nanoparticles were obtained by the co-axial electrospray. The resultant nanoparticles were evaluated on their morphology, particle size, encapsulation efficiency, releasing kinetics, and antimicrobial properties. The scanning electron microscopy (SEM) was used for morphology and size analysis. The results have indicated that the particles are sphere shaped with the size ranged from 81.21 nm - 84.85 nm. The encapsulation efficiency is 84.17 ± 0.04%. Compared to the nanoparticles without the shell layer, the releasing kinetics has demonstrated a significant slower release pattern at the first several hours after dissolved in water, with only 30% of the total essential oils released during the first 10 h. The antimicrobial efficacy of the packaging materials was evaluated against Escherichia coli and Staphylococcus aureus, and the results indicated that the nanoparticles had exhibited a significant antimicrobial activity. The results have confirmed that the shell of the nanoparticles can provide additional protection over the essential oil and can modulate the release pattern of the core materials over the time. Further studies will be carried out to study the effect of varied shell composition and thickness on release pattern of the antimicrobial agents.

9:20 Investigating chemical safety of a new N-halamine rechargeable antimicrobial coating for food processing equipment Yelena Sapozhnikova1, yelena.sapozhnikova@usda.gov, Raegyn Taylor1, Buket Demir2, Mingyu Qiao3. (1) Agricultural Research Service, USDA, Wyndmoor, Pennsylvania(2) Halomine, Inc., Ithaca, New York Novel N-halamine based antimicrobial coatings are highly advantageous due to their unique properties and low cost. Recently, their applications have been investigated in food safety, health care, water and air disinfection, and many other areas. In this study, we evaluated chemical migration of active components from a novel antimicrobial N-halamine polymer coating (Halofilm) designed for food processing equipment. Along with migration studies, stability and recovery tests were performed with formulation components: polyethylenimine (PEI), Trizma® base, and hydantoin acrylamide (HA) and dopamine methacrylamide (DMA) that are monomeric units of the N-halamine polymer. Four different treatment groups — negative control, positive control, Halofilm coating without chlorination, and Halofilm coating with chlorination — were tested at 40C with three food simulants (10, 50 and 95% ethanol/water) to mimic various food properties. Overall, measured concentrations of the migrated active components were consistent among food simulant types. When comparing migration results from different coating types, addition of the chlorination step led to fewer detections, possibly indicating a stabilizing effect on the polymer in the presence of food simulant. Only HA compound was detected in Halofilm coated and chlorinated tiles and at levels less than 0.05 mg/kg. Additionally, high resolution mass spectrometry (HRMS) analysis was employed to screen for migration of other extractable and leachable (E&L) chemicals, which led to the identification of eight possible common E&L chemicals.

10:00 Food safety applications of reversible guanylhydrazone antimicrobial agents William Hart-Cooper, hartcoop@gmail.com, Jong H. Kim, Jennifer Wilson-Welder, Kaydren Orcutt, William J. Orts. USDA Agricultural Research Service, Albany, California Guanylhydrazones, an emerging class of broad-spectrum antimicrobial agents, are promising alternatives to traditional preservatives, disinfectants, food processing aids and antibiotics. When diluted in water, hydrazones dissociate to relatively inactive, biodegradable subunits, reducing environmental persistence, ecological toxicity, and the potential for antibiotic resistance. Industry standard preservative and disinfectant tests show comparable performance between guanylhydrazones and traditional biocides, including isothiazolinones, formaldehyde releasers, quaternary ammonium compounds (“quats”), bleach and peroxides. Efficacy against bacteria, mold and yeast in food and consumer products are demonstrated. Antibiotic-alternative applications, such as treatments for digital dermatitis in livestock, show comparable performance between a prototypical guanylhydrazone and gold-standard antibiotics. Dissociation and mineralization studies, combined with a hazard analysis, show order-of-magnitude reductions in persistence and toxicity, both human and environmental, compared to traditional biocides.

10:25 Antimicrobial efficacy of fatty acid amide derivatives for inhibition and reduction of Listeria monocytogenes and other bacterial strain Ocen M. Olanya1, modesto.olanya@usda.gov, Yosief Hailemichael2, Richard Ashby3, Brendan Niemira1, Dike Ukuku1, Sudarsan Mukhopadhyay1, Joseph Msanne3, Majher I. Sarker3, Xuetong Fan1. (1) Food Safety and Intervention Technologies Research Unit, USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania (2) USDA-ARS ERRC (former employee), Wyndmoor, Pennsylvania(3) Sustainable Biofuels and Co-Products Research Unit, USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania Pathogenic bacteria such as Listeria are persistent impediments to food and consumer safety, especially on minimally processed fresh produce. The need for novel biodegradable compounds to mitigate foodborne pathogens, and enhance quality and consumer safety has increased,

due to demand-driven and consumer-oriented interests in food safety. Therefore, novel biorational inactivation measures are needed to combat bacterial contamination in food. The objective of this research was to determine the efficacy of pyrrolidine derivatives of decanoic (DEPY), lauric (LAPY), myristic (MYPY) and palmitic (PAPY) fatty acid amides (FA) for in-vitro inhibition and inactivation of Listeria monocytogenes, Bacillus subtilis (Natto), Streptococcus mutans and Streptococcus sobrinus; and to assess the FA amide efficacy for reduction of Listeria on produce. Significant inhibition ($P<0.05$) of bacterial strains by FA amides was observed. Similarly, inhibition was also significant ($P<0.05$) among Listeria strains with improved efficacy at higher concentrations of FA amides (10,000-20,000ppm). The in-vitro growth inhibition of B. subtilis, S. sobrinus and S. mutans was in the order of LAPY>MYPY>PAPY>DEPY. In co-inoculation assays, LAPY treatment significantly reduced Listeria populations by 1.55 to >5.0 Log CFU/mL at 5 to 250 ppm concentration range. Listeria populations on pathogen-inoculated produce were significantly ($P<0.05$) reduced by 0.51 to >3.00 Log and pathogen inactivation was significantly greater on carrots than alfalfa, soybean, and pistachio. These results demonstrate the antibacterial efficacy of these FA amides against L. monocytogenes and other bacteria. Biorational applications of these FA amides on produce in post-harvest interventions can enhance food safety.

10:50 Novelty of extraction of Rosmarinic acid from balm-mint /lemon balm (Melissa officinalis) using alkylation hydrocarbons at retrogression temperature for the use as food preservative and treatment of chronic viral diseases Salako N. Olatunji, salakoolatunji9@gmail.com. Chemical and Environmental technology, Center for Countermeasure against Chemical and Biological Warfare Agents, Oshodi, Lagos, Nigeria There several kinds of Organic or Natural Preservative agents that could be use as food additive, antioxidant and food flavoring. It is imperative for the quality control personnel or the scientist to find the best agent or natural preservative ingredient that could prevent the mucous and rancid from growing in the food product, and also would not be toxic to the respiratory tract of the ingested person, and would not affect the phase material and react with the product. It turns out that two components from Rosemary plant, Rosmarinic acid and Carnosic acid are responsible for long -time effect. Both inhibit the free radical chain reaction that leads to oxidation of fats and oil. However, they aren't responsible for flavor of rosemary. There is common preservative known to Chemists as butylated hydroxytoluene, commonly known as BHT, butylated hydroxy anisole, commonly known as BHA and tert-butylhydroquinone are antioxidants that prevent rancidity in fats and oils. Studies say they may cause cancer in rodents. Others preservative that helps fend off molds and other microbes are Potassium Sorbate and Sodium benzoate. These anti-microbes are widely used and generally view as save, not consumers can find their Chemical names off-putting (dislike it because it is Chemical). However, to prevent the growing of rancid and microbes in your product, you will have to use an organic synthesizing preservative agent that can serve as antioxidants and also add some flavor to your ingredients, and does not have toxicity effect when consume. The Organic preservative recommend for you to use is Rosmarinic acid and Carnosic acid derived from rosemary plant. The biosynthesis of Rosmarinic acid uses 4-coumaroyl-CoA from the general phenylpropanoid pathway as hydroxycinnamoyl donor. The hydroxycinnamoyl acceptor substrate comes from the shikimate pathway: shikimic acid, quinin acid and 3,4-dihydroxyphenyllactic acid derived from L-tyrosine.

Renewable Polymer Materials: Preparation, Processing, Application, and Disposal

8:05 Lignin-based thermoset and composite polymers for the circular economy Mahdi M. Abu-Omar, abuomar@chem.ucsb.edu, Melissa Sanchez, Peter C. Ford. Chemistry and Biochemistry, U. of California Santa Barbara Lignocellulose is the most abundant renewable carbon source on our planet. It offers an alternative and a complementary source to petrochemical refining for chemical production. However, utilization of biomass is underdeveloped. In particular, lignin is the largest source of naturally occurring phenols and is typically a waste byproduct of the paper industry and the biorefinery. Our research group has developed selective reaction chemistries that convert lignin into phenolic synthons. The renewable bio-phenols can be upgraded to polymers with advanced thermo-mechanical properties that rival those from petroleum. More than 40 million tons of thermosetting plastics are produced annually and 70% of those are epoxy polymers. The synthesis of bio-based epoxide provides a pathway for making renewable thermoset plastics. We describe in this study the use of a genetically modified high-S poplar lignin to produce 4-propyl-2,6-dimethoxyphenol (DMPP), which is converted to the tri-functional compound propylpyrogallol (DMPPO) by a reaction catalyzed by niobia oxide (Nb_2O_5) in water. The conversion of DMPPO to a novel tri-epoxide and its use to make thermoset polymers will be described. The implication and use of lignin synthons to make renewable and recyclable thermoset polymers will be discussed.

8:35 Design of thermoset polymerization and materials for energy and environmentally efficient applications Robert D. Allen, robert.allen@nrel.gov. Polymers and Composites for a Circular Economy, National Renewable Energy Laboratory, Golden, Colorado Thermosetting polymers are used in high performance applications including adhesives and composites. Network-forming curing of rigid thermoset polymers typically demands medium-to-high temperatures to avoid vitrification and extended cure times to insure complete polymerization. Large form-factor composite structures are particularly economically sensitive to cure times and temperatures. As part of an exploration on renewable thermoset chemistries, we have developed a dual cure strategy that combines two orthogonal polymerization mechanisms. We plan to discuss overall energy required for curing, control variables, morphology control, resulting mechanical properties and our attempts to circularize these thermoset materials. We have also developed a rubbery thermosetting platform that has demonstrated biodegradability. Synthesis, characterization and structure property relationships of this elastomeric platform will be discussed.

9:00 Trojan horse repeat sequences for triggered chemical recycling of polyesters for films and bottles Eric W. Cochran, ecochran76@gmail.com, Dhananjay Dileep, Ting-Han Lee, Michael J. Forrester, Tung-Ping Wang, Baker W. Kuehl, Demetrius Finley, Alexsei Ananin, George A. Kraus. Chemical and Biological Engineering, Iowa State U., Ames In this talk I will share or latest progress in low-energy poly(ethylene terephthalate) (PET) chemical recycling in water. In one example, PET copolymers with diethyl 2,5-dihydroxyterephthalate (DHTE) undergo selective hydrolysis at DHTE sites, autocatalyzed by neighboring group participation. Liberated oligomeric subchains further hydrolyze until only small molecules remain. Poly(ethylene terephthalate-stat-2,5-dihydroxyterephthalate) copolymers were synthesized via melt polycondensation and then hydrolyzed in 150–200 °C water with 0–1 wt% $ZnCl_2$, or alternatively in simulated sea water. Degradation progress follows pseudo-first order kinetics. With increasing DHTE loading, the rate constant increases monotonically while the thermal activation barrier decreases. The depolymerization products are ethylene glycol, terephthalic acid, 2,5-dihydroxyterephthalic acid, and bis(2-hydroxyethyl) terephthalate dimer, which could be used to regenerate virgin polymer. Composition-optimized copolymers

show a decrease of nearly 50% in the Arrhenius activation energy, suggesting a 6-order reduction in depolymerization time under ambient conditions compared to that of PET homopolymer. This study provides new insight to the design of polymers for end-of-life while maintaining key properties like service temperature and mechanical properties. Moreover, this chemical recycling procedure is more environmentally friendly compared to traditional approaches since water is the only needed material, which is green, sustainable, and cheap. The process can also be adapated to other "Trojan Horse" repeat units that offer advantages over the initially studied DHTE system.

9:25 Degradable and thermally stable Spiro polycycloacetals from renewable resources Minjie Shen, Srikanth Vijjamarri, Hongda Cao, Fahimeh Khakzad, Yanchun Tang, Elvis Enebeli, Megan L. Robertson, mlrobert@central.uh.edu. U. of Houston, Texas A series of partially bio-based spiro polycycloacetals were synthesized using bio-renewable feedstocks, such as vanillin and its derivative syringaldehyde, along with pentaerythritol and commercially available co-monomers including 4,4′-difluorobenzophenone and bis(4-fluorophenyl) sulfone. These spiro polycycloacetals displayed high thermal stabilities (degradation temperatures in the range of 343 – 370 °C, as quantified by 5% mass loss) and glass transition temperatures (in the range of 179 – 243 °C). Importantly, these polymers were effectively degraded to small molecules under acid-catalyzed hydrolytic conditions in less than 7 h. The kinetics of hydrolytic degradation was quantified through in situ NMR analyses.

10:05 Developing bio-based covalent adaptable network polymers with designed recyclability Ning Yan, ning.yan@utoronto.ca. Dept. of Chemical Engineering & Applied Chemistry, U. of Toronto, Ontario, Canada Pollution from waste plastics are exerting significant negative impacts on our ecosystem. Among various types of waste plastics that are typically end up in landfills, thermoset materials constitute a significant portion due to their lack of recyclability. Meanwhile, there is a growing interest in developing chemicals from bio-based building blocks to enhance sustainability. By integrating covalent adaptable networks (CAN) into a polymer's molecular structure, we can impart designed recyclability into the material to allow it to be repeatedly reformed after usage under external stimuli, such as under heat and pressure. This approach results in a new class of self-healing, recyclable, and reprocessable vitrimer materials that can extend product service life, reduce landfill wastes, and help realize the circular economy concept. We have developed various bio-based CAN materials using starch, chitosan, and lignin as the precursor. They all exhibited self-healing properties and recyclability with some materials even demonstrated upcycling abilities that allowed them to be strengthened as they were reformed. The synthesis methods, mechanisms for dynamic bond exchanges, and unique material attributes of these bio-based CAN materials will be discussed in this presentation. These novel bio-based polymers show great potential to replace fossil fuel dependent plastics to improve sustainability and reduce landfill wastes.

10:30 Developing a roadmap for bio-derivable and recyclable composites: Re-design and scale-up considerations Nicholas Rorrer, nicholas.rorrer@nrel.gov, Erik Rognerud, Michael McGraw, Ryan Clark, Robert D. Allen. National Renewable Energy Laboratory, Golden, Colorado Composites, often in the form of fiber reinforced plastics, are used in multiple facets of modern life from snowboards to vehicles, to wind turbines and beyond. Despite their prolific, and often renewable energy related uses, they are currently subject to a linear material economy from emission intensive precursors; thus, there is an opportunity to re-design these materials to be both bio-derivable and recyclable. In the present work, we provide a roadmap of what application considerations must be considered for vacuum assisted resin transfer molding (VARTM) processes for large composites materials at scale (e.g. infusible viscosities, moderate cure times, proper fiber adhesion, low cost, and maximum peak exotherm) when implementing bio-derivable and recyclable materials. We also provide illustrative concepts utilizing polyester covalently adaptable networks, from epoxy-anhydride chemistry, to achieve these goals. We further provide considerations when developing recycling process (e.g. maintenance of fiber sizing and orientation) and demonstrate these practices using low temperature methanolysis. Accompanying technoeconomic and life cycle analysis further illustrate the decarbonization benefits to bio-derivable and recyclable thermosets while informing future research and recycling processes. Finally, we provide a brief introduction to synergistic work within our team exploring how to further decarbonize the manufacturing of these materials.

10:55 Natural epoxy oil (Euphorbia oil) polymerization in liquid carbon dioxide-green media Zengshe Liu, kevin.liu@usda.gov. NCAUR, ARS, USDA, Peoria, Illinois Vegetable oils possess renewable advantages with non-toxic, non-polluting, biodegradable and environmentally friendly properties. Due to these properties, vegetable oils have been used in a variety of industrial applications, such as plastics, lubricants, adhesives, fuels/biodiesel, coatings, printing inks, varnish solvents and surfactants. Many researchers have reported the production of biodegradable polymers from vegetable oils, specifically from epoxidized soybean oil (ESO). However, ESO must be synthesized using conventional synthetic routes and some of the synthesized epoxide rings can degrade during the process. A plant oil with an epoxidized ring has been investigated to overcome this shortcoming. One such plant oil is euphorbia oil (EuO). This report discusses the ring-opening polymerization of EuO in liquid carbon dioxide-green solvent using boron trifluoride diethyl etherate (BF3OEt2) catalyst. A variety of analytical techniques have been used to characterize the materials, including FTIR, 1H-NMR, 13C-NMR, differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and gel permeation chromatography (GPC). Using subcritical carbon dioxide (CO2) and pressure of 65.5 bar, the ring-opening polymerization of euphorbia oil (RPEuO) occurred under mild conditions, such as at room temperature. It was found that the cross-linked polymers of RPEuO had glass transition temperatures ranging from -15.0 °C to -22.7 °C. RPEuO polymers were thermally stable below 220 °C, and decomposition occurred above 340 °C, according to TGA results.

11:20 Development of high-performance recyclable structural composites from vegetable oils Baoming Zhao, baoming_zhao@wsu.edu, Yiding Cao, Jinwen Zhang. Composite Materials and Engineering Center, Washington State U., Pullman The environmental impact of plastics has spurred the development of recyclable polymers from renewable feedstocks. Vegetable oils (VO), one of the most widely available and inexpensive biomass resources, have long been investigated as polymer precursors. However, most VO-based thermosets suffer from inferior thermomechanical performance. To address this issue, we developed a unique structural design that transforms VO into highly functional epoxy monomers and formulated high-performance epoxy resins with high bio-contents. In contrast to most VO-based bio-epoxies, which have limited reactivity and result in poor thermomechanical performance, our VO-epoxy incorporates a cyclic ring that enhances resin performance. The resin with 62.5 wt% bio-content exhibited mechanical, thermal, and weathering properties statistically similar to a commercial BPA epoxy. Furthermore, our VO-epoxy employs

terminal glycidyl ester type epoxides, which not only impart high reactivity to the epoxy but also make the resulting resin and composite inherently recyclable.

Sustainable Agriceuticals

8:03 In vitro study of polymethoxyflavones (PMFs) from orange peel for their potential to inhibit trimethylamine (TMA) and trimethylamine-N-oxide (TMAO)-producing enzymes and reduce TMA/TMAO production Yu Wang1,2, yu.wang@ufl.edu, Hana Lee1,2. (1) Food Sci. and Human Nutrition, U. of Florida Inst. of Food and Agricultural Sciences, Gainesville(2) Citrus Research and Education Center, U. of Florida Inst. of Food and Agricultural Sciences, Gainesville Orange peel, a by-product of orange juice production, is a rich source of polymethoxyflavones (PMFs) known for their health benefits. With cardiovascular disease (CVD) emerging as the leading cause of mortality worldwide, there is a need to reduce TMA-producing enzymes such as cntA/B and cutC/D that accelerate atherosclerosis and CVD. This study aimed to evaluate the effects of 13 naturally occurring PMFs on the inhibition of TMA/TMAO-producing enzymes and measure their potential to reduce CVD risk in vitro. Among the tested PMFs, nobiletin, 5-hydroxy-3,6,7,8,3',4'-hexamethoxyflavone, and sinensetin effectively reduced TMA production by inhibiting the cntA/B enzyme. On the other hand, 6,7,8,3',4'-pentamethoxyflavone, 3,6,7,8,2',5'-hexamethoxyflavone, and 3,5,6,7,8,3',4'-heptamethoxyflavone showed promising activities in inhibiting the cutC/D enzyme and reducing TMA production. Additionally, 3,6,7,8,2',5'-hexamethoxyflavone reduced TMAO production in TMA-induced HepG2 cells by down-regulating flavin-containing monooxygenase 3 and up-regulating farnesoid X receptor mRNA expression levels. These findings suggest that PMFs from orange peel could reduce the risk of CVD by inhibiting TMA and TMAO-related enzymes.

8:23 Elderberry fermentation promotes structural and metabolic changes to the gut microbiota Lin Liu[1], linshu.liu@usda.gov, Jenni Firrman[1], Adrienne Narrowe[1], Karley Mahalak[1], Johanna M. Lemons[1], Pieter Van den Abbeele[2], Aurélien Baudot[2], Stef Deyaert[2], Margaret Slavin[3], Liangli Yu[3]. (1) USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania (2) Cryptobiotix SA., Ghent, Belgium(3) Dept. of Nutri. and Food Sci., U. of Maryland at College Park Elderberries (EB) are a rich resource of polyphenolic compounds, such as anthocyanins and terpenes, etc.; the type and amount of those bioactives vary from fruit, flower, leaf and stem, but also depend on the species, growth environment, and processing conditions. EB polyphenols are consumed orally after processing as tinctures, syrups, capsules, or teas. From there they enter the gastrointestinal tract (GIT), where they are fermented by the gut microbiota. EB consumption is reported as having beneficial effects on human health; it can augment the immune system, relieve cold and flu symptoms, and help mitigate stress and inflammation. The mechanisms by which EB exerts these functions is not well studied, and for the most part, the physiologic pathways are unknown. Research on the interplay between EB and microbes that reside in the GIT is an emerging topic in recent years, which demonstrated the prebiotic property of EB, and its effect on some bacteria at the species level. In the present study, the effect of EB extract on the microbiome was tested using the fecal samples of 6 adults, using a previously described SIFR® ex vivo fermentation technology. Bacterial cell number and microbial composition were determined using flow cytometry and Shallow Shotgun sequencing technology, respectively. Metabolic activity was monitored by measuring total gas (H_2, H_2S, CO_2, and NH_3) released and the amount of short chain fatty acids (SCFA) produced. ANOVA was used to determine statistical significance. In this study, EB extract caused an increase in cell counts and alpha diversity, a slight increase to the Shannon index, and a limited, donor-dependent shift in beta-diversity. However, the relative amounts of P. Actinobacteria, P. Verrucomicrobia, and G. Ruminococcaceae were enhanced. The changes in these taxa corresponded to levels of SCFAs produced, especially propionate and butyrate. The present research showed that an abundance of physiologically active compounds could be produced by EB fermentation through modification of the gut microbiota. The information provided may be useful for further mechanistic studies and the development of EB-based functional foods.

8:43 Interaction between extracts of black cumin, turmeric, and Ceylon cinnamon and the human gut microbiome Karley Mahalak1, karley.mahalak@usda.gov, Lin Liu1, Adrienne Narrowe1, Jenni Firrman1, Johanna M. Lemons1, Pieter Van den Abbeele2, Aurélien Baudot2, Stef Deyaert2, Margaret Slavin3, Liangli Yu3. (1) Dairy and Functional Foods RU, US Dept. of Agriculture, Wyndmoor, Pennsylvania(2) Cryptobiotix SA, Ghent, Belgium(3) Dept. of Nutri. and Food Sci., U. of Maryland at College Park Many spices are used for both culinary purposes and in traditional herbal medicine practices. Three such spices are black cumin seed, turmeric root, and Ceylon cinnamon bark and are often associated with providing anti-inflammatory, antimicrobial, antidiabetic, and gastroprotective properties, among others. However, most studies on the health effects of these spices have not been performed in humans. Since many of the claimed health effects for the three spices involve gastrointestinal health, we explored the impact of black cumin seed extract (BCE), turmeric root extract (TRE), and Ceylon Cinnamon extract (CCE) on the human gut microbiome in vitro. To do so, we performed an ex vivo analysis over 48 hours, with fecal inoculum from 6 individual adult donors using the SIFR® technology. Using shotgun sequencing and flow cytometry, we determined that only treatment with CCE reduced microbial population growth when compared with control, and CCE and TRE increased the number of observed species, whereas BCE decreased in terms of Shannon's diversity index compared with control. Gas chromatography-Flame ionizing detection analysis was performed to understand the metabolic output of the gut microbiome with these treatments via short-chain fatty acid (SCFA) analysis. BCE treatment caused the greatest change in SCFA production compared with control, including an overall increase in SCFAs along with an increase in acetate, butyrate, and propionate. BCE also caused a significant decrease in pH compared with control and with TRE and CCE. These changes, along with changes caused by treatment of the gut microbiota with CCE and TRE, indicate that extracts from these spices may have an impact on the human gut microbiome that may provide an explanation for some of their purported beneficial health effects.

9:03 Human gut microbiome is rapidly and extensively altered by Senna sp. seed extracts Adrienne Narrowe1, adrienne.narrowe@usda.gov, Lin Liu1, Jenni Firrman1, Karley Mahalak1, Johanna M. Lemons1, Pieter Van den Abbeele2, Aurélien Baudot2, Stef Deyaert2, Margaret Slavin3, Liangli Yu3. (1) Dairy and Functional Foods Research Unit, Eastern Regional Research Center, USDA Agricultural Research Service, Wyndmoor, Pennsylvania(2) Cryptobiotix SA, Ghent, Belgium(3) Dept. of Nutri. and Food Sci., U. of Maryland at College Park Senna obtusifolia (alt. Cassia obtusifolia) is a globally distributed plant of which the leaves, roots, and seeds have multiple traditional medicinal and nutritional uses. The seeds are rich in anthraquinones, including emodin, which contributes to the plant's established laxative effects, and studies on a limited number of microorganisms have demonstrated the selectively potent antimicrobial property of seed extracts. Here we used carbohydrate-free ethanol extracts of S. obtusifolia seeds to assess the specific effects of the polyphenolic

compounds on the human gut microbiome via short-term incubation using the SIFR® (Systemic Intestinal Fermentation Research) technology. After a 48-hour human fecal incubation, we measured total bacterial cell counts and fermentation products including pH, gas production and concentrations of short chain fatty acids. The initial and post-incubation microbial community structure and functional potential were characterized using shotgun metagenomic sequencing. S. obtusifolia seed extracts displayed strong, taxon-specific anti-microbial effects as indicated by significant reductions in cell counts (40%) and intra-sample community diversity. Members of the Bacteroidetes and Firmicutes were nearly eliminated over the 48-hour incubation with a resultant increase in the proportion of Enterobacteriaceae. The active persistence of the members of the Enterobacteriaceae despite the reduction in overall cell numbers was demonstrated by increased fermentative outputs including high concentrations of gas and acetate with correspondingly reduced pH. A potential mechanism by which these bacteria may detoxify or utilize phenolic components of the S. obtusifolia seeds was identified by analysis of the functional capacity of the microbial community, which suggested that the extracts selected for taxa that encode genes to breakdown polyphenolic compounds. As the effects of functional foods on the human digestive tract are mediated by interactions with the gut microbiome, research regarding these interactions yields knowledge to empirically guide existing usage and to unlock new potential for bioactive compound discovery.

9:23 Monitoring the cellular response to whole food digests Johanna M. Lemons1, johanna.lemons@usda.gov, Elliot S. Friedman2, Dylan Curry2, Fuhua Hao3, Andrew Patterson3, Lin Liu1, Gary D. Wu2. (1) Dairy and Functional Foods, USDA Agricultural Research Service, Wyndmoor, Pennsylvania(2) Division of Gastroenterology, U. of Pennsylvania Perelman School of Medicine, Philadelphia(3) Biochemistry & Molecular Biology, The Pennsylvania State U., U. Park There is a large body of research examining the health benefits of food derived compounds, dubbed nutraceuticals. These molecules include polyphenols, fiber, polyunsaturated fatty acids and are often a subset of those found in healthy foods, like fruits, vegetables, fish, and nuts. Targeted mechanistic studies have described the mode of action for many individual compounds, but these are rarely consumed in isolation. A reductionist approach fails to capture the collective/synergistic cellular effects of all compounds derived from a particular food matrix. Indeed, human nutrition research is increasingly focused on the benefits of consuming specific whole food diets, not individual nutrients. We have developed a method of making cell culture media from whole foods or meals using an in vitro processes that mimics human digestive physiology. Other than the nutrients derived from the foods, the culture media is fully defined so alterations in cellular response can be directly attributed the nutrient composition of the digest. Using metabolomics, we show that the in vitro digests release nutrients in a predictable fashion. Preliminary results provide evidence for differential effects of food digests on both the growth and barrier function of Caco-2 cells, a commonly used model of the small intestinal epithelium. We aim to differentiate cellular utilization versus cellular transport of nutrients as well as monitor the effect of different food digests on global transcriptional changes. So far, we have utilized this platform to ask whether the cellular response is different when exposed to plant versus meat products with different degrees of food processing, but it could also be leveraged to explore how different foods impact immunity, disease state, pathogen engraftment, drug uptake and changes in gut microbiome diversity.

9:43 2′- Fucosyllactose modulates the function of intestinal microbiota to reduce intestinal permeability in mice colonized by feces from healthy infants Bailiang Li, 15846092362@163.com, Qingxue Chen, Zhengtao Guo, Rui Zhang. Northeast Agricultural U., Harbin, China 2′-Fucosyllactose (2'-FL) shows the potential to support intestinal health as a natural prebiotic that bridges the gap between infant formula feeding and breastfeeding. However, the effect and mechanism of 2'-FL in improving intestinal permeability are not clear. In this study, we constructed human microbiota-associated (HMA) mouse models by colonizing healthy infant feces in mice with antibiotic-depleted gut microbes. The protective effect of 2'-FL on the intestinal permeability was explored using the HMA mouse models, and the combination of macrogenomics was used to analyze the possible mechanisms by which the microorganisms reduced the intestinal permeability. The results showed that 2'-FL decreased the levels of the serum markers of intestinal permeability (enterotoxin and DAO). Macrogenomics revealed the enrichment of Bifidobacteria and increased the expression of glycoside hydrolases (GHs), including GH31, GH28, and GH5. In conclusion, 2'-FL strengthened intestinal permeability function by improving microbial composition to control the translocation of harmful substance.

10:13 Lactobacillus plantarum ZJUIDS04 alleviates DSS-induced colitis by regulating the immune response and modulating gut microbiota Chongwei Yu, Qinchao Ding, Daxi Ren, dxren@zju.edu.cn. Zhejiang U. Inst. of Dairy Science, Hangzhou, China Gut microbiota dysbacteriosis has always been considered as a key factor in the pathogenesis of inflammatory bowel disease (IBD). Probiotics could improve intestinal symptoms and reduce damage in patients with IBD by gut modulation. In this study, we evaluated the therapeutic effect of Lactobacillus plantarum ZJUIDS04 on dextran sulfate sodium (DSS)-induced colitis in C57BL/6 mice. Results showed that after Lactobacillus plantarum ZJUIDS04 intervention DSS-induced colitis mice, the disease activity index (DAI) and colonic tissue damage and inflammatory response were reduced, colonic shortening was inhibited, the expression of intestinal tight junction (TJ) proteins (ZO-1, occludin and claudin-1) was recovered. Furthermore, 16S rRNA sequencing demonstrated that Lactobacillus plantarum ZJUIDS04 reduced intestinal microbiota dysbiosis in DSS-induced colitis mice, including a decrease in Proteobacteria at the phylum level and Escherichia-Shigella at the genus level, an increase in Akkermansia, and an increase in short-chain fatty acid (SCFA) content. Overall, Lactobacillus plantarum ZJUIDS04 pretreatment effectively alleviates sodium dextrose sulfate-induced colitis by modulating the immune, maintaining the intestinal barrier responses and improving the microbial community.

10:33 Potential health benefits of upcycled romaine lettuce powder on metabolic syndrome Eli Teran-Cabanillas1, eteranc@uas.edu.mx, Karla F. Garcia Rocha1, Ulises Osuna Martinez1, Wallace H. Yokoyama2, Roberto Avena Bustillos2. (1) Nutrition, U. Autonoma de Sinaloa, Culiacan, Mexico(2) USDA-ARS Western Regional Research Center, Albany, California During harvesting of Romaine lettuce, the outer leaves are discarded in the field, which presents an excellent opportunity for upcycling. We previously developed Romaine lettuce powder (RLP) using these outer leaves, which possesses high levels of fiber, total soluble phenolics (TSP), and a remarkable antioxidant capacity. In this study, we assessed the preventive effects, and health benefits of RLP in mice fed with a high-fat diet that induced metabolic syndrome (MS). The mice that received a 10% RLP supplement in their high-fat diet showed reduced glucose and insulin levels and the prevention of insulin resistance. Additionally, adipose tissue and liver weight were lower in the group fed with a high-fat diet supplemented with 10% RLP compared to the high-fat and standard diet. Moreover, mice fed with 10% RLP showed reduced

microvesicular steatosis and hepatic vasodilation, compared to the high-fat diet-fed mice, indicating a potential positive effect of lettuce powder on liver health. Our findings suggest that incorporating RLP into the diet may also benefit human health.

10:53 Potential of mealworm (Tenebrio molitor larva) protein: Improvement of its techno- and health functional properties via various extraction methods and purification Eunyoung Oh1,2, Yookyung Kim1,2, yookyung_kim@korea.ac.kr. (1) Dept. of Human Ecology (Food Sci. and Nutrition), Graduate School, Korea U., Seongbuk-gu, Seoul 136-701, Korea (the Rep. of)(2) Interdisciplinary Program in Sustainable Living System, Graduate School, Korea U., Seongbuk-gu, Seoul 136-701, Korea (the Rep. of) Mealworm (Tenebrio molitor larva) is an edible insect considered a highly nutritious protein source. Due to their lower environmental impact, the insect could be regarded as a sustainable protein replacement, contributing to improved food product applications via protein extraction. Bioactive peptides produced from protein hydrolysis are easily digestible and have specific biological activities in the body. Indeed, they have recently received attention as alternative chemotherapeutic agents by modulating and improving physiological functions. To investigate the effects of protein extraction methods on techno- and health functionalities, we obtained extracts using four different treatments: alkali (AE), enzyme (EE), salt (SE), and pressure (insoluble protein: PEF; soluble protein: PES). Additionally, we prepared fractions with subsequential fractionation and purification process to determine the novel peptides preventing muscle atrophy. Mealworm protein hydrolysate was purified by molecular weight cut-off (MWCO), anion exchange (AEX), and reverse-phase HPLC (RP-HPLC) and evaluated its expression levels of myostatin (a negative regulator of muscle synthesis). As a result, EE (1.66±0.30 mg/ml) had the lowest IC50 value of ABTS scavenging activity among all the samples (AE: 10.68±0.48 mg/ml; SE: 2.72±0.24 mg/ml; PEF: 3.98±0.05 mg/ml; PES: 2.38±0.38 mg/ml). The IC50 values of DPPH scavenging capacity of SE (3.27±0.58 mg/ml) and PES (3.16±0.32 mg/ml) were lower compared to that of AE (10.91±1.28 mg/ml), EE (4.34±0.44 mg/ml), and PEF (6.35±1.44 mg/ml). Solubility levels of EE (ranged from 99.13% to 99.89%) and SE (91.53%~99.53%) were significantly higher than those of AE (0.12%~29.56%), PEF (6.92%~99.93%), and PES (54.47%~99.87%) at different pH levels. We also evaluated their myostatin expression levels of fractions and determined the most-effective fractions in each purification step. As a result of peptide profiling, seven peptide sequences were identified. Overall, our findings suggest that protein extraction methods significantly influence their techno- and health functionalities. The purification of bioactive peptides could have improved potential for preventing muscle atrophy, thereby providing health benefits.

11:13 Prebiotic potential of water-soluble yellow mustard mucilage: Microbial evaluation on gut health promotion CheKenna Fletcher, cfletch6@tnstate.edu, Ying Wu. Agricultural and Environmental Sciences, Tennessee State U. College of Agricultural Human and Natural Sciences, Nashville Gut health is a crucial part of one's overall health as it can affect many parts of the body. Both probiotics and prebiotics can stimulate the growth of healthy bacteria in the gut. Currently, novel materials are sought as encapsulation agents for probiotics to provide additional health benefits to enhance the health of the gut. Water soluble yellow mustard mucilage (WSM) was well proven with antioxidant activities and can protect bioactive compounds from gastrointestinal environment. It was also reported with great emulsification and stabilization effect. However, the probiotic potential of WSM has not been evaluated previously. Therefore, in the current study, WSM solutions were prepared to treat bacterial strains including Lactobacillus casei, L. acidophilus, and Bifidobacterium breve. The growth performances of the tested strains were recorded to compare with the prebiotic treatment groups including inulin and galacto-oligosaccharides, at similar concentrations. The immunomodulatory activity was measured by the ability to regulate the production of the pro-inflammatory chemokine IL-8 following TNF-α stimulation of HT-29 cells. The results have indicated that the WSM solutions have exhibited promoting effect on the tested probiotics. It also exhibited better effect on regulating chemokine IL-8 compared to the other prebiotic parallels. The results have indicated that when using WSM as an encapsulation, WSM may not only protect the probiotic strains over the gastrointestinal environment but also promote the growth of the probiotics at neutral pH conditions. Further studies will be carried out to investigate the encapsulated synbiotic products using WSM, and the corresponding promoting effect on gut health.

11:33 Functionalized nanoclays as sustainable carriers for antimicrobials and festicides Ofer Prinz Setter, Sandeep Sharma, Hanan Abu Hamad, Naama Ivanir, Ester Segal, esegal@technion.ac.il. Biotechnology and Food Engineering, Technion Israel Inst. of Technology, Haifa, Israel The magnitude of global food loss and waste together with the increasing extent of plant diseases, which are estimated to destroy a third of all food crops annually, pose major threats to global food security, economy, and the environment. These staggering figures emphasize the need to develop multifaceted sustainable solutions to reduce food loss throughout the entire supply chain and protect crops. This work describes the use of halloysite nanotubes (HNTs), a natural mineral clay composed of alternating layers of silica and alumina geologically rolled into mesoporous tubular particles which are abundant and considered as environmentally-friendly, as a smart carrier for a wide range of bioactive molecules. Upon careful functionalization of these nanotubes, we demonstrate that they can carry a range of sensitive antimicrobials and release them in a sustained or a triggered manner. These carriers can be also modified to selectively bind to target bacterial cells in suspension. Such systems can allow us to treat target cells within a challenging heterogeneous population while minimizing the impact on the natural flora. Thus, the intriguing nano-bio interface of HNTs enables to design tailored solutions for numerous agricultural, environmental, biotechnological, and even medical challenges, and may present a safer, sustainable, and more affordable alternative for other synthetic nanomaterials. Yet, future research has to fully elucidate the long-term impact of HNTs (pristine and modified) on human health and ecology.

Virtual Session - ACS Microbiome Consortium Kick off Symposium

10:05 Investigating the molecular mechanism of anthocyanins in ameliorating type 2 diabetes and ulcerative colitis from the perspective of modulating gut microbita composition and metabolites Wei Chen, zjgsuchenwei@zjgsu.edu.cn. Dept. of Food Sci. and Nutrition, College of Biosystems Engineering and Food Sci., Zhejiang U., Hangzhou, China Anthocyanins are phenolic compounds that exerts various biological activities, such as anti-diabetic, anti-obesity, anti-inflammation, antioxidant, etc. Increasing evidence indicates that anthocyanins show beneficial effects on type 2 diabetes (T2D) and dextran sulfate sodium (DSS) induced ulcerative colitis, but the underlying mechanism remains unclear. In the present study, the hyperglycemia-lowering activity of pelargonidin-3-O-glucoside (Pg3G) purified from wild raspberry was investigated in high-glucose/high-fat (HG+HF)-induced hepatocytes and db/db diabetic mice. The results suggested that Pg3G promoted glucose uptake in HG+HF-induced hepatocytes. In vivo study showed that Pg3G contributed to the improvement of insulin sensitivity, glucose tolerance, and induction of autophagy.

Pg3G modified the gut microbiota composition, which was indicated by an increased abundance of Prevotella, and elevated Bacteroidetes/Firmicutes ratio. Pg3G administration also significantly increased the fecal concentration of total SCFAs (short chain fatty acids), including propionic acid, acetic acid, isobutyric acid, butyric acid, and valeric acid in diabetic mice. The results indicated an involvement of SCFAs on the protective effect of Pg3G against T2D. Then, the protective action of mulberry anthocyanins (MAS) on dextran sulfate sodium (DSS) induced colitis was investigated. Mice were treated MAS by gavage for 1 week, and then DSS was added to the drinking water for 7 days. MAS was administered for a total of 17 days. The results suggested that oral gavage of MAS reduced the disease activity index (DAI), prevented colon shortening, attenuated colon tissue damage and inflammatory response in mice with DSS-induced colitis. In addition, analysis of 16S rRNA amplicon sequences showed that MAS reduced the DSS-induced intestinal microbiota dysbiosis, which was indicated by a reduction in Escherichia-Shigella, an increase in Akkermansia, Muribaculaceae and Allobaculum. Collectively, the results unveil novel mechanisms for natural anthocyanins preventing type 2 diabetes and ulcerative colitis through modulating gut microbita composition and metabolites, suggesting the potential application of anthocyanins for type 2 diabetes and ulcerative colitis therapeutics.

10:50 Modulatory effects of tea consumption on gut microbiota and gut microbiota-related metabolites Mingzhi Zhu, mzzhucn@hotmail.com, Jian-An Huang, Zhong-hua Liu. Hunan Agricultural U., Changsha, Hunan, China Tea is one of the most popular beverages worldwide, which possesses a wide range of beneficial effects for human health. Tea polyphenols (TP) and tea polysaccharides (TPS) are considered as the main active ingredients of tea. However, the bioavailability of TP is generally low, with only a small portion directly absorbed in the small intestine; TPS cannot be absorbed by the small intestine completely. The majority of ingested TP and TPS reach the large intestinal lumen, and interact with gut microbiota. Gut microbiota has been demonstrated to be tightly associated with host health. The interactions of TP and TPS with gut microbiota will lead to the alterations of gut microbiota composition and the production of gut microbiota-related metabolites including short chain fatty acids, amino acids, bile acids, accordingly exerting their biological effects both locally and systemically. Some specific gut bacteria have been found in the process of TP and TPS intervention. We further discuss how TP and TPS impact the host health via gut microbiota from the viewpoint of gut organ/tissue axis. Tea consumption and dietary supplementation with tea active ingredients represent an attractive alternative toward promoting human health.

11:10 Systematic evaluation of metabolites composition and antioxidant activity of anthocyanin-rich berry extracts subjected to gut microbiota fermentation Lianghua Xie, 11613026@zju.edu.cn, Wei Chen. Dept. of Food Sci. and Nutrition, College of Biosystems Engineering and Food Sci., Zhejiang U., Hangzhou, China Anthocyanins are naturally occurring compounds widely exist in berries, and increasing evidence demonstrates that the beneficial properties attributed to the intake of berry fruits (blackberry, mulberry, blue honeysuckle, blueberry, raspberry, strawberry, bayberry) are associated with the presence of high content of anthocyanins. Recent studies have found that anthocyanins are susceptible to metabolism by gut microbiota, and the metabolites of anthocyanins subjected to gut microbiota fermentation were reported to show potent biological activities. In the present study, three representative anthocyanin-rich berry extracts (blackberry, mulberry and blue honeysuckle) were prepared and subjected to in vitro human gut microbiota fermentation at different time intervals (0 - 48 h) to study their gut metabolites and antioxidant properties. The content of cyanidin-3-O-glucoside was found to be the highest in blackberry, which degraded completely after 6 h of fermentation. Cyanidin-3-O-glucoside and cyanidin-3-O-rutinoside were the major anthocyanins in mulberry extracts. Cyanidin-3-O-glucoside was identified as the predominant anthocyanin in blue honeysuckle extracts. After gut microbiota fermentation, the contents of anthocyanins were increased initially, then decreased with time, and some anthocyanin metabolites (such as gallic acid, ferulic acid, 3,4-Dihydroxybenzoic acid, 2,4,6-trihydroxybenzoic acid, 2,4,6-trihydroxybenzaldehyde, etc.) were detected. Gut metabolites of blackberry extracts were found to improve the glucose consumption and glycogen content significantly in HepG2 cells. Furthermore, gut metabolites of blackberry extracts significantly ameliorated high glucose plus palmitic acid (HG + PA)-induced ROS, mitochondrial membrane collapse, and glutathione depletion in HepG2 cells. Cellular study indicated that mulberry extracts possessed reactive oxygen species scavenging capacity after gut microbiota fermentation. Digested blue honeysuckle extracts at a concentration 1.0 mg/mL exhibited significant ($p < 0.05$) protective effect against EC-induced cytotoxicity in Caco-2 cells via inhibiting ROS and superoxide anion accumulation, attenuating GSH depletion, and inhibiting mitochondrial membrane potential collapse. In conclusion, this study reported the metabolites composition and antioxidant activity of anthocyanin-rich berry extracts subjected to gut microbiota fermentation, which suggests berry as a dietary source to be considered as functional food.

11:30 Development and utilization of lactic acid bacteria resources Zhihong Sun, sunzhihong78@163.com, Feiyan Zhao. Inner Mongolia Agricultural U., Hohhot, China Lactic acid bacteria are indispensable strategic resources for the sustainable development of related industries such as fermented dairy products, probiotics, medicine and so on. Since 2001, our team has collected 5,188 samples of naturally fermented dairy products, fermented foods, breast milk and baby feces from 27 countries including China, Mongolia, and Russia, and isolated and identified 37,309 lactic acid bacteria strains, including 33 genera, 138 species, and subspecies, among which, the largest lactic acid bacteria resource pool in the world has been established. The "10k-strain Lactic Acid Bacteria Genome Project" was launched and an accurate probiotic screening platform based on genomic big data and artificial intelligence was constructed. According to the characteristics of intestinal microorganisms and the interaction of intestinal microflora in the population of China, the screening technology of probiotic lactic acid bacteria was developed. A total of 68 probiotics lactic acid bacteria with beneficial functions such as immune regulation, intestinal flora regulation, blood lipid reduction, and blood pressure reduction were screened out, including Lacticaseibacillus casei Zhang, Bifidobacterium animalis subsp. lactis V9, Lactiplantibacillus plantarum P-8, Bifidobacterium animalis subsp. lactis Probio-M8, and Lacticaseibacillus rhamnosus Probio-M9. Completed 32 clinical studies of probiotic lactic acid bacteria, exploring their beneficial functions of preventing upper respiratory tract infection, relieving stress and anxiety, and relieving polycystic ovary syndrome. The results showed that Lacticaseibacillus casei Zhang helped rejuvenate the human intestinal flora and rapidly activated the production of immunoglobulin G; Bifidobacterium animalis subsp. lactis V9 promotes the proliferation of intestinal short-chain fatty acid-producing bacteria, and the interaction of short-chain fatty acids and neurotransmitters regulates the level of pituitary hormones secreted by the pituitary gland of patients with polycystic ovary syndrome through the intestine-brain axis. Lactiplantibacillus plantarum P-8 remarkably increase that content of beneficial bacteria such as Leuconostoc and Lactobacillus in the intestinal tract and relieves the stress of mental anxiety and adult stress.

12:05 Impact of gut microbiota on avenanthramide metabotype from whole grain oat intake Shengmin Sang, ssang@ncat.edu. North Carolina Agricultural and Technical State U., Kannapolis As a distinct grain, oat has been widely accepted as a key food for human health. It is becoming increasingly evident that individual differences in metabolism determine how different individuals benefit from diet. Both host genetics and the gut microbiota play important roles on the metabolism and function of dietary compounds. Recently, we used the combination of in vitro incubation assays with human gut microbiota and mouse and human S9 fractions, chemical analyses, germ-free (GF) mice, 16S rRNA sequencing, gnotobiotic techniques, and a human feeding study to pinpoint the mechanism of individual variations in response to whole grain (WG) oat intake. Our results demonstrated that gut microbiota mediates the metabolism of avenanthramides (AVAs), the signature bioactive polyphenols of WG oat, into their dihydro forms, dihydro-AVAs (DH-AVAs). We observed inter-individual variations on the metabolism of AVAs to DH-AVAs associated with Faecalibacterium prausnitzii (F. prausnitzii) relative abundance. The AVAs converting capabilities of the fecal slurries from each subject were consistent with their urinary pharmacokinetic results of DH-AVAs in a human feeding study taking oat bran as breakfast. Moreover, as opposed to GF mice, F. prausnitzii-monocolonized mice were able to metabolize AVAs to DH-AVAs. These findings demonstrate that the presence of intestinal F. prausnitzii is indispensable for proper metabolism of AVA in both human and mice. We propose that the abundance of F. prausnitzii can be used to subcategorize individuals into AVA metabolizers and non-metabolizers after WG oat intake. Our work paves the way for future explorations of how F. prausnitziiimpacts the health benefits of oat intake.

12:50 Gut microbiota, metabolites and pancreatic diseases Jia Sun, 65022900@qq.com. Jiangnan U., Wuxi, Jiangsu, China Gut microbiota and metabolites play a crucial role in human physiology. Importantly, they influence the susceptibility of the host to pancreatic diseases. Diseases intrinsic to the pancreas such as pancreatitis, pancreatic cancer and type 1 diabetes are reported to be associated with gut dysbiosis, implying an indispensable role of gut microbiota in pancreatic diseases. One of the primary modes by which the gut microbiota interacts with the host is through their metabolites. Based on this, we proposed a pathogenic pathway “gut microbiota—metabolites—antimicrobial peptides—immune deregulation—pancreatic diseases” and deciphered the mechanisms linking gut microbiota to pancreatic diseases (Immunity, 2015; Gastroenterology, 2022). Besides, we found that therapeutic interventions (probiotics, prebiotics and gut microbial metabolites) could modulate the structure of gut microbiota and production of their metabolites, thereby affecting immune homeostasis and alleviating pancreatic diseases (Acta Pharm Sin B, 2021&2023; Br J Pharmacol, 2019&2021; Mol Nutr Food Res, 2019&2022; J Agric Food Chem, 2020&2023). Collectively, a better understanding of the host-microbiota interactions would help identify novel microbial targets for future precision therapeutic modulation of pancreatic diseases.

1:10 Akkermansia muciniphila-derived outer membrane vesicles alleviate ulcerative colitis by regulating the intestinal barrier Ting Zheng1,2, 17861506680@163.com, Jiankun Li1,2, 1328247259@qq.com, Yukun Yao1,2, Yisuo Liu1,2, Qiqi Liu1,2, Huaxi Yi1,2, yihx@ouc.edu.cn. (1) Ocean U. of China, Qingdao, Shandong(2) Food Laboratory of Zhongyuan, Luohe, China The development of ulcerative colitis is linked to disruption of the intestinal barrier, and the regulation of intestinal barrier has become a significant treatment for ulcerative colitis. Akkermansia muciniphila-derived outer membrane vesicles (Akk OMVs) are nano-vesicles that contain multiple bioactive macromolecules with the potential to modulate the intestinal barrier. The effect of Akk OMVs on the intestinal barrier of mice with ulcerative colitis was investigated. The results showed that Akk OMVs could effectively alleviate colitis symptoms, improve blood in stool and weight loss, inhibit the shortening of the colon, and reduce edema and inflammatory infiltration of colonic tissue in mice. Meanwhile, Akk OMVs significantly decrease serum inflammatory factors (IL-6, IL1β, IL-17A, TNF-α), DAO, DLA, and LPS levels, and significantly up-regulate serum IgA and sIgA levels, increase colonic tissue tight junction proteins (ZO-1, Occludin, JAM-1, Claudin-1, MUC2) and the levels of short-chain fatty acids propionic acid, butyric acid, isobutyric acid and isovaleric acid in the feces of mice ($P<0.05$). In conclusion, Akk OMVs could improve intestinal barrier function and ameliorate ulcerative colitis by modulating the inflammatory response, decreasing intestinal permeability, promoting the synthesis of short-chain fatty acids, and regulating intestinal barrier gene expression.

1:30 Health effects of pectin: reshaping gut microbiota and circulating metabolites Shaoping Nie, spnie@ncu.edu.cn, Huizi Tan, Linlin Fan, Quanyong Wu, Qianhuang Xiao, Menglin Chen. State Key Laboratory of Food Sci. and Tech., China-Canada Joint Laboratory of Food Sci. and Tech. (Nanchang), Key Laboratory of Bioactive Polysaccharides of Jiangxi Province, Nanchang U., Jiangxi, China Pectin is one of the functional dietary fibers widely existing in plant cell walls. It has been under long-term development as a safe and natural food additive, and the application scope may be directly influenced by the degree of esterification (DE). In this study, the differentiated effects of high-DE and low-DE pectin on health conditions associated with colonic inflammation or induced by a high-fat diet and low-dose antibiotics. Low-esterified pectin displayed significant improvements in pathological markers such as body weight, cytokine expressions, fasting blood sugar, intestinal barrier, and liver functions. The relevance of the varied profiles of gut microbiota and serum metabolites mediated by pectin to the health indicators was investigated. The beneficial roles of Bifidobacterium longum, which is one of the dominant intestinal bacteria, were further analyzed to decipher the underlying mechanism of gut microbiota on the health effects of pectin. The results provide evidence for the further analysis of the structure-function relationship of pectin and the development of customized food and healthcare products.

WEDNESDAY AFTERNOON

Chemical Intervention Technology to Improve Microbial Stability of Food

2:05 Photo-sensitive vitamin compounds as potential antimicrobial agents for food safety applications Gang Sun1, gysun@ucdavis.edu, Zheng Zhang1, Luxin Wang2. (1) Biological and Agricultural Engineering, U. of California Davis(2) Food Sci. and Tech., U. of California Davis Recent research results have revealed several vitamin compounds possessing photo-sensitive functions and could effectively produce reactive oxygen species (ROS) under different lighting conditions. These compounds, sharing structural features as photosensitizers, are water soluble and insoluble vitamin K and vitamin B2 derivatives. The light-induced ROS could demonstrate efficient antimicrobial functions in different media under UVA or daylight exposure. Due to the fact of edible natures and the photo-induced antimicrobial functions, these compounds could have great potentials in microbial control of food products for improved safety performance. This presentation will provide a detailed overview of the structural features and photo-reaction mechanisms, as well as dominating ROS produced, suitable application conditions, and limitations, of these vitamin compounds.

2:30 Photodynamic inactivation of plant pathogenic fungus on fresh produce using food-grade plant-derived antimicrobials and sunlight Yoonbin Kim1, csbkim@ucdavis.edu, Cuong H. Nguyen1, Ahmed El-Moghazy1, Hefei Zhao1, Selina Wang1, Nitin Nitin1,2, nnitin@ucdavis.edu. (1) Dept. of Food Sci. and Tech., U. of California Davis(2) Dept. of Biological and Agricultural Engineering, U. of California Davis Fungal pathogens are a major challenge in agriculture production, resulting in a significant loss in crop yields and excessive use of chemical fungicides. Antimicrobial resistance among fungal pathogens against conventional fungicides further highlights the need to develop sustainable alternatives. This study aimed to develop photodynamic antifungal treatments using food-grade extracts and compounds with ambient sunlight to create sustainable solutions to control fungal pathogens in agricultural production. The food-grade extracts and compounds evaluated in this study include olive pomace extract (OPE) and curcumin. The efficacy of the photodynamic approach was evaluated against Alternaria alternata on a tomato leaf and Botrytis cinerea on a strawberry plant as model systems, respectively. The results demonstrate a significant reduction (ca. 2.3 log reductions) in the number of culturable A. alternata conidia inoculated on tomato leaf (ca. 4.73 ± 0.21 log conidia/cm2) within 30 min of the photodynamic treatment using OPE and sunlight. Based on the in vivo study, the combined treatment of OPE with sunlight effectively suppressed the spread of Alternaria infection on the tomato leaf. The size of the Alternaria infection increased significantly on the tomato leaf that are treated only with water, OPE, or sunlight within 5-7 days of incubation. In contrast, the photodynamic treated samples showed no significant increase even after 10 days of incubation. The antifungal activity of the combined treatment of curcumin and sunlight was evaluated against B. cinerea infection on a strawberry plant. The number of culturable B. cinerea conidia inoculated on the strawberry plant showed ca. 2.7 log reduction within 30 min of the photodynamic treatment, whereas those treated only with water, curcumin, or sunlight showed ca. 0.0, 0.5, and 1.1 log reductions, respectively. Interestingly, the antifungal efficacy of the combined treatment was further enhanced by depositing the curcumin on the cellulose nanofiber (CNF). The populations of conidia inoculated on the strawberry plant decreased below the detection limit (1.0 log conidia/cm2) within 30 min when treated with CNF-bound curcumin and sunlight. Together, these results suggest a strong potential for photodynamic antifungal treatments using food-grade extracts and compounds as a safe and sustainable antifungal strategy to effectively control plant pathogens on fruits and vegetables.

2:55 Chlorine dioxide fumigation of fresh produce and nuts: microbial reduction and quality change Xuetong Fan, xuetong.fan@usda.gov. USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania There have been a number of salmonellosis outbreaks associated with fresh produce and nuts, such as tomatoes and almonds. Gaseous chlorine dioxide is a potent fumigant against various microorganisms. Therefore, the effectiveness of gaseous chlorine dioxide in inactivating Salmonella spp. were evaluated on tomatoes, blueberries and almonds. Results show that the efficacy of gaseous chlorine dioxide depends on the concentration, duration, and the temperature and relative humidity during treatments. More than 4 log reductions of Salmonella populations can be achieved on the surfaces of fresh produce and almonds, with appropriate treatment conditions. In general, there are limited changes in sensorial or nutritional quality of tomatoes and blueberries after treatment. However, chlorine dioxide induces the formation of a few chlorine-containing compounds in almonds, which mostly dissipate during storage. In addition, increased rate of lipid oxidation and production of volatile acids, aldehydes and alcohols are observed in almonds during storage. Overall, our results demonstrated that the application of chlorine-dioxide fumigation should be carefully evaluated in order to determine conditions that exert minimal impact on quality attributes, while achieving desirable pathogen reductions.

3:35 Combined effects of microencapsulated essential oils and γ-irradiation on microbiological and physicochemical properties of dry fermented sausages during ripening and storage Monique Lacroix, monique.lacroix@iaf.inrs.ca. Armand Frappier Health Biotechnology, Institut national de la recherche scientifique, Laval, Quebec, Canada The present study illustrates the effect of combined treatments of encapsulated essential oils and γ-irradiation (1.5 kGy) on Escherichia coli O157:H7, Listeria monocytogenes, molds and yeasts, lactic acid bacteria (LAB), and total mesophilic bacteria (TMF), as well as pH, water activity, color, and texture in dry fermented sausages during ripening and vacuum packed during storage at room temperature (20 - 21 °C) for 20 weeks. Combined treatments showed synergetic effects on inhibiting Escherichia coli O157:H7 cocktail and LAB, and also exhibited strong inhibition of Listeria monocytogenes, molds and yeasts, and TMF. The combined treatments did not affect the texture of the sausages and the encapsulation process of the essential oils contributed to the color protection of the sausages.

4:00 Withdrawn

4:25 NMR-based metabolomic investigation on antimicrobial mechanism of Salmonella on pea sprouts treated with Nanoemulsified basil essential oils and ultrasonic Liu Zifei, e0506474@u.nus.edu. Dept of Food Sci. and Tech., National U. of Singapore Development of novel and effective food fungicide to ensure the microbiological safety of fresh produce has gained considerable attention, while the sanitizing mechanism of ultrasound and essential oil has not been explained fully at metabolomics level. This study investigated the antibacterial mechanism of ultrasound combined with nanoemulsified basil essential oil (NBEO_US) on Salmonella enterica strains (ATCC 6962, ATCC 13076 and ATCC 14028) inoculated onto pea sprouts. The results indicated that the NBEO_US treatment resulted in a substantial decrease in bacterial counts (2.01-2.69 log CFU/g reductions), significant nucleic acid leakage (OD260 nm of 1.313-1.661) and protein leakage (22.27-23.70 μg/ml), while disruption of the integrity and permeability of the cell membrane was observed through transmission electron microscopy. Additionally, the 1H NMR-based metabolomics showed that 60 metabolites were identified from the Salmonella enterica strains. Furthermore, the flux of labeled metabolites indicated that NBEO_US disrupted energy and amino acid metabolism in bacterial cells, including glycolysis and amino acid biosynthesis. NBEO_US could also affect the Embden-Meyerhof-Parnas pathway of Salmonella enterica strains and reduce the activity of three key enzymes (hexokinase, pyruvate kinase and phosphofructokinase). In conclusion, this study provides insight into the antimicrobial mechanism of Salmonella enterica strains and offers a basis for enhancing the application of NBEO_US in controlling foodborne pathogens in fresh produce.

4:50 Development of bacteriophage added coating material to reduce Escherichia coli O157:H7 contamination in mushroom Eylul Evran, sefikaevran@hacettepe.edu.tr, Emine K. Tayyarcan, Ismail H. Boyaci. Food Engineering, Hacettepe U., Ankara, Turkey Escherichia coli O157:H7 (E. coli O157:H7) is a serious foodborne pathogen for human. With the presence of inadequate hygiene conditions during product collection, packaging, or handling, it can contaminate food and cause food-borne diseases. Edible mushrooms can cause some diseases in humans. If the fertilizer used during production is not well sterilized or appropriate conditions are not provided during collection and packaging, pathogenic bacteria like

E. coli can transmit to mushroom and can cause food poisoning in human. For this reason, different methods should be developed to prevent pathogenic bacterial contaminations in mushroom. Today, phage therapy is an alternative method to antibiotics for bacterial infections. Bacteriophages, called phages, are viruses that only infect bacteria. Today, lytic phages can be used against pathogenic bacteria that develop antibiotic resistance. In recent years, investigating the use of phages in food packaging materials is among the most popular topics. The release, stability, and effectiveness of phages on pathogenic bacteria in food packaging material are frequently studied. In this study, we performed the isolation and characterization of phages that are effective against E. coli O157:H7 bacteria that can be found in mushroom. We determined the growth parameters during the characterization stages and investigated whether they could maintain their stability with the change of physical parameters such as temperature and pH. We then coated the mushroom by mixing phage with different coating materials (sodium alginate and whey protein concentrate) and investigated the behavior of the phage during storage at 4 and 15°C and its effect on the pathogen. Efficiency of plating (EOP) and one step growth size experiments showed that phages are highly effective against E. coli O157:H7. According to results, phage coated material reduced the bacterial count compared to control group. Thus, it will be shown that phages are bioprotective agents that can be used safely as food packaging material and can be a solution for safer food production.

Food Toxicants: Occurrence, Detection, Formation Mechanism and Mitigation

2:05 Detection and occurrence of PFAS in food and food packaging Yelena Sapozhnikova1, yelena.sapozhnikova@usda.gov, Raegyn B. Taylor1, Megha Bedi2, Carla Ng3. (1) Agricultural Research Service, USDA, Wyndmoor, Pennsylvania(2) Dept. of Civil & Environmental Engineering, U. of Pittsburgh, Pennsylvania Per- and polyfluoroalkyl substances (PFAS) are wide-spread, persistent and bioaccumulative contaminants with documented human health impacts. Monitoring of PFAS in food and food packaging is imperative for understanding human exposure. Analytical efforts on PFAS analysis have largely focused on water, but analysis of food, and the development of efficient analytical protocols for food, has recently gained more attention. We have developed and validated analytical methods for analysis of 33 PFAS in food (fish, meat and eggs) and food packaging materials. Seafood is considered a dominant non-occupational source of human exposure to PFAS, thus we investigated the occurrence and levels of PFAS in fish and seafood, including farm-raised and wild-caught species with origins from US and internationally from 19 countries. Low levels (ng/g) of PFAS were detected in 74% of the samples with PFHxS most frequently detected. Even fewer analytical methods have been published for PFAS monitoring in food packaging, where PFAS are both intentionally and non-intentionally added substances. We analyzed PFAS in globally sourced food packaging from the US and 23 other countries. Different food packaging types, including greaseproof papers, paperboard trays, wrappers, cardboard etc. were selected representing food choice for different consumer groups (e.g. adults vs. children). The combined approach of targeted analysis, total oxidizable precursor (TOP) assay and non-targeted analysis was employed to identify and characterize PFAS chemicals. Overall, 84% of food packaging samples had detectable levels of at least one of the targeted PFAS with 6:2 DiPAP most frequently detected. More realistic migration tests were conducted using the US Food and Drug Administration (FDA) protocols to study PFAS migrating into food simulants, and 4 migrated PFAS (PFHxS, PFHxA, PFHpA and 6:2 DiPAP) were measured at ng/g levels with amounts increasing over the 10-day migration test.

2:25 Analysis of Alternaria and Fusarium toxins in cereals and cereal-based food products via LC-MS/MS Fabian Dick, fabian.dick@tum.de, Alena Dietz, Michael Rychlik. Chair for Analytical Food Chemistry, Technische U. Munchen, Bayern, Germany Cereals are often infected by mycotoxigenic Fusarium species, that often infect plants during growth, and Alternaria, which are known as saprophytic plant pathogens. Mycotoxins produced by Fusarium include type A trichothecenes T2- and HT2 toxin, type B trichothecenes deoxynivalenol and nivalenol, zearalenone as well as the emerging mycotoxins enniatins and beauvericin. Alternaria is known to produce tenuazonic acid, tentoxin and dibenzo-α-pyrones like alternariol and alternariolmethylether. Many of those mycotoxins are also occurring in modified forms, e.g. conjugated with glucose or sulphate, which are expected to be converted to their free form during digestion. In the present study we developed a multi-mycotoxin method to analyse 23 different Alternaria and Fusarium toxins in cereals in one 23 min long LC-MS/MS run. After triple extraction the sample work-up involves a modified QuEChERS clean-up followed by dispersive solid phase extraction. The method was validated according to Hädrich and Vogelgesang (1998) and includes the modified mycotoxins AOH-3-G, AOH-9-G, AOH-3-S, AME-3-G, AME-3-S and DON-3-G. The screening of over 100 different cereals and cereal-based products showed the prevalent co-occurrence of Alternaria and Fusarium toxins in wheat, rye, spelt and rice. The analysed toxin contents for Fusarium toxins where in all samples below the regulatory limits. While there are no regulatory limits for Alternaria toxins the EU introduced an indicative level of 2 µg/kg for AOH and AME in cereal-based foods for infants and young children in the commission recommendation (EU) 2022/553 of 5 April 2022. Almost 10% of the analysed samples show the transgression of the indicative value while the modified mycotoxins would add even more to the total exposure.

2:45 Analysis of volatile compounds and α-dicarbonyl compounds in Robusta coffee by soaking with various amino acids, organic acids and monosaccharides Kwang G. Lee, kwglee@dongguk.edu. Food Sci. and Biotechnology, Dongguk U., Jung-gu, Seoul, Korea (the Rep. of) In order to compensate for the disadvantages of Robusta coffee, various ingredients such as amino acids, organic acids and monosaccharides were added before coffee roasting. After coffee roasting volatiles and α-dicarbonyl compounds (α-DCs) were analyzed. In coffee samples treated with amino acids (1% and 3% of leucine, glycine, and alanine), the total volatiles (sum of peak area ratios for each compound) ranged from 21.08±0.92 to 35.67±0.77. As the concentration of amino acids increases, the processed non-polar amino acids act as an inhibitor of the Maillard reaction, reducing all of the pyrazine and pyrrole components. Among the three amino acids, when treated with L-leucine and L-alanine, the production of α-DCs was significantly reduced ($p<0.05$). Four organic acids (malic, citric, tartaric, and succinic acid) were used at concentrations of 1, 2, and 3% (w/v), and the soaking time was 1 hour. Furfural and 5-methyl furfural increased after organic acid pre-treatment. In 3% malic acid soaked Robusta coffee, furfural and 5-methyl furfural increased by 90.99% and 24.92%, respectively, compared to the control (Robusta). In 3% malic acid sonicated (280W, 1 h) Robusta coffee, furfural and 5-methyl furfural increased by 236.03% and 114.77%, respectively. The levels of α-DCs (glyoxal, methylglyoxal and diacetyl) were significantly ($p<0.05$) decreased in all Robusta coffees after organic acid pre-treatment. Among organic acids, tartaric acid was the most effective. Robusta coffee soaked and sonicated in tartaric acid solution decreased α-DCs (glyoxal, methylglyoxal and diacetyl) by up to 44% and 58%, respectively, compared to the control. Robusta coffee beans were soaked with D-xylose and D-ribose solutions (0, 3, 6, and 9% w/v). The levels of pyrazines, pyridine, pyrroles and furans were

diminished by 85%, 77%, 23%, and 48% compared to the control after pentose pretreatment ($p < 0.05$). The total amount of α-DCs was decreased significantly (70%) in all treated samples compared to the control ($p < 0.05$). The concentration of acetic acid was increased only in the samples pretreated with autoclave ($p < 0.05$). The principal component analysis showed that the pentose pretreatment treated with autoclave decreased the level of pyrazines and increased the level of 1-furfurylpyrrole, methyl furfuryl disulfide,4-ethyl-2-methoxy-phenol, furfuryl acetate, 2-acetylpyrrole, 2-methoxyphenol, pyridine, and acetic acid.

3:05 Differential induction of shiga toxin in environmental Escherichia coli strains Michelle Q. Carter2, michelle.carter@usda.gov, Xiaohua He1. (1) Foodborne Toxin Detection and Prevention Research Unit, Western Regional Research Center, USDA, Albany, California(2) Produce Safety and Microbiology Research Unit, Western Regional Research Center, USDA, Albany, California Shiga toxin-producing Escherichia coli (STEC) can cause severe diseases in humans including hemolytic uremic syndrome. Production of Shiga toxins (Stxs), especially Stx2a, is thought to be correlated with STEC virulence. Since stx genes are located in prophage genomes, induction of prophages is required for effective Stxs production. Here, we investigated the production of Stxs in a group of environmental STEC O145:H28 strains under stresses STEC encounter in natural habitats and performed comparative analysis with two clinical strains, one linked to a 2010 U.S. lettuce-associated outbreak and the other linked to a 2007 Belgium ice cream-associated outbreak. Among all stx2a positive environmental strains, only the Stx2a-prophage in cattle isolate RM9154-C1 was clustered with the Stx2a-prophages in the U.S. outbreak strain, the Stx2a-phage induced from a STEC O104:H4 strain linked to the 2011 outbreak of enterohemorrhagic infection in Germany, and the Stx2a-prophage in STEC O157:H7 strain EDL933, a prototype of enterohemorrhagic E. coli. Furthermore, the Stx2a-prophage in strain RM9154-C1 shared the same chromosomal insertion site and carried the same antiterminator Q gene and the late promoter PR' as the Stx2a-prophage in the U.S. outbreak strain. Following mitomycin C or enrofloxacin treatment, the production of Stx2a in strain RM9154-C1 was the highest among all environmental strains tested. In contrast, following acid challenge and recovery, the production of Stx2a in strain RM9154-C1 was the lowest among all the environmental strains tested, at a level comparable to both outbreak strains. A significant increase in Stx2a production was detected in all strains when exposed to hydrogen peroxide, although the induction fold was much lower than those by other inducers. This low-efficiency induction of Stx-prophages by hydrogen peroxide, a natural inducer of Stx-prophages, supports the hypothesis of bacterial altruism in controlling Stxs production, a strategy that assures the survival of the STEC population as a whole by sacrificing a small fraction of cells for Stxs production and release. Differential induction of Stxs among strains carrying nearly identical Stx-prophages suggests a role of host bacteria in regulating Stxs production.

3:40 Development of tools for mycotoxin analysis in foods Kai Zhang, kai.zhang@fda.hhs.gov. Center for Food Safety and Applied Nutrition, US FDA, College Park, Maryland To protect and promote food safety, the FDA has established regulatory levels of mycotoxins in a wide range of food and feed products and has incorporated mycotoxin analysis into regulatory monitoring and surveillance programs. Due to variations in the physicochemical properties of mycotoxins and the complex process of mycotoxin analysis, the development of robust analytical protocols for mycotoxin detection must address challenges related to sampling, sample homogenization, subsampling, mycotoxin co-occurrence, method validation, and the availability of certified matrix reference materials. Furthermore, much of the sample preparation for mycotoxin analysis is performed manually, resulting in laborious and low- throughput operations for routine sample analysis. Therefore, in recent years, we have developed practical tools for mycotoxin analysis to address these challenges. This presentation will review some of the existing technical issues and difficulties encountered in the analysis of mycotoxins in food samples and will highlight tools for automated sample preparation, the validation and extension of LC-MS-based methods for mycotoxin analysis, the characterization of sample homogeneity using laser diffraction particle size measurements and real-time imaging analysis, and the application of mycotoxin certified matrix reference materials to evaluate method uncertainty and establish metrological traceability of measurements. Our results demonstrate that the incorporation of these newly developed tools not only enhances the FDA's ability to monitor mycotoxins in foods, but also sheds the light on future directions for mycotoxin research at the FDA.

4:00 Geographical discrimination of 94 geographically authentic wheat samples and non-targeted metabolomics of moldy wheat by ultra-performance liquid chromatography-quadrupole time-of-flight mass spectrometry Boyan Gao[1], raphaelgao1985@gmail.com, Mengchu Jin[1], Yinghua Luo[3], luoyinghua@cau.edu.cn, Liangli Yu[2]. (1) Shanghai Jiao Tong U., China(2) U. of Maryland at College Park(3) China Agricultural U., Beijing The present research aimed to investigate lipid compositions of Chinese wheat samples and clarify the major markers that contribute to the geographical differences. A total of 94 wheat samples from eight main wheat-producing provinces in China were evaluated to differentiate their lipid compositions. Based on the data collected from ultra-high-performance-liquid-chromatography tandem time-of-flight mass spectrometry (UPLC-Q/TOF MS), an optimized non-targeted lipidomic method was utilized for analyses. As the results, 62 lipid compounds, including fatty acids, phospholipids, galactolipids, triglycerides, diglycerides, alkylresorcinol, and ceramide were tentatively identified. After that, the identification of moldy wheat samples was studied using ultraperformance liquid chromatography-quadrupole time-of-flight mass spectrometry (UPLC-QTOF-MS) coupled with chemometrics. The non-targeted PCA model for identifying moldy wheat from normal wheat was established by using previously established compounds database of authentic wheat samples. The partial least squares-discriminant analysis (PLS-DA) was performed. By optimizing the model parameters, correct discrimination of the moldy wheat as low as 5% (w/w) adulteration level could be achieved. Results from this study offered an effective method toward screening wheat safety.

4:20 Using mass spectrometry and whole genome sequencing to relate shiga toxin production with stx phage induction in shiga toxin-producing Escherichia coli (STEC) Christopher J. Silva1, christopher.silva@usda.gov, Beatriz Quiñones1, Bertram Lee1, Bianca A. Amézquita-López2, Melissa L. Erickson-Beltran1. (1) Produce Safety and Microbiology Research Unit, USDA, Agricultural Research Service, Western Regional Research Center, Albany, California(2) Facultad de Ciencias Químico Biológicas, U. Autónoma de Sinaloa, Culiacán, Mexico Shiga toxin-producing Escherichia coli (STEC) are a significant cause of foodborne illness worldwide. An STEC produces Shiga toxins (Stx) when a temperate stx phage is induced to undergo lytic replication, lysing the STEC and releasing the Shiga toxins. More than one stx phage can infect a host STEC and, upon lysis, releases more than one subtype of Shiga toxin. The present study developed an innovative multiplex mass spectrometry-based assay capable of simultaneously quantifying different subtypes of Shiga toxins in a sample. The assay employed the multiple reaction monitoring method (MRM) to quantify the characteristic tryptic peptides from 17 distinct Shiga toxin subtypes

(Stx1a, Stx1c, Stx1d, and Stx2a-m,o) relative to added uniformly 15N-labeled internal standard peptides. These peptides were derived from the tryptic digestion of a single uniformly 15N-labeled artificial protein, containing the required internal standards. Twenty-four STEC isolates comprised eleven different serotypes, some of which are associated with severe human illness. The STEC were isolated from fecal samples in a major agricultural region of Northwestern Mexico that actively exports fresh produce to the US. High-resolution genome sequencing showed that each isolate contained two or more stx phages. Each isolate was cultured to induced Shiga toxin production. Our MRM-based method was used to quantify the amounts of the Shiga toxin subtypes in the cultures. Our results indicate that the MRM-based assay can accurately determine a relationship between stx phage induction and Shiga toxin production. These studies have set a foundation for a better characterization of the conditions regulating the expression of multiple Shiga toxin subtypes, enabling a better assessment of the virulence potential of STEC isolates from relevant produce production regions.

Renewable Polymer Materials: Preparation, Processing, Application, and Disposal

2:05 Additive manufacturing advancing sustainability Timothy E. Long, telong@asu.edu, Charlotte Barker, Cody W. Weyhrich, Ren Bean, Jianheng Wen, Garvit Nayyar. Arizona State U., Tempe Additive manufacturing has numerous applications in a variety of industries, including aerospace, automotive, healthcare, and consumer goods. It can be used to produce complex shapes, customize products, and create prototypes quickly and cost-effectively. Additionally, additive manufacturing has the potential to be more sustainable than traditional manufacturing by reducing waste and lowering material usage. 3D printable polyimides provide an avenue for the fabrication of complex structures consisting of one of the most performant synthetic polymers currently available. Leveraging the complex design afforded by vat photopolymerization enabled dematerialization of high-performance parts with printed polyimide octet lattices comprised of 70 vol. % air and 30 vol. % solid materials. Unsaturated polyesters provide opportunities in lithographic additive manufacturing through subsequent free radical processes, where resulting printed parts contain ester functional groups susceptible to hydrolysis leading to depolymerization with specific environmental stimuli. Additive manufacturing of latexes enables the novel processing of high molecular weight materials from water that otherwise requires dilution with volatile organic solvents. Discrete particles within a latex decouple the relationship between viscosity and high molecular weight, which allows high molecular weight polymers to be utilized as precursors for vat photopolymerization. Furthermore, layer-by-layer processing drives product lightweighting to the forefront, curing polymer only where desired, thus reducing the amount of material required. Driven by changes in a world that demand material sustainability, additive manufacturing provides a pathway to dematerialization and end-of-life strategies for polymeric materials.

2:35 Plant-based Biofoam to replace Styrofoam for temperature-controlled packaging applications Xiao Zhang, x.zhang@wsu.edu. Voiland School of Chemical Engineering and Bioengineering, Washington State U., Richland The global polymer foam market is estimated to reach USD 153.8 billion by 2027. A majority of polymer foams today are made of polyurethane (PU), polystyrene (PS), polyvinyl chloride (PVC), phenolic, and polyolefin, which are all currently produced from petroleum-derived resins. The lack of sustainability and recyclability of current foams poses an urgent need to find alternative technologies to produce foam materials from environmentally benign and sustainable resources such as plant-based feedstock. We have developed a technology for producing biobased foams from plant based nanomaterials which are ultralight, super strong, and provide excellent insulation, fire resistance, and mechanical properties. This presentation will highlight our recent progress toward commercialized plan based biofoam temperature-controlled packaging applications.

3:00 Efficient production of aliphatic α,ω-dicarboxylic acids using mild aqueous catalytic oxidation of low-density polyethylene Oleg Davydovich, odavydo@sandia.gov, Daniella Martinez, Jay Salinas, Ryan D. Davis, Estevan Martinez, Hemant Choudhary, Michael Kent. Sandia National Laboratories, Albuquerque, New Mexico Aqueous oxidative depolymerization of commercial low-density polyethylene (LDPE) film (Tm ~ 120 °C) was investigated using various homogeneous first-row transition metal catalysts under mild aqueous conditions (130 – 150 °C and 7 bar O_2 pressure). Oxidation of LDPE resulted in high yields of low molecular weight aliphatic dicarboxylic acids (up to 70 % yield as determined by carbon balance) with minimal loss of yield. The water-soluble products were characterized using size exclusion chromatography (SEC) and Fourier-transform infrared spectroscopy (FTIR) to determine the extent of depolymerization and their functional group composition, respectively. Electrospray ionization mass spectrometry confirmed the identity of the oxidized products to be primarily C_8-C_{16} aliphatic dicarboxylic acids. Oxidation was shown to be scalable and amenable to other common commercial LDPE products. Given the high yield, use of aqueous conditions, abundant first-row transition metal catalysts, and mild reaction temperatures, this process offers a promising “green” route to chemically convert LDPE to useful dicarboxylic acid intermediates.

3:25 Biodegradability and antifungal property of nanosilver-imbibed cotton fabric Sunghyun Nam1, sunghyun.nam@ars.usda.gov, Haile Tewolde2, Zhongqi He1, Kanniah Rajasekaran1, Jeffrey Cary1, Gregory Thyssen1, Christine Sickler1. (1) USDA-ARS, New Orleans, Louisiana(2) USDA-ARS, Mississippi State Studies were conducted to examine the biodegradability and antifungal property of cotton fabric imbibed with nanosilver as a potential means to control fungal infection during seed germination. Nanosilver particles with a diameter of approximately 23 nm, were synthesized in situ in unscoured and unbleached cotton fabrics without using any external agents. A simple one-step heat treatment allowed the unscoured and unbleached cotton to naturally generate nanosilver. The nanosilver-imbibed and untreated control cotton fabrics were buried in Leeper silty clay loam soil at a depth of about 11 cm. After a 16-week burial period, the untreated control cotton fabric experienced approximately 32% weight loss, whereas the nanosilver-imbibed cotton fabric showed no weight loss. The observed distinctive resistance to biodegradation for the treated cotton fabric was attributed to the antifungal properties of nanosilver. The antifungal property of the fabric was evaluated using a green fluorescent protein (GFP)-expressing Aspergillus flavus, and the results demonstrated that fungal growth and colonization was 56 times lower in the nanosilver-imbibed cotton fabric compared to the untreated control cotton fabric.

3:55 Lignin-based PU foams Mojgan Nejad1, nejad@msu.edu, Christian Henry3, Enoch Acquah4, Kevin Dunne2. (1) Forestry and Chemical Engineering, Michigan State U., East Lansing(2) Material Science, Michigan State U., East Lansing(3) Forestry, Michigan State U., East Lansing(4) Chemical Engineering, Michigan State U., East Lansing This study focused on partially replacing petroleum-based polyol with lignin in flexible foams and fully in rigid polyurethane (PU) foams. The goals were to enhance lignin utilization and ultimately increase the biobased carbon content of the PU foams without compromising thermo-mechanical properties. Foam samples were analyzed by measuring their densities, tensile

strengths, ultimate elongations, tear strengths, compression force deflections, support factors, fire performance, thermal conductivities, and compression sets. Biobased carbon content and biodegradability study were also performed on developed PU flexible foams. We successfully replaced up to 100% of fossil-fuel-based polyol in PU rigid foams but could only replace up to 20% of the polyol with lignin in flexible foams. The lignin-based polyisocyanurate rigid foam (100% substitution) met all the standard requirements for insulation applications, but more work is needed to reduce the cell size of lignin-based foams. On the other hand, the lignin-based foams made with partially (20%) replacing commercial polyol met all the requirements for seating applications, and the lignin portion of foams were degraded in thermophilic composting conditions (58°C) in less than three months.

4:20 Graphene Quantum Dots Improve the Dispersion of Cellulose Nanocrystals and Thermo-mechanical Properties of High Density Poly(ethylene) based Composites Saptaparni Chanda1, Dilpreet S. Bajwa1, dilpreet.bajwa@montana.edu, Sreekala G. Bajwa2, Cecily Ryan1. (1) Mechanical and Industrial Engineering, Montana State U., Bozeman, Montana, US(2) College of Agriculture, Montana State U., Bozeman Cellulose nanocrystals (CNC) have been demonstrated to be an effective reinforcement in polymeric composites because of their inherent biodegradability, universal accessibility, and superior mechanical properties. The central challenge is the uniform dispersion of CNCs in a hydrophobic polymer matrix because of CNC's hydrophilic nature. In this research, a safe, effective, and ecofriendly surface modification technique was used to prepare a hybrid system of cellulose nanocrystal (CNC)/graphene quantum dots (GQD). This hybrid system of CNC/GQD was incorporated in high-density polyethylene (HDPE) separately to process composites via the melt blending extrusion process. The CNC/GQD inclusion complex properties were evaluated using Zeta potential measurement, Raman spectroscopy, X-Ray Photoelectron 16 Spectroscopy (XPS), and X-Ray Diffraction (XRD) analysis. The composite properties were studied using analytical, mechanical, and techniques. The electrical properties were determined using electrical impedance spectra analysis. Raman spectroscopy, XPS, and XRD analysis confirmed the interaction of CNC and GQD. The SEM micrographs of the cross-sections of GQD-induced composites showed uniform fibrillar morphology and no signs of agglomeration. The GQD-incorporated composites exhibited better thermal stability and mechanical properties than neat HDPE. The composites showed a purely capacitive response for an AC electrical system. The results indicate the improved dispersion of CNC in the polymer matrix, which improved the composite's overall properties. The CNC/GQD inclusion complex exhibited its energy storage capacity.

4:45 Strong and ultrafast healing lignin-based copolymer elastomers via a grafting strategy Yaqiong Zhang, zyq100@ahau.edu.cn, Yangtao Ou, Jiajing Huang. Dept. of Material Sci. and Eng., Anhui Agricultural U., Hefei, Anhui, China Lignin-based composite elastomer materials have received tremendous interest on accounts of its attracting advantages. The combination of lignin and controlled/living radical polymerization techniques can open new avenues for designing high-performance elastomers. In this work, reversible addition-fragmentation chain transfer (RAFT) polymerization was used to fabricate a variety of lignin-graft-poly(butyl acrylate-co-acrylic acid) (Lignin-g-P(BA-co-AA)) copolymer elastomers by adjusting the feed ratios and lignin contents. Interestingly, these lignin-based copolymer elastomers exhibit excellent tensile strength, high toughness, and ultrastretchability. In addition, the incorporation of lignin endows these composite elastomers with unexceptionable photothermal performance, leading to extraordinary self-healing efficiency of 97.1% under near-infrared laser irradiation.

5:10 Uniform, size controllable, and pH-sensitive protein microgels as efficient aqueous bio-lubricants: a soft ball-bearing mechanism study Yifu Chu, yifu4@ualberta.ca, Lingyun Chen. Dept. of Agricultural, Food and Nutritional Science, U. of Alberta, Edmonton, Canada Aqueous lubrication is crucial in biological interfaces such as the oral cavity, joints, and eyes, which rely on aqueous lubricants like saliva, synovial fluids, and tears to reduce sliding friction. Biopolymer microgel suspensions are soft colloidal systems that have attracted a lot of research attention owing to their biocompatibility, unique rheological properties, environmental sensitivities, and high surface-to-volume ratio as compared to their bulk hydrogel counterparts. Recently, microgels emerged as novel aqueous lubricants in the food and biomedical fields for their soft nature that traps water in their micron-structure, and the "ball-bearing lubrication" effect. In our lab, we developed a facile method to fabricate uniform size-controllable whey protein microgels through protein-polysaccharide water-in-water emulsions. The protein microgels are crosslinked via disulfide bonding, and their size can be precisely controlled (1, 6, and 20 μm) by modulating the protein-polysaccharide interactions, such as electronic repulsive force and hydrophobic interaction. This facile microgel production does not require chemical modification or high energy input, ensuring safe use as food ingredients with significant industry interests. The microgels assembly of the shape and distribution of fat droplets in food emulsions and their suspension showed a shear thinning effect and higher rheological performance than traditional oil-in-water emulsions. The microgel suspension (50% vol) demonstrated superior lubricating performance in both boundary and mixed regimes under neutral pH and was capable of exceeding the lubricity of human saliva in tribological tests using a rheometer with ring-on-plate geometry. Our findings also indicated that the "soft ball-bearing" mechanism is responsible for the superlubricity of our microgels, resulting from two factors: 1) they can trap water molecules and generate interparticle electrostatic repulsion owing to their soft nature, leading to hydration lubrication; 2) they can act as micron-scale "ball bearings" to decrease the sliding friction. These findings demonstrated that the biocompatible protein microgel aqueous lubricants have the potential for various food and biomedical applications, such as preparing fat-reduced food formulations with an improved creamy mouthfeel and dry-mouth therapy for healthier outcomes.

5:35 Antimicrobial, catalytic and thermophysical applications of internally synthesized Cu2O nanoflowers in cotton fibers Matthew B. Hillyer, Matthew.Hillyer@USDA.gov, Sunghyun Nam, Jacobs H. Jordan, Michael W. Easson, Crista Madison, Doug Hinchliffe. Cotton Chemistry & Utilization Research Unit, US Dept. of Agriculture, New Orleans, Louisiana Cotton fabrics infused with metal oxide nanoflowers for antibacterial applications, catalytic activity and enhanced material functionalities are becoming increasingly popular. Copper oxide nanomaterials have gained popularity for their synthetic versatility, microbicidal properties and cost-effectiveness compared to other metals. This study has presented a method in which cuprous oxide nanoflowers (Cu2O NFs) are synthesized in situ from a copper (II) precursor under mild conditions and without added chemical reducing agents. The internal formation of Cu2O NFs (72.0 ± 51.8 nm) within the cotton fiber structure was confirmed by TEM. These Cu2O NF cotton fabrics demonstrated remarkable laundering durability, releasing only 19% of copper content after 50 home laundering cycles determined by ICP-MS and UV-vis using a calculated calibration curve ($R2 = 0.9979$). The washing durability of the internally-produced Cu2O NFs was verified by the persistence of superior broad-spectrum

antibacterial, antifungal and antiviral activity with greater than 99.99% inhibition against K. pneumoniae, E. coli, S. aureus and A. niger and ≥90% inhibition against Human coronavirus, strain 229E, even after 50 home laundering cycles. In addition, the Cu2O NF cotton exhibited remarkable catalytic activity for the degradation of organic dyes, hydrogen peroxide production, and enhanced thermophysical properties which will be discussed.

THURSDAY MORNING August 17
Food Toxicants: Occurrence, Detection, Formation Mechanism and Mitigation

8:05 Thermostability modification of zearelenone lactonase by two different methods Wei Xu, weixu@jiangnan.edu.cn, Binbin Ouyang, Wanmeng Mu. Jiangnan U., Wuxi, Jiangsu, China Zearalenone (ZEN) is a nonsteroidal estrogenic mycotoxin biosynthesized by several Fusarium species, which widely exists in musty maize and its co-products. ZEN exhibits a pronounced binding affinity to estrogen receptors, and also causes adverse effects such as reproduction, carcinogenicity, genotoxicity, and immunotoxicity. In addition to ZEN, its derivatives include α/β-zearalenol (α/β-ZOL), and α/β-Zearalanol (α/β-ZAL) are also found toxic to some extent. So far, a potent ZEN-degrading lactonase from Gliocladium roseum (ZENG) was identified. ZENG exhibited its optimal pH and temperature at 7.0 and 38 °C. ZENG was active against ZEN, α-ZOL, and α-ZAL, and the specificity activity was 315, 187, and 117 U/mg, respectively. However, ZENG lost more than 90% activity after incubation at 50 °C for 2 min. Two methods, including structure-guided modification and molecular dynamic (MD) simulation, were implemented to address the problem. Firstly, multiple sequence alignment of ZEN lactonases having different thermostabilities were implemented. Two residues were found to be conserved for most lactonases (H134 and S136) but varied largely in the enzyme from Rhinocladiella mackenziei (Rmzhd), which has a higher thermostability. Considering the special position of H134 and S136, three double-site mutants were constructed accordingly. Finally, two mutants, including H134L/S136L and H134F/S136F, displayed a significant improvement in thermostability compared with the wild-type enzyme. Secondly, employing the crystal structure of Clonostachys rosea (ZHD101) as a template, two potential hotspots, S162 and S220, in ZENG were found during MD simulation. As a result, mutants S162R and S220R were obtained with increased thermostability. Additionally, the half-life of the S162P/S220R mutant at 55 °C was significantly increased by 36.8-fold, and the melting temperature (Tm) was significantly increased from 49.3 to 57.5 °C. Results showed that improved thermostability of S162P/S220R was related to the decreased root mean square fluctuations (RMSF) value, enhanced structural stability, and increased hydrogen bonds.

8:25 Baseline determination of azole-resistant aspergilli in California farms: Correlation between azole resistance and aflatoxin production Jong H. Kim, Jongheon.Kim@USDA.gov, Kathleen L. Chan, DeAngela Ford, Siov L. Sarreal, Jeffrey D. Palumbo. USDA-ARS Foodborne Toxin Detection and Prevention Research, Albany, California Azoles are used as antifungals for treating clinical and agricultural fungal pathogens. The triazole class of fungicides are demethylase inhibitors that interfere with lanosterol 14 alpha-demethylases (cytochrome P450 (CYP) enzymes) and disrupt cell membrane biosynthesis. Since more than 25% of total fungicide sales are azoles such as metconazole and tebuconazole, azole fungicides could provide environmental selection pressure for the emergence of pan-azole-resistant fungal pathogens including aflatoxin (AF)-producing Aspergillus flavus and Aspergillus parasiticus. Recently, fungicide potentiation of mycotoxin production in resistant fungi has been reported, not only debilitating public food safety but also causing significant economic losses once incorporated into food supply chain. In this study, A. flavus and A. parasiticus field strains isolated from ten counties in California (for the period 1992-2015) were investigated for their azole resistance and aflatoxin production. Azole-resistant, toxigenic Aspergillus strains were screened via voriconazole, itraconazole and posaconazole (VIP)-check testing, where one AF overproducer (A. flavus TM-079) and three less toxigenic strains (A. flavus TM-001; A. parasiticus TM-120, 123) were identified. We found: (1) fungicide resistance of aflatoxigenic mutants was unique to azoles; no differences in susceptibility to other fungicides were identified, (2) A. flavus TM-079 exhibited highly increased aflatoxin B (AFB) production, whereas A. flavus TM-001 produced significantly low level of AFB, (3) A. parasiticus TM-120 and TM-123 also showed significantly reduced aflatoxin G (AFG) production, (4) metconazole and tebuconazole could enhance AF production, where the enhancement depended on azole concentrations (low or high) or target strains, (5) AF over-production by A. flavus TM-079 was not linked to stress-dependent fungal fitness. Altogether, the results from this study would provide new control points for preventing AF production by aspergilli in the fields.

8:45 Dilute-and-shoot quantification of As, Cd, Pb, Be, Ni, Co, Cu, Mn, Se, Zn, Ba, Ag, and V in fruit juices by ICPMS based on matrix overcompensation calibration Guoying Chen, guoying.chen@usda.gov, Bunhong Lai. Agricultural Research Service, US Dept. of Agriculture, Wyndmoor, Pennsylvania A dilute and shoot protocol was developed for multielemental (As, Cd, Pb, Be, Ni, Co, Cu, Mn, Se, Zn, Ba, Ag, and V) quantification in fruit juices by inductively coupled plasma mass spectrometric (ICPMS). Fruit juices were diluted in 1:50 ratio in 1% HNO3-0.5% HCl-5% ethanol; ethanol was added to all samples and the standard series to overcompensate matrix effects of carbon origin. This new correction strategy, termed as matrix overcompensation calibration (MOC), achieved quantitative (92-102%) recovery as well as quantitation comparable to traditional standard addition calibration (SAC). Ge, Rh, Tb, and Ir were used as internal standards. Reliable quantification of all juice matrices was enabled by MOC using a single calibration curve. Significant advantages were gained in time, labour, productivity, and argon consumption.

9:05 Technologies for the detection of bacterial and plant toxins that impact food safety and security Christina Tam, christina.tam@usda.gov, Priscila Alves, Larry H. stanker, Luisa Cheng. Foodborne Toxin Detection and Prevention Research Unit, USDA-ARS Pacific West Area, Albany, California Bacterial and plant toxins can have tremendous impacts on food safety and security. Botulinum neurotoxins and abrin are two examples of extremely potent bacterial and plant toxins that are potential bioterror weapons. Lack of antidotes and/or limited treatment therapies after abrin and botulinum neurotoxin intoxication can lead to high morbidity and mortality. Of critical importance due to the potency of these two foodborne toxins is for the development of new reagents and technologies to be able to detect the toxins with high sensitivity (low concentrations) in relevant food matrices. Rapid, sensitive, and portable detection technologies for these toxins would greatly enhance food safety and security. Additionally, the development of new reagents and therapeutics to address the lack of therapies after intoxication would reduce morbidity and mortality. Mitigation efforts to inactivate these toxins would require understanding their stability and bioavailability especially in food matrices and under relevant food processing conditions.

9:40 Chlorothalonil induces metabolic syndrome in mice by regulating host gut microbiota and bile acids metabolism via FXR pathways Wentao Zhu, wentaozhu@cau.edu.cn. China Agricultural U., Beijing Background: The most commonly used organochlorine

pesticide nowadays, chlorothalonil (CHI), is ubiquitous in a natural environment and poses many adverse effects to organisms. Unfortunately, the toxicity mechanisms of CHI have not been clarified yet. Results: This study found that the CHI based on acceptable daily intake (ADI) level could induce metabolic syndrome (MetS) in mice, including obesity, hepatic steatosis, dyslipidemia, and insulin resistance. In addition, exposure to reglementary-dose CHI could induce an imbalance in the gut microbiota of mice, resulting in a significant increase in the ratio of Firmicutes to Bacteroidetes. Furthermore, the results of the antibiotic treatment and gut microbiota transplantation experiments showed that the reglementary-dose CHI could induce MetS in mice in a gut microbiota-dependent manner. Based on the results of targeted metabolomics and gene expression analysis, the reglementary-dose CHI could disturb the serum metabolism of bile acids (BAs) in mice, causing the inhibition of the signal response of BAs receptor farnesol X receptor (FXR) and leading to glycolipid metabolism disorders in liver tissue and epididymal white adipose tissue (epiWAT) of mice. The administration of FXR agonist GW4064 and CDCA could significantly improve the reglementary-dose CHI-induced MetS in mice. Conclusions: In conclusion, the reglementary-dose CHI was found to induce MetS in mice by regulating the gut microbiota and BAs metabolism via the FXR signaling pathway. This study provides evidence linking the gut microbiota and pesticides exposure with the progression of MetS, demonstrating the key role of gut microbiota in the toxic effects of pesticides.

10:00 Chemopreventive effect of natural dietary compounds on food-borne toxicants induced colon carcinogenesis Min-Hsiung Pan, mhpan@ntu.edu.tw. Inst. of Food Sci.s and Tech., National Taiwan U., Taipei The chemopreventive effect of natural dietary compounds on colon carcinogenesis induced by food-borne toxicants has been a topic of interest in recent research. Several studies have demonstrated that natural dietary compounds derived from common dietary foods and plants exhibit beneficial effects in preventing and suppressing colon carcinogenesis induced by toxicants such as benzo[a]pyrene (BaP) and 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP). These food-derived carcinogens are known to cause mutagenic activity and disrupt normal biological functions, leading to adverse health effects. Therefore, metabolic regulation of these hazardous chemicals is important for reducing toxicity. Natural dietary compounds may act through various mechanisms such as activation of detoxifying enzymes, inhibition of metabolic activation of carcinogens, and modulation of cell signaling pathways. This review aims to summarize current research on the chemopreventive effect of natural dietary compounds on food-borne toxicant-induced colon carcinogenesis, highlighting potential mechanisms of action and future research directions.

10:20 Effects of sulfonation on metabolic fate of deoxynivalenol in nursery pigs Wes Mosher1, moshe096@umn.edu, Dana Yao1, Richard Faris3, Molly McGhee3, Chi Chen1,2. (1) Food Sci. and Nutrition, U. of Minnesota Twin Cities, St Paul(2) Animal Science, U. of Minnesota Twin Cities, St Paul(3) Cargill Animal Nutrition, Elk River, Minnesota Chronic exposure of deoxynivalenol (DON), a common trichothecene mycotoxin in corn and cereal grains, compromises feed intake, growth, immune response, and reproduction of production animals. Chemical derivatization of DON through sulfonation has been developed as a mitigation approach to reduce the bioavailability of DON in animal feeds, but the exact impacts of sulfonation on the biotransformation and excretion of DON in animals were not well characterized. In this study, a total 48 nursery pigs were fed 4 experimental diets containing 1.2 ppm or 4.1 ppm DON with or without 0.25% NoTox™ Ultimate D additive, a sulfite-based sulfonation agent, for 21 days. DON metabolites in urine and fecal samples were determined by liquid chromatography-mass spectrometry analysis. The results showed that DON was completely metabolized in nursey pigs as it was not detected in urine and fecal samples. The sulfite additive led to the formation of three DON sulfonate (DONS) metabolites, and increased deepoxy-deoxynivalenol (DOM), a microbial metabolite of DON, in feces. In urine, sulfonation decreased DON-3-glucuronide and DON-15-glucuronide but increased DOM-3-glucuronide and DOM-15-glucuronide. Overall, sulfonation decreased the absorption of free DON in nursery pigs, making it more available for gut microbes to form DOM, an inert metabolite, for excretion.

Oat Bioactives and their Health Benefits

8:05 Pharmacokinetics of novel biomarkers of oat intake after single and repated intakes of liquid and solid oat products Marina Armeni, Rikard Fristedt, Nina Jansson, Otto Savolainen, Rikard Landberg, rikard.landberg@chalmers.se. Dept. of Life Sciences, Chalmers U. of Technology, Gothenburg, Sweden A high whole grain intake has been consistently associated with lower risk of developing type 2 diabetes, cardiovascular disease and some cancers in observational studies. Little is known about the role of specific grains, partly due to difficulties in measuring the intake of specific grains and the lack of objective biomarkers. We have evaluated and found alkylresorcinols useful as specific biomarkers of whole grain wheat and rye intake but specific biomarkers of oats intake are lacking. Avenathramids and avenacosides are oat specific compounds that have been suggested as biomarkers of oat intake. However, information about their pharmacokinetics, including their dose-response and relative bioavailability after intake from solid and liquid food matrixes in humans are lacking. The aim of this project was therefore to evaluate avenanthramides and avenacosides as specific biomarkers of oat product intake in humans. We recruited 23 healthy subjects for a study to evaluate biomarker candidates after single and repeated doses of solid and liquid oat-based products, respectively, in a cross-over design. The study was started by provision of a single dose of avenanthramides and avenacosides through a single meal based on a solid or a liquid oat-based product in cross-over. Blood and urine samples were collected during 24h and a fecal sample was provided before the single meal at base-line for determination of microbiota and its interaction with oats and the biomarker candidates. Subjects were then fed three different intake levels three times per day during five days and blood and urine samples were taken during the repeated sampling and at the end of the five days. The procedure was repeated for the other product after one week wash-out period with habitual diet. A LC-MS/MS method was used for qunaitative analysis of avenanthramides and avenacosides in blood samples from all participants. Basic pharmacokinetic parameters such as half-life, Cmax, tmax and AUC were estimated and results from pharmacokinetic modelling based on single dose data and validated by repeated dose response measurements will be presented. The results from the study are expected to provide key information for evaluation of the usefulness of avenantrhamides and avenacosides as biomarkers of whole grain oat intake and will also provide key information about intake levels and frequencies needed to obtain specific plasma concentrations of these compounds from liquid and solid oat products.

8:40 Oats lower biological age in adults at risk for cardiovascular disease YiFang Chu, yifang.chu@pepsico.com. Health & Nutrition Science, PepsiCo, Chicago, Illinois Despite being largely preventable, cardiovascular disease (CVD) is still the leading cause of death globally. Recent studies suggest that the immune system, particularly a form of systemic chronic inflammation (SCI), is involved in the mechanisms leading to CVD; thus, targeting SCI

may help prevent or delay the onset of CVD. In a recent placebo-controlled randomized clinical trial, an oat product providing 3 g of β-Glucan improved cholesterol low-density lipoprotein (LDL) levels and lowered cardiovascular risk in adults with borderline high cholesterol. Here, we conducted a secondary measurement of the serum samples to test whether the oat product has the potential to reduce SCI and improve other clinical outcomes related to healthy aging. We investigated the effects of the oat product on a novel metric for SCI called Inflammatory Age (iAge), derived from the Stanford 1000 Immunomes Project. The iAge® predicts multimorbidity, frailty, immune decline, premature cardiovascular aging, and all-cause mortality on a personalized level. A beneficial effect of the oat product was observed in subjects with elevated levels of iAge at baseline (>49.6 iAge® years) as early as two weeks post-treatment. The rice control group did not show any significant change in iAge . Interestingly, the effects of the oat product on iAge® were largely driven by a decrease in the Eotaxin-1 protein, an aging-related chemokine, independent of a person's gender, body mass index, or chronological age. Thus, we describe a novel anti-SCI role for oats that could have a major impact on functional, preventative, and personalized medicine.

9:05 Oat protein modulates cholesterol levels and improves cardiac systolic function in high-fat, high-sucrose fed rats Sijo Joseph1,2, sijo.joseph@agr.gc.ca. (1) Food and Human Nutritional Sciences, U. of Manitoba, Winnipeg, Canada(2) Agriculture and Agri-Food Canada, Winnipeg, Manitoba Oats are recognized to provide many health benefits that are mainly associated with its dietary fibre,β-glucan. However, the protein derived from oats is largely understudied with respect to its ability to maintain health and attenuate risk factors of chronic diseases. The goal of the current study was to investigate the metabolic effects of oat protein consumption in lieu of casein as the protein source in high fat, high sucrose (HF/HS) fed Wistar rats. Four week old rats were divided into three groups and were fed three different experimental diets: a control diet with casein as the protein source, a HF/HS diet with casein or a HF/HS diet with oat protein for 16 weeks. Heart structure and function were determined by echocardiography. Blood pressure measurements, an oral glucose tolerance test, and markers of cholesterol metabolism, oxidative stress, inflammation and liver and kidney damage were also performed. Our study results show that incorporation of oat protein in the diet was effective in preserving systolic heart function in HF/HS fed rats. In addition, oat protein lowered serum total- and LDL-cholesterol. To conclude, oat protein provides hypocholesterolemic and cardioprotective benefits in a diet induced model of metabolic syndrome

9:30 Phytochemical-rich sprouted oats as a novel functional food to attenuate gut inflammation Pei-Sheng Lee, peisheng7@gmail.com, Juanjuan Hu, Shengmin Sang. Center for Excellence in Post-Harvest Technologies, North Carolina Agricultural and Technical State U., Greensboro Inflammatory bowel disease (IBD) is a chronic inflammation of the gastrointestinal tract that has become a worldwide disease, especially prevalent in western countries. Oat (Avena sativa L.) is a known healthy food that contains numerous bioactive phytochemicals, such as avenanthramides and avenocosides, which promote intestinal health and exhibit antioxidative and anticancer effects. Sprouting enhances the content of protein, essential amino acids, and phytochemicals during germination, making sprouted oats more effective in improving gut health than regular oats. To determine the anti-inflammatory activity of germinated oats, we screened products from oats produced under varying germination conditions using LPS-induced nitric oxide (NO) production in macrophages (RAW 264.7 cells) as an anti-inflammatory assay. The product with the highest anti-inflammatory ability was further tested in a mouse model of dextran sodium sulfate (DSS)-induced colitis. This presentation will report our recent findings on the anti-inflammatory effects of the in-house produced sprouted oats, evaluated using both an in vitro assay and a mouse model.

10:15 Germination and false germination increase the levels of bioactive steroidal saponins in oats Juanjuan Hu, jhu@aggies.ncat.edu, Changliing Hu, Yantao Zhao, Shengmin Sang. Center for Excellence in Post-Harvest Technol, North Carolina Agricultural and Technical State U., Greensboro Oat (Avena sativa L.) is widely recognized as a healthy food due to its many health benefits, including reducing the risk of certain cancers, cardiovascular diseases, and type 2 diabetes, as well as lowering blood cholesterol levels. These benefits are attributed not only to the soluble dietary oat fiber but also to the unique oat phytochemicals, such as steroidal saponins, avenanthramides, triterpenoid saponins, phenolic acids, and flavonoids. Recently, there has been growing interest in sprouted oats for their enhanced nutritional and bioactive potential, with some studies demonstrating increased levels of avenanthramides and phenolic acids during germination. However, no study has yet investigated the alteration of steroid saponins during germination and false germination, nor to identify the optimal conditions that promote desirable changes. To fill this knowledge gap, the present study aims to investigate the influence of germination duration (1, 3, 5, and 7 days) and temperature (20, 25, and 30°C) on the chemical profile change of ten major steroidal saponins in both germinated and false germinated oats, as well as evaluate their anti-inflammatory activity. Our results demonstrate that germinating oats at a temperature of 20°C for seven days significantly increases the total levels of steroidal saponins, with a doubling effect to 3266 μg/g. Notably, AVE-E, the most potent anti-inflammatory steroid saponin in oats, displayed a remarkable increase in content, becoming the most prominent steroidal saponin with a 21-fold surge from 64 μg/g to 1421 μg/g after 7 days of germination at 20°C. Furthermore, we propose the hydrolysis of sugar moieties from AVE-A and B to form lower molecular weight steroidal saponins as a plausible metabolic pathway based on the variation trend and structures of these compounds. To the best of our knowledge, this is the first study to provide evidence that germination and false germination can be used to increase the steroidal saponins in oats and therefore enhance the bioactivity of oats. Our findings can serve as a reference for developing germinated oats as novel value-added products for consumers to prevent chronic diseases.

10:40 Assessing the impact of nitrogen supplementation in oats across multiple growth locations and years with targeted phenotyping and high-resolution metabolite profiling approaches Will Allwood1,2, will.allwood@hutton.ac.uk, Pilar Martinez-Martin3, Yun Xu4, Alexander Cowan3, Simon Pont1, Irene Griffiths3, Julie Sungurtas1, Sarah Clarke5, Royston Goodacre4, Athole Marshall3, Derek Stewart6,7, Catherine Howarth3. (1) Environmental and Biochemical Sciences, The James Hutton Inst., Dundee, United Kingdom(2) U. of Dundee, United Kingdom(3) Aberystwyth U. Inst. of Biological Environmental and Rural Sciences, Aberystwyth, Ceredigion, United Kingdom(4) Dept. of Biochemistry and Systems Biology, U. of Liverpool, United Kingdom(5) ADAS Gleadthorpe, Mansfield, Nottinghamshire, United Kingdom(6) The James Hutton Inst., Dundee, United Kingdom(7) Heriot-Watt U. School of Engineering and Physical Sciences, Edinburgh, United Kingdom Introduction: Oats are known as being a health beneficial cereal, high in dietary fibre (e.g. β-glucans), as well as antioxidants (e.g. avenanthramides), minerals and vitamins. UK agricultural guidelines on nitrogen (N) level are suboptimal. In this study the response of yield, grain quality and grain metabolites to increased N levels were investigated. Methods:

Four varieties (Mascani, Tardis, Balado, Gerald) were grown in a N response trial (0 control, 50-280 kg N/ha), over two UK locations and growth seasons. Grain yield and milling quality were assessed. β-glucan, total protein and oil content were quantified via near-infrared (NIR) spectroscopy. Oat metabolites were assessed by Gas Chromatography - Mass Spectrometry (GC-MS) and a newly developed and validated Ultra High Performance Liquid Chromatography (UHPLC) - High Resolution (HR)MS/MS method optimised towards high chromatographic resolution. Results: N had a significant effect on grain yield. Grain quality traits displayed significant differences between varieties and N application levels. β-glucan content significantly increased with N level. The GC-MS and LC-MS/MS methods captured a wide range of compounds, inclusive of amino acids, organic acids and sugars (GC-MS), vitamins, membrane lipids, and a range of secondary metabolites, including the avenanthramides and their glucosides, avenacins, avenacosides, hordenines and isovitexins (LC-MS/MS). Amino acid metabolism was upregulated by N, as were total protein levels, whilst organic acids were decreased (carbon skeleton scavenging). High N appeared to increase TCA turn over and reduce sugar levels to provide the plant with energy and reductant power to aid N assimilation. N was also directed towards the production of N containing phospholipids (e.g. Phosphatidyl Choline's (PC), Ethanolamine's (PE), and inositol's (PI)), likely as a scavenging and storage strategy. High levels of N application negatively impacted the total oat oil levels, and perhaps most significantly, the levels of health-beneficial avenanthramides. Conclusion: Although N addition significantly increased grain yield and β-glucan content, oat varietal choice as well as negative impacts upon health beneficial secondary metabolites and the environmental burdens associated with inorganic N fertilisers, require further consideration.

11:05 Variations in avenanthramide concentration in oats Lovemore Malunga, lovemore.malunga@agr.gc.ca. Agriculture and Agri-Food Canada, Morden Research Development Center, Winnipeg, Manitoba, Canada Avenanthramides are phenolic compounds unique to oat and may promote good health when consumed in adequate concentration. Genotypic and environmental factors affecting the concentration of avenanthramides were studied in Canadian oat. Twenty eight cultivars were grown for three years at three locations across Canada in a randomized complete block design with three field replicates. A UPLC–PDA system was used to analyze avenanthramides extracted from oat-groat flour. The mean concentration of total avenanthramide in oat was 49.9 μg/g with a 73 % coefficient of variation. The concentration of avenanthramides were significantly ($p<0.0001$) affected by the genotype, environment, and their interaction. The cultivar (C), growing location (L), CxL, and CxLxY explained 24, 21, 20, and 22% of the variation in the avenanthramide concentration, respectively. Understanding phenolic compounds' genotypic and environmental triggers may help agronomists and breeders strategize in selecting and growing oat cultivars of interest.

Renewable Polymer Materials: Preparation, Processing, Application, and Disposal

8:05 Bioorthogonal protein engineering Yoshihiro Ito1,2, y-ito@riken.jp. (1) Emergent Bioengineering Materials Research Team, Rikagaku Kenkyujo Sohatsu Bussei Kagaku Kenkyu Center, Wako, Saitama, Japan(2) Nano Medical Engineering Laboratory, Rikagaku Kenkyujo Kaitaku Kenkyu Honbu, Wako, Saitama, Japan Recombinant DNA technology has provided various designs of proteins with canonical amino acids. Bioothogonal protein engineering is for specific incorporation of non-canonical functional amino acids into proteins. Here some methodologies are shown. One is enzymatic ligation or modification of polypeptides for incorporation of non-canonical amino acids. As the enzyme, we employed sortase and tyrosinase. By these methods, incorporation of phosphorated serine or 3,4-dhydroxyphenylalanine, which plays an important role in the underwater adhesive proteins, into growth factor proteins was performed. The bioinspired growth factors were adhesive onto various materials and enhanced cell growth or differentiation on the modified surfaces. The long-lasting effect and high local concentration of adhesive growth factors significantly induced the enhancement. Another approach is usage of ribosome (in vitro translation system) and misacylated (non-canonical amino acid carrying) tRNA. Genetic PEGylation which is genetical incorporation of polyethylene glycol of different lengths into the side chains of polypeptides using stop-anticodon and frameshift anticodon-containing tRNAs which are acylated with PEG-carrying amino acids. In addition, not only rational design but also evolutionary engineering method which is the selection from random sequences has been also developed. These engineering technologies contribute the preparation of new class of functional proteins.

8:35 Development of soy protein-based hydrogels for a wide range of applications Long Jiang2,1, long.jiang@ndsu.edu, Qian Ma1,2, Raj S. Hazra1,2. (1) Material and Nanotechnology Program, North Dakota State U., Fargo(2) Mechanical Engineering, North Dakota State U., Fargo Soy protein is a natural polymer mainly used in human and animal foods and supplements. Non-food uses of soy protein have been developed and some of them have achieved commercial success including soy-based wood adhesive and thermoplastics. The functional groups in soy protein including amine, hydroxyl, thiol, and carboxyl allow it to form physical and chemical bonds with other polymers/agents relatively easily. In this presentation, the development of soy-based hydrogels with strong anti-drying performance and impressive flexibility, stretchability, and conductivity under very low temperatures (e.g. -40C) will be discussed. The factors that affect these properties will be evaluated. Their potential applications in biomedical, structure monitoring, and energy storage in a cold climate will be demonstrated. Future directions of development will be offered.

9:00 Zinc-coordinated chitosan nanocrystal for quercetin delivery Peihua Ma, peihua@umd.edu, Qin Wang, Cheng-I Wei. Nutri. and Food Sci., U. of Maryland at College Park There has been an increased demand for phytochemicals in food and nutraceutical in part due to an increase in consumers' health awareness. Delivery systems are commonly used for quercetin application, but key factors are scale-up, cost, clean-labeled and regulation. Here, we proposed a novel zinc-coordinated chitosan nanocrystal (Zn-ChNCs) for quercetin delivery which is easy to be fabricated, and high loading capacity is achieved by controlling the formation of nano-channels between chitosan chains. We first designed this novel structure with molecular simulation techniques and on this basis, we systematically characterized the prepared Zn-ChNCs on crystallography, morphology, and spectroscopy aspects. The particle size of synthesis is around 230.14 nm with a porosity of 64.6%. We finally encapsulated quercetin into Zn-ChNCs by immersion. The encapsulation rate and stability of the obtained material were characterized, which satisfied potential application. We hope this research will provide new ideas for developing food delivery systems and contribute to developing other metal-polysaccharide coordinated porous materials.

9:25 Utilization of hemp biomass waste: Physicochemical properties of protein isolated from leaves, flowers, and stems of industrial hemp after cannabidiol extraction Jerel Crew, jcrew@tnstate.edu, Ying Wu, ywu@tnstate.edu. Tennessee State U., Nashville Industrial hemp (Cannabis sativa L.) has garnered considerable interest in recent years due to its legalization and potential use in

various industries. This study aims to explore the use of hemp biomass protein as a novel ingredient in food and non-food systems. Hemp biomass was usually disposed of after cannabidiol (CBD) extraction from the flowers, leaves, and stems of industrial hemp. The current study has recovered about 60% of total protein in biomass waste by aqueous extraction and isolation at pH 4.5. Physicochemical characterization of the isolated protein was conducted to investigate the solubility, surface tension, amino acid profile, viscosity, water-holding and oil-holding capacities, zeta-potential and emulsification property. The major amino acid composition was ASP, GLU, GLY, VAL, ALA, VAL, and LEU. Its solubility reached the lowest point of around 14% at the pH 3 region and reached 52% at pH 8. Its zeta-potential value was beyond -30mV when pH reached 6 and above. Surface tension was observed to be far superior than pigeon pea and soy protein. The flow curves showed the material behaved shear-thinning and concentration dependent. These findings indicate that hemp biomass protein has promising emulsification properties, making it a potential alternative to conventional protein ingredients in various food and delivery systems such as packaging, encapsulation, and controlled release. Future studies are warranted to investigate its potential applications in food, cosmetics, and other industries.

10:05 Fabrication of Bio-based multiple-functional materials for a beneficial food-energy-water nexus Zhaohui Tong, zt7@gatech.edu. Chemical and Biomolecular Engineering, Georgia Inst. of Technology, Atlanta Our society is facing long-term challenges in the water-food-energy nexus, such as extreme climate change, resource and energy depletion, air pollution, food scarcity, and water and soil contamination. To tackle these sustainable concerns and challenges, our team has been dedicated to synthesizing value-added multiple-functional biomaterials from renewable resources, especially bio-based waste from biorefinery, agriculture, and forestry. The adaption of chemical functionalization and self-assembling methodologies to renewable starting materials for functional materials is very challenging due to bio-based feestocks' macromolecular structures, heterogeneous properties, poor solubility, and the disturbance of impurities. In this talk, we will focus on how we explore new modification and functionalization methods or reaction systems to attack these technical barriers. We will use some examples to describe a series of recently fabricated multiple-function biomaterials for applications in the areas of environmental mitigation and human health. For example, a glycerol-based intelligent food packaging film for a universal, accurate, easy-to-use, and real-time food spoilage monitoring system. Besides, smart materials with controllable release functions have been synthesized from low-cost biomass residues to improve nutrient (N, P, and micronutrients) utilization efficiency in agriculture and reduce environmental pollution to soil and water. The biocompatible and tunable biocomposites can achieve prolonged, stimuli-driven, and slow drug-release functions. Ultimately, we would like to utilize a waste-treat-waste approach to fabricate value-added functional materials to achieve a high-efficiency circular bioeconomy.

10:30 Oxidized chitin nanocrystals-enhanced colorimetric sensor array for accurate monitoring of beef freshness combined with deep learning models Xiaoxue Jia, jiaxx@umd.edu, Peihua Ma, Qin Wang. Nutri. and Food Sci., U. of Maryland at College Park Food waste poses a serious threat to the sustainability of agri-food systems. Food freshness monitoring reduces waste caused by food spoilage and promotes sustainability. We aimed to develop a biodegradable and safe material from inedible portions of seafood to monitor food freshness. Chitin was extracted from shrimp shells and oxidized with TEMPO. The oxidized chitin nanocrystals (O-ChNCs) were employed to prepare colorimetric sensor arrays (CSAs) that were able to monitor food freshness through color changes. The results showed that the oxidation procedure downsized chitin to the nanoscale, which enlarged surface areas and increased reactive sites with gases. TEMPO modification converted hydroxyl groups to carboxyl groups and endowed O-ChNCs with high negative charges. These modifications enhanced electrostatic interactions of O-ChNCs with ammonium cations, which were validated with three representative food spoilage gases (methylamine, trimethylamine, and ammonia). The CSAs prepared from O-ChNCs were more sensitive and showed faster color change compared to those prepared from untreated chitin nanocrystals. To accurately distinguish the color changes, four convolutional neural network (CNN) architectures were engaged and successfully discriminated freshness with an accuracy of over 96% during real-time monitoring of real beef samples stored at room temperature for 4 days. The highest accuracy of 99.27% was achieved by ResNet-50. The overall results indicated that the newly developed O-ChNCs-based CSAs coupled with CNN achieved fast and reliable monitoring of beef freshness. This study not only achieves freshness monitoring and reduces food waste, but also effectively utilizes inedible wastes and finds novel applications, thereby contributing to food sustainability.

10:55 Modified cellulose nanocrystals as functional nanofillers for antibacterial food packaging Yixiang Wang, yixiang.wang@mcgill.ca, Shuting Huang. Food Sci. and Agricultural Chemistry, McGill U. Faculty of Agriculture and Environment, Sainte-Anne-de-Bellevue, Quebec, Canada Considering the increasing food safety concerns, the development of antibacterial food packaging has attracted more and more attention. Cellulose nanocrystals (CNCs) are promising candidates for the fabrication of functional nanofillers due to their unique morphology and availability for modification. Herein, we aim to develop an approach to producing CNC-based antibacterial nanofillers that can be easily incorporated into commercial plastic films for active packaging. Particularly, CNCs extracted from cotton textile waste were modified with methacrylamide (MAM) and incorporated into cellulose acetate (CA) and poly(vinyl chloride) (PVC) films by the solution casting method. Addition of MAM-CNCs significantly improved the mechanical and UV barrier properties of CA and PVC films. After chlorination, the composite films with 3% MAM-CNCs exhibited excellent antibacterial efficacy against common foodborne pathogens, e.g., higher than 6 log reduction of S. aureus and E. coli after 1 h of contact at 37 °C. This antibacterial capacity could be recharged by chlorination without affecting the mechanical performance of plastic films. Subsequently, the effects of different CNC modifications on the performance of compostable materials were investigated. CNCs were modified with MAM, cetyltrimethylammonium bromide, and zinc oxide, respectively, and then applied on the surface of polylactic acid (PLA) films by spray-coating. Compared to neat PLA films, PLA/CNC films exhibited improved mechanical strength with maintained flexibility, lower gas permeability, and faster compost disintegration rate, and extended the shelf life of wrapped pork samples from 3 days to >10 days. Therefore, this work demonstrates the potential of utilizing modified CNCs to fabricate active food packaging.

11:20 Influence of pH, ethanol content, ionic environment, and casein concentration on electrospinnablility of casein dispersions Deepika Sharma, deepi.nids21@gmail.com, Gregory R. Ziegler, Federico M. Harte. Dept. of Food Sci., The Pennsylvania State U., U. Park The low molecular weight of casein proteins (19–25 kDa) and their strong affinity to form casein micelles in native milk (ca. 250 nm in diameter) or aggregates in caseinate dispersions, limits the electrospinnablility of caseins. The study reports the influence of pH, ethanol content, ionic environment, and casein concentration on the solubility, solution viscosity, surface tension and conductivity of

casein-based spinning dopes intended to fabricate bead-free casein nanofibers. The conductivity of the electrospinning dopes increased with an increase in casein concentration and decreased with the increase in ethanol content. A homogenous dispersion of casein was observed for mixtures with 20 wt. % casein prepared using 60 % ethanol/water mixture at pH 10. Minimum viscosity (0.4 Pa.s) and surface tension (60.6 mN/m) with comparatively higher conductivity (897.7 μS/cm) was observed for solutions containing 2 wt. % of tetrasodium pyrophosphate (TSPP) with respect to casein content, which resulted in the formation of nanofibers with a minimum number of bead defects (BN ~ 6 x 10-3/ μm2) and minimum average fiber diameter (FD) of ~ 424 nm. Further, the viscosity dependence on casein concentration at constant relative TSPP content was like polyelectrolytes and casein nanofibers with minimum bead defects obtained at a concentration ~ 2 to 2.5 times the entanglement concentration (Ce). Therefore, the study demonstrates the influence of solution characteristics on the electrospinnablility of casein proteins to fabricate novel biodegradable, and biocompatible, casein-based nanostructured mats with potential for food, cosmetic, packaging, and biomedical applications.

Smart Food Safety

8:05 Non-targeted analysis using high-resolution mass spectrometry as a smart and innovative tool to assess the safety of food contact materials Stephane Bayen1, stephane.bayen@mcgill.ca, Barbara Hales2, Cindy Goodyer5, Ziyun XU1, Lei Tian3, Lan Liu4. (1) Dept. of Food Sci. and Agricultural Chemistry, McGill U., Montreal, Quebec, Canada(2) McGill U. Faculty of Medicine and Health Sciences, Montreal, Quebec, Canada(3) McGill U. Faculty of Agriculture and Environment, Sainte-Anne-de-Bellevue, Quebec, Canada(5) McGill U. Health Centre, Montreal, Quebec, Canada Plastic-based materials used as food contact materials (FCMs) are of particular concern considering the diversity of chemical residues which may migrate from these materials into our food. A range of intentionally added substances in FCMs, such as plasticizers and flame retardants, have been identified to have detrimental impact for human health. We recently correlated the levels of bisphenols (endocrine disrupters) in fresh food in Canada with their use as color developers in thermal labels on food packaging [https://doi.org/10.1021/acs.est.2c09390]. In addition, non-intentionally added substances, including breakdown products, impurities, and unwanted side products, may also migrate from FCMs into contacted food and have emerged as a concern for the food industry due to a lack of detailed guidance for their assessment. Recent advances in the fields of chromatography and mass spectrometry have greatly enhanced the capacity to analyze trace contaminants in agri-food matrices. In particular, non-target analysis (NTA) based on high-resolution mass spectrometry (HRMS) has emerged as a novel approach to detect and identify unknown or unexpected contaminants not captured by the conventional targeted methods. In this talk, key applications of suspect and non-targeted analyses for plastic-derived chemicals in FCMs will be presented. First, screening methods using LC-QTOF-MS will be introduced for contaminant analysis in food, and we will show how their application has revealed the contamination of agri-food systems by previously unreported manmade chemicals, all with plastics as a common origin. Some recent studies on the NTA of migrants from FCMs using LC-QTOF-MS will be presented; these results demonstrate the capacity of NTA to uncover new contaminants of concern. Innovative tools, e.g. quantitative structure retention time relationships, will be described to improve the identification of unknowns. Using this LC-QTOF-MS approach, large chemical fingerprints can be recorded for each sample, offering novel perspectives on the plastic-derived chemical mixtures present in FCMs.

8:45 EpCAM : Eco-friendly, Polymer-based nanozyme integrated with colorimetric sensing platform for agricultural biomolecule detection Dong Hoon Lee, dhl5@illinois.edu, Mohammed Kamruzzaman. Dept. of Agricultural and Biological Engineering, U. of Illinois Urbana-Champaign Agricultural biomolecules, including pesticides and antioxidants have a significant impact on agricultural quality control and human health. Researchers recently contrived nanozyme for use in agricultural applications for detecting these biomolecules. However, most of the nanozymes they contrived are noble-metal nanoparticles or MOF (Metal-Organic Framework)-derived nanostructure which is a comparably toxic (e.g., MOF) and expensive material (e.g., Gold nanoparticle). To overcome these drawbacks, bio, and eco-friendly materials-based nanozyme with cost-effectiveness are required. To address this needs, we have introduced an eco-friendly, fully polymer-based nanozyme with peroxidase-like activity. As our nanozyme is made entirely by biopolymers, we expect it to be highly biocompatibility and cost-effective compared to the conventional nanozyme utilized in agricultural applications, such as MOF and engineered AuNP. Furthermore, our nanozyme has decent catalytic performance (LOD of H2O2, up to 100nM) and good stability with its catalytic consistency on a broad range of pH conditions. Our nanozyme-integrated colorimetric detection platform enables to proceed fast antioxidant detection (e.g., H2O2), and other agricultural (e.g., pesticide) and food biomolecule (e.g., vitamin C) in agriculture and food samples. We also provide the RGB-scale smartphone-based simple readout platform to provide the Point-of-Use detection platform for agricultural biomolecules. We envision our nanozyme can be utilized for various agricultural applications in the future.

9:15 Phage-based nanobots to recognize, separate, and concentrate bacteria for food and water safety Caitlin M. Carmody, Sam R. Nugen, snugen@cornell.edu. Food Sci., Cornell U., Ithaca, New York Immobilization of bacteriophages onto solid supports such as magnetic particles has demonstrated ultralow detection limits as biosensors for the separation and detection of their host bacteria. While the potential impact of magnetized phages is high, the current methods of immobilization are either weak, costly, inefficient, or laborious making them less viable for commercialization. Here, we genetically engineered bacteriophages to allow synthesis of a monomeric streptavidin on the phage capsid during infection of the bacterial host. The monomeric streptavidin was fused to a capsid protein (Hoc) to allow site-specific self-assembly of up to 155 fusion proteins per capsid. Phages were genetically engineered using CRISPR/Cas9 to modify the capsid protein Hoc with an mSA fusion. Additionally, a gene for the luciferase NanoLuc was inserted into the phage genome resulting in expression during host infections. The modified phages were then conjugated to biotin-modified magnetic nanoparticles and used to capture E. coli (ECOR13) from 100 mL water samples. Following capture, separation, concentration, and resuscitation, the samples were analyzed for active NanoLuc using a luminometer. The assay's signal increased proportionally with E. coli (ECOR13) concentration. The assay resulted in a 4.68 ± 1.82 luminescence signal:noise ratio for 10 ± 4 CFU/100 mL, and 23.85 ± 13.11 luminescence signal:noise ratio for 89 ± 19 CFU/100 mL. The limit of detection (LOD) for ECOR 13 in 100 mL of water using the mSA-modified phage assay was calculated to be ~5 CFU/100 mL. Significance: This work highlights the creation of genetically modified bacteriophages with a novel capsid modification, expanding the potential for bacteriophage functionalized biotechnologies.

9:55 Probiotic biopolymer-based encapsulation enhances limonene oil stability and antimicrobial efficacy Sangeeta Balyan1,3,

sangeetabalyan05@tamu.edu, Nitin Dhowlaghar2,3, nd288@tamu.edu, Bhimu S. Patil1,2,3. (1) Dept. of Food Sci. & Technology, Texas A&M U. System, College Station(2) Dept. of Horticulture Sciences, Texas A&M U. System, College Station(3) Vegetable and Fruit Improvement Center, Texas A&M U. System, College Station The potential of plant essential oils, such as limonene, as natural flavor additives and preservatives in food products is hindered by their limited solubility, stability, and bioavailability. To overcome these challenges, we tested exopolysaccharide (EPS) extracted from probiotic lactic acid bacteria as a novel food-grade emulsifier to enhance the stability and antimicrobial activity of limonene. The EPS-based emulsions successfully encapsulated S-limonene and D-limonene, with mean particle sizes of 450 and 462 nm, respectively, and a low polydispersity index. Upon optimization of EPS and oil concentrations, the droplet size decreased, and the emulsion stability increased, due to the irreversible adsorption of EPS at the oil-water interface. The Fourier transform infrared spectra indicated the presence of cyclohexane-1-ene in both emulsions, reflecting the presence of limonene oils, which reinforced the interfacial network. Moreover, the emulsions demonstrated excellent stability under various processing conditions. The combination of EPS and limonene oils exhibited enhanced antimicrobial activity against Escherichia coli O15:H7 and Listeria monocytogenes V7 strain, compared to free oils. In conclusion, this study presents a promising approach for enhancing the stability and antimicrobial activity of natural essential oils using EPS-based emulsions from probiotic bacteria.

10:25 Point-of-need microfluidic device to safeguard food integrity Yaxi Hu[1], huyaxi2004@gmail.com, Xiaonan Lu[2], Yunxuan Chen[3]. (1) Chemistry, Carleton U. Faculty of Science, Ottawa, Ontario, Canada(2) McGill U. Faculty of Agriculture and Environment, Sainte-Anne-de-Bellevue, Quebec, Canada(3) The U. of British Columbia Faculty of Land and Food Systems, Vancouver, Canada Food safety and food fraud are the two major issues impacting food integrity. Globally, ~ 600 million people annually suffer from foodborne illnesses related to the consumption of unsafe food. Although typically not resulting in illness, food fraud issues have been estimated to cause approximately $65B USD in damages to the food industry each year. The prevalence of food safety and food fraud issues can be partially attributed to the lack of rapid and cost-effective analytical methods that are suitable for frequent routine analysis needed by the food industry and inspection agencies. To tackle this challenge, we have developed analytical methods harnessing the advantages of isothermal nucleic acid amplification and microfluidic “lab-on-a-chip” platform for rapid, accurate and cost-effective detection of two representative food safety and food fraud issues, namely Salmonella enterica contamination and pomegranate juice adulteration. By delicate design, we developed simple sample-to-answer microfluidic devices that integrate the DNA extraction, isothermal amplification and results readout functions onto a single device. Without the need of any laboratory specific infrastructure, the devices achieved sensitive detection of 32, 44, and 58 CFU/mL Salmonella in lettuce, chicken breast and milk with a 6-hour incubation; and 2 µL pomegranate juice and 5 µL apple and grape juice in fresh fruit juice mixtures. The overall analysis for Salmonella detection was achieved in~ 30 min, while the analysis for the authentication of pomegranate juice could be completed in ~1 h. The cost for each safety and authenticity test was estimated to be ~ $4 USD including the cost for fabrication of the microfluidic devices and the use of reagents at the laboratory scale. These simple sample-to-answer hybrid paper/polymer-based lab-on-a-chip devices are expected to have high potential for being adopted by government laboratories and the food industry to rapidly and routinely analyze the safety and authenticity of food products.

Sustainable Agriceuticals

8:03 Effect of polyphenol extract-derived postbiotics on microbiota dysbiosis in HF-induced obese mice Hyunsook Kim1, hyunsk15@hanyang.ac.kr, Kun-Ho Seo2, Hye-Young Youn3. (1) Food and Nutrition, Hanyang U., Seongdong-gu, Seoul, Korea (the Rep. of)(2) Konkuk U., Gwangjin-gu, Seoul, Korea (the Rep. of) Postbiotic for weight management by bioconversion of whey (WHE) and polyphenol-rich citrus pomace extract (CPX) using kefir lactic acid bacteria (LAB) was developed. WHE and CPX bioconverted by kefir LAB (CPB) were fed to C57BL/6J mice on high-fat diets for five weeks and compared with oral administrations of saline (CON), WHE, CPX, and kefir LAB. CPB group showed significantly reduced HF-induced body weight gain, adipose tissue weight/body weight ratio, hypertriglyceridemia, and adipocyte diameter along with increased gene expression related to energy expenditure in adipose tissue, compared to the CON. Abundance of gut microbiota related to butyrate production was significantly altered in the CPB group compared with the CON group. There was a significant correlation between obesogenic biomarkers and the abundance of butyrate-producing and obesogenic gut microbiota. In conclusion, kefir LAB-derived bioconversion of WHE and CPX may be effective in improving obesity-related microbiota dysbiosis.

8:33 Macro and nanocapsules of essential oil in the protein/pectin system stabilized by ultrasound Shahnozabonu Alieva, Gulru Kodirova, Jamshed Bobokalonov, Zamira Sherova, Zayniddin Muhidinov, muhidinovzayniddin@gmail.com. V.I. Nikitin Inst. of Chemistry, Dushanbe, Tajikistan Recently, there has been a growing interest in using bioactive compounds (BAC) isolated from plant sources in functional foods and pharmaceuticals. It is known that the food matrix, molecular size, and environments of the gastrointestinal tract can interfere with the bioavailability and stability of the BAC. Protecting BAC with nanoencapsulation technology can increase their stability in the GI tract. Therefore, this work is devoted to studying a delivery system based on macro- and nanocapsules of essential oils in emulsion for the control release, and protection of BAC (essential oils). Also, the effect of various amplitudes of ultrasounds on the stability of essential oil/water emulsion in the protein/pectin system was investigated. The average size of the resulting nano- and microcapsules (d4.3), the zeta potential, the particles' specific surface area, and the dispersion system's viscosity were analyzed. It was shown that depending on the applied force, the ultrasound wave initiates the formation of a pectin layer with different charge densities on the surface of emulsion particles. The ultrasound amplitude was optimized to produce particles with an average size and a high specific surface area of 32967 cm square per gram of emulsion. The resulting nano- and macroparticles with essential oil showed good antimicrobial, antifungal, and antiviral activity. The developed delivery systems with specific characteristics may well meet the requirements of the antibacterial drugs market. Overall, it is eventually recommended to use the developed system as an antibacterial agent; however, toxicity investigation and precise in vivo experiments are required.

8:53 Multi-crosslinked hydrogels with multi-functions for seawater-immersed wound healing Xian-Ai Shi, shixa@fzu.edu.cn, Yicheng Lv, JM Yang. Fuzhou U., Fujian, China Seawater-immersed wounds are associated with tissue necrosis, infection, prolonged healing period, and high mortality because of high salinity, hyperosmosis, and the presence of various pathogenic bacteria in seawater. However, current wound dressings can hardly achieve strong and stable wet adhesion and antibacterial properties, thus limiting their application to seawater-immersed wounds. Here a multifunctional hydrogel (OD/EPL@Fe) comprising catechol-modified oxidized hyaluronic acid (OD), ε-poly-L-lysine (EPL), and

Fe3+ was prepared primarily through Schiff-base reaction, metal chelation, cation–π, and electrostatic interaction. The hydrogel with high wet adhesion (about 78 kPa) was achieved by combining the mussel-inspired strategy, dehydration effect, and cohesion enhancement, which is higher than that of commercial fibrin glues and cyanoacrylate glues. Meanwhile, the hydrogel can eliminate Marine bacteria (V. vulnificus and P. aeruginosa) and inhibit their biofilm formation. In addition, the hydrogel demonstrated injectability, self-healing, reactive oxygen species scavenging activity, photothermal effect, seawater isolation, on-demand removal, and hemostatic properties. In vivo results showed that the hydrogel had good adhesion to dynamic wounds in a rat neck full-thickness skin wound model. In particular, the hydrogel exhibited antibacterial, anti-inflammatory, and antioxidant properties in a rat seawater-immersed infected wound model and accelerated the reconstruction of skin structure and functions. The results demonstrated that the OD/EPL@Fe would be a potential wound dressing for seawater-immersed wound healing.

9:13 Chemical composition of honeysuckle (Lonicerae Japonicae) extracts and their potential in preventing COVID-19 and scavenging free radical capacities Boyan Gao[1], raphaelgao1985@gmail.com, Huoying Chen[1], chhy@sjtu.edu.cn, Liangli Yu[2]. (1) Shanghai Jiao Tong U., China(2) U. of Maryland at College Park Honeysuckle (Lonicerae japonicae) has been used in functional tea products. The chemical compositions of the water and ethanol extracts of honeysuckle were examined in the present study, along with their potential in inhibiting SARS-CoV-2 spike protein binding to ACE2, suppressing ACE2 activity and scavenging reactive free radicals. Thirty-six compounds were tentatively identified from the honeysuckle extracts using HPLC-MS/MS, with ten reported for the first time in honeysuckle. Both honeysuckle extracts inhibited the binding of SARS-CoV-2 spike protein to ACE2, as well as ACE2 activity. The ethanol extract exhibited a 100% inhibition on binding of the SARS-CoV-2 spike protein to ACE2 at 100 mg botanical equivalent/mL, whereas the water extract had a 65% binding inhibition at the same concentration. Furthermore, the water extract exhibited 90% ACE2 activity inhibition, which was stronger than that of the ethanol extract (62% inhibition) at the same botanical weight concentration. In addition, higher total phenolic contents and greater scavenging activities against hydroxyl (HO), DPPH and ABTS radicals were observed in the water extract than the ethanol extract counterpart on a dry botanical weight concentration basis. These findings suggest honeysuckle has the potential to reduce the risk of SARS-CoV-2 infection and the development of severe COVID-19 symptoms.

9:33 Associations of diet quality, mediating metabolomics, with frailty and sarcopenia: Findings from the UK biobank Zuobing Chen, czb1971@zju.edu.cn. The First Affiliated Hospital, School of Medicine, Zhejiang U., Hangzhou, China Background: Frailty and sarcopenia are common geriatric syndromes that require appropriate management. Healthy diet is a modifiable factor that has been shown to benefit physical health. However, the associations of diet quality on frailty and sarcopenia remain unclear. Moreover, not much is known about diet-related metabolomic biomarkers that may mediate the associations. Objective: To examine the associations of dietary patterns with frailty and sarcopenia and to investigate the potential mediation effects of metabolomics in the associations. Methods: Overall, 296,065 participants from the UK Biobank were included for frailty and sarcopenia analysis, respectively. We use the Oxford WebQ to record the diet. Frailty was measured by five items: involuntary weight loss, tiredness, weakness, slow walking speed, and low physical activity. Sarcopenia was defined as low grip strength. Generalized linear regression models were used to investigate the associations of adherence to four dietary patterns, alternate Mediterranean diet (aMED), Recommended Food Score (RFS), Dietary Approaches to Stop Hypertension (DASH), and Mediterranean-DASH Intervention for Neurodegenerative Delay diet (MIND), with frailty and sarcopenia. Metabolomics were assessed using multivariable linear regression models and the mediation analysis. Results: Higher diet quality scores were all independently associated with frailty and sarcopenia (all P for trend<0.001). After multivariable adjustments, for aMED, RFS, DASH and MIND, the odds ratios (95% confidence intervals, CIs) for the highest tertile group versus the lowest tertile group were 0.74 (0.67,0.81), 0.66 (0.62, 0.72), 0.75 (0.70, 0.81) and 0.75 (0.70, 0.81) for frailty, 0.82 (0.77, 0.88), 0.78 (0.74, 0.83), 0.82 (0.78, 0.87) and 0.87 (0.82, 0.94) for sarcopenia, respectively. Conclusions: Adherence to aMED, RFS, DASH, and MIND were negatively associated with frailty and sarcopenia, and diet-related metabolomics mediated the association. Our findings reveal novel mechanistic insights into the diet quality in the frailty and sarcopenia, leading to healthy aging.

10:03 Combination of cinnamon bark and astragalus extracts reduces metabolic dysfunction and improves microbiome composition in mice fed high-fat diets Hyunsook Kim2, Priscila Alves1, Wallace H. Yokoyama1, wally.yokoyama@ars.usda.gov. (1) Healthy Processed Foods Research, USDA, Albany, California(2) Dept. of Food and Nutrition, Hanyang U., Seoul, Korea (the Rep. of) Mice fed a high fat diet (HF) containing 0.1% cinnamon extract (CNMN) and 0.1% astragalus (ASTR) extract (CNMN+ASTR) for four weeks significantly reduced (P<0.05) body weight gain, total body weight, epididymal adipose weight, and blood glucose compared to mice fed HF diet alone. Individually, 0.2% CNMN or 0.2% ASTR tended to lower body and organ weights as well as lower blood glucose compared to the HF diet alone suggesting a synergism between CNMN and ASTR. CNMN tended to lower LDL, HDL, TOTAL-cholesterol, and lower LDL/HDL ratio. 0.2% CNMN, 0.2% ASTR, and 0.1% CNMN+0.1% ASTR.

10:33 Milk fat globule membrane regulates the physicochemical properties and surface composition of prepared infant formula powders by improving the stability of the emulsion Qingxue Chen, Fangqin Xiang, Xinming Ma, Bailiang Li, 15846092362@163.com. Northeast Agricultural U., Harbin, China Milk fat globule (MFG) in infant formula (IF) powders are maintained by a membrane structure composed of proteins and phospholipids, which is reconstructed in homogenization. Milk fat globule membrane (MFGM) is a structure naturally present in breast milk and has great potential for emulsification. However, it is currently unclear whether the improved emulsion stability of MFGM can have a profound effect on the final prepared IF powder. Therefore, this study investigated the effects of MFGM on the particle size, stability, rheology, and microstructure of emulsions. Further, IF powders with MFGM were prepared, and the physicochemical properties, surface composition of the powders were examined. The results showed that MFGM reduced the particle size of the emulsion, improved the emulsion stability, increased the viscosity, and improved the microstructure of the MFG, and these results indicated that MFGM improved the stability of the emulsion. Furthermore, MFGM reduced the moisture content of the powder, increased the glass transition temperature (Tg), and reduced the presence of surface fat, indicating that MFGM improved the powder stability. This was attributed to the fact that MFGM promoted the structure of more protein/phospholipid-coated MFG to enhance emulsion stability, thus improving the powder is physicochemical properties and stability.

10:53 Identification of exposure biomarkers for apple consumption by targeted metabolomics approach Junhe Yu, junhe1017@163.com, Yingdong Zhu, Weixin Wang, Shengmin Sang. Center for Excellence in Post-Harvest Technologies, North Carolina A&T State U., Kannapolis Apple consumption is widely recommended in dietary guidelines worldwide due to its potential to prevent chronic diseases. However, accurately assessing apple intake in large human studies remains a challenge because of the recognized bias associated with self-reporting methods, particularly in reporting the precise type and quantity of apple intake. In this study, major polyphenols in apples, including dihydrochalcones (DHC), flavan-3-ols, flavonols, anthocyanins, and phenolic acids, were firstly profiled. To identify specific exposure biomarkers for precise assessment of apple consumption, a crossover human study with 11 healthy subjects was then conducted. Urine and blood samples were collected at different time points after a single dose of apple consumption. Metabolic fingerprints of major apple polyphenols were extensively investigated using targeted LC/MS-based metabolomic approaches, leading to the identification of over 40 apple polyphenols and their metabolites in humans. Based on the pharmacokinetic profiles of these metabolites, we grouped them as short-term, mid-term, and long-term exposure biomarkers. We also established a panel of urinary markers consisting of multiple metabolites of DHC, flavan-3-ols, flavonols, and anthocyanins as specific biomarkers to cover multiple time points and longer time periods for the correct and objective monitoring of apple consumption. By establishing specific exposure biomarkers and a panel of urinary markers, our study can help to reduce the bias associated with self-reporting methods and improve the accuracy of dietary assessment of apple consumption, thus facilitating the evaluation of the potential health benefits of this fruit.

11:13 Changes in functional properties of eggplant during pickling process using fermented rice bran Haruna Kamo, Yukiharu Ogawa, ogwy@faculty.chiba-u.jp. Graduate School of Horticulture, Chiba Daigaku, Matsudo, Chiba, Japan Rice is a plant seed of Caryopsis species, which consists of a pericarp, seed coat, germ, and endosperm. The color of a normal pericarp is light brown; therefore, it is called brown rice. Because of the low sensory traits, the pericarp, seed coat, germ, and a part of the aleurone layer on the endosperm are usually removed from the brown rice grain. Those removed portions are called rice bran, which can be regarded as a byproduct of rice postharvest processing. Rice bran contains a lot of nutritional substances, including substances with functional potential. Such rice bran is traditionally used as a pickling bed to produce Japanese fermented pickles using fresh vegetables. The rice bran pickling bed is mixed with salt and naturally fermented by bacterial flora, mainly lactic acid bacteria. The functional substances in rice bran could be absorbed in the pickles during fermentation. However, the nutritional and functional characteristics of resulting pickles vary by the pickling conditions and materials. This study investigated changes in the functional properties of eggplant as a pickled material during the pickling process with fermented rice bran. A commercially produced fermented rice bran bed (7% of salt concentration) and fresh eggplant were used in this study. The pickling process was set for 24 h at 23 °C. Moisture content, total phenol content, total flavonoid content, DPPH, and ABTS of the eggplant were measured at 6 h intervals during the pickling process. The results showed that the values of all functional parameters increased 1.5 times from the start to 18 h of the pickling but decreased to lower than the initial values at 24 h of the pickling. This could indicate that the functional property of pickles transferred from the fermented rice bran, but it would have optimized values during pickling.

11:33 Whey protein hydrolysate alleviated atherosclerosis and hepatic steatosis by regulating lipid metabolism in apoE-/- mice fed a Western diet Kai Wang, Yuqing Tan, yuqingtan@cau.edu.cn. Food Sci. and Nutritional Engineering, China Agricultural U., Beijing Whey protein hydrolysate (WPH) has been proved to possess various biological activities associated with the amelioration of cardiovascular disease (CVD). The objective of this study was to investigate the antiatherosclerotic and hepatoprotective effects of WPH on apolipoprotein E knockout (apoE-/-) mice fed with a Western diet for 15 weeks. Results revealed that WPH markedly inhibited the development of atherosclerotic lesions in the aorta and steatosis injury in the liver. The serum lipid and inflammation levels were both reduced after WPH supplemented in apoE-/- mice. In addition, WPH inhibited the lipid accumulation in the liver, thereby decreasing the hepatic inflammation level and oxidative stress injury. Mechanism investigation revealed that WPH down-regulated the expression of cholesterol biosynthesis genes while up-regulated the expression of cholesterol uptake and excretion genes in the liver. Meanwhile, the de novo lipogenesis was inhibited while the fatty acids β-oxidation was activated in the liver by WPH supplementation. Notably, the n-3 polyunsaturated fatty acid (PUFA)/n-6 PUFA ratio in serum and liver of the WPH-H group were 2.69-fold ($p < 0.01$) and 3.64-fold ($p < 0.01$) higher than that of the Model group. Collectively, our results proved WPH possesses potent antiatherosclerotic and hepatoprotective activities and has the potential to be used as a novel functional ingredient for the management of CVD.

ACS Microbiome Consortium Kick off Symposium

8:05 Algorithms and analysis approaches in microbiome research Weibin Zeng, wb.zeng@louisville.edu. U. of Louisville, Kentucky Microbiome research is a rapidly growing field that has the potential to revolutionize our understanding of human health and disease. As the field has grown, so too has the need for sophisticated computational tools to help analyze the vast amounts of data generated by microbiome studies. This presentation is to give an overview of the algorithms and approaches for analyzing microbiome data, their challenges and limitations, with focus on some case studies, and discuss how mathematical and statistical tools and algorithms are helping to advance our understanding of the role of the microbiome in health and disease.

8:50 Sudden change in diet acutely affects the gut microbiome response after an in vitro resistant starch supplementation Ida Gisela Pantoja Feliciano1, ida.g.pantojafeliciano.civ@army.mil, J. Philip Karl2, Matthew Perisin3, Laurel A. Doherty1, Holly L McClung2, Nicholes J Armstrong2, Rebecca Renberg4, Kenneth Racicot1, Tobyn Branck1, Steve Arcidiacono1, Jason W. Soares1. (1) Soldier Effectiveness Directorate (SED), U.S. Army DEVCOM Soldier Center, Natick, Massachusetts(2) Military Nutrition Division, U.S. Army Research Inst. of Environmental Medicine (USARIEM), Natick, Massachusetts(3) U.S. Army DEVCOM Army Research Laboratory, Adelphi, Maryland(4) General Technical Services, U.S. Army DEVCOM Army Research Laboratory, Adelphi, Maryland Gut microbiome homeostasis in vivo is due to complex microbial interactions which can be perturbed by acute stress-induced changes in the gastrointestinal environment, potentially leading to dysbiosis. Diet in particular, can greatly influence the dynamics of gut microbiome composition and metabolism. In our laboratory we used an in vitro gut model to investigate the influence of a sudden change in diet, namely 21 days sole sustenance on the Meal, Ready-to-Eat (MRE) U.S. military combat ration relative to volunteers on habitual diet (HAB), on population dynamics within the gut microbiome using resistant starch (RS) as a substrate. Fecal samples collected from individuals before and after consuming their habitual diet or only MREs for 21

days underwent 24hr in vitro fermentation in nutrient-rich media supplemented with RS under ascending colon domain-specific conditions. 16S rRNA amplicon, Whole Genome Sequencing (WGS) and specific statistical analysis were used to measure community composition and functional potential. 11 taxa showed differential changes in relative abundance; as an example, we can mention Dorea spp which notably increased in the MRE day 21 group after 10hr of exposure to starch-supplemented medium relative to the other groups. Nine Carbohydrate-active enzyme (CAZymes) showed interesting patterns due to MRE day 21 group, specifically GH13_14 significantly higher at 10 and 24hr in MRE day 21 group compared to the other groups. These findings revealed how gut microbial metabolic capacity is acutely altered as a function of a sudden change in diet. Additionally, this study begins to identify candidate nutritional intervention substrates for modulating the gut microbiome to impact on health and performance.

9:10 Deciphering diet-microbiota interactions by integrating metabolomics and metagenomics with topological data analysis Leah Guthrie1, lguthri1@stanford.edu, Justin Sonnenburg1,2,3. (1) Microbiology and Immunology, Stanford U. School of Medicine, California(2) Chan Zuckerberg Biohub, San Francisco, California(3) Center for Human Microbiome Studies, Stanford, California Integrating diet data with microbiome composition, metagenomics, and metabolome datasets is critical for understanding diet-microbiome-metabolite interactions. Inferring these interactions has multiple challenges, including collecting dietary data that accurately reflects intake at a resolution relevant to microbial community structure and metabolism and identifying analytical frameworks for multivariate compositional datasets that enable the discovery of meaningful diet-microbiome-metabolome relationships. We tackle these challenges using a chemoinformatic approach to convert dietary log data into compound matrices and apply topological data analysis approaches to define diet-metabolite and diet-microbiome interactions. First, we determine a high-level structure of microbial communities with subpopulations associated with distinct dietary patterns. We identify diet-metabolite-microbiome interactions that are not revealed by macronutrient level profiling by reanalyzing data from three dietary intervention studies. We also identify microbiome features related to microbiome composition and microbiome-dependent metabolic output that are the most sensitive to and predictive by diet chemical composition. Our chemical-centric approach can aid in assessing participant responsiveness to a dietary intervention based on their baseline microbiome.

9:30 Chemistry in the rhizosphere: Using fabricated ecosystems and exometabolomics to match plants with beneficial microbes Trent Northen, TRNorthen@lbl.gov. E O Lawrence Berkeley National Laboratory, California Rhizosphere microbiomes are important drivers of plant health and soil carbon cycling. Metabolites mediate critical plant-microbe interactions and can be directly probed using exometabolomics. However, the large variability and lack of control in natural environments makes it difficult to determine causal mechanisms. Using exometabolomics we have found that aromatic acids are a key class of metabolites in structuring rhizosphere communities. To address this need, we have developed methods for making and using fabricated plant ecosystems (EcoFABs) complete with synthetic rhizosphere microbial communities. Using these capabilities, we have found that aromatic acids and other related metabolites are secreted by plants under nutrient stress and are preferentially used by rhizosphere bacteria. These findings lay a foundation for matching plant hosts with beneficial microbes.

10:00 Microbiome data augmentation using deep learning models Liqing Zhang, lqzhang@vt.edu. Computer Science, Virginia Polytechnic Inst. and State U., Blacksburg Microbiome sequencing technology has proven to be a valuable tool in generating rich information and has been widely used across various domains. However, this type of data also presents several challenges such as lack of generalizability, high dimensionality with low sample size, and missing data. In this presentation, I will discuss several projects that have utilized recent developments in deep learning to address these challenges and further advance our understanding of the microbiome.

10:20 Applying metagenomic sequencing to decipher the human gut microbiome Matthew R. Olm, mattolm@stanford.edu, Dylan Dahan, Bryan Merrill, Matthew Carter, Justin Sonnenburg. Microbiology and Immunology, Stanford U. School of Medicine, California The gut microbiome is a key modulator of human immune and metabolic health. Changes in the microbiome brought on by the industrialized lifestyle have been linked to increasing rates of immune disorders in the West, yet little is known about the microbiome of non-industrialized populations. Here we addressed this gap by profiling the gut microbiome of the Hadza, modern-day hunter-gatherers in Tanzania, using state-of-the-art metagenomics techniques. We discover key differences in microbiome composition and function across lifestyles, including changes related to strain acquisition and microbial adaptation to inflammation. These results extend our understanding of microbiome variation across the globe, provide important context for interpreting changes brought on by industrialization, and highlight the power of metagenomic sequencing to probe this essential component of our human physiology.

10:40 Interplay between gut microbiota and curcumin. **M. Luo**, H. Xiao NO ABSTRACT

11:00 Identification, distribution and structural diversity of Fusarium molecules with potential to modulate plant-microbiome interactions Hye-Seon Kim1, hyeseon.kim@usda.gov, Guixia Hao1, Carson Andorf2, Robert Proctor1. (1) Mycotoxin Prevention and Applied Microbiology Research Unit, USDA Agricultural Research Service, Peoria, Illinois(2) Corn Insects and Crop Genetics Research Unit, USDA Agricultural Research Service, Ames, Iowa Plant microbiomes include rhizosphere, endosphere and phyllosphere components that can vary in composition of microbial species. Plant microbiota can positively or negatively impact plant development, fitness and/or health. Some of these impacts are caused by two types of microbial molecules: proteins and secondary metabolites. The proteins include effectors, which are relatively small and often cysteine-rich peptides that elicit or suppress responses in plants and/or other members of the microbiome. The secondary metabolites include plant growth promoting compounds, such as auxins and gibberellins, and harmful compounds, such as toxins. A common constituent of plant microbiomes is Fusarium, a species-rich fungal genus that includes both endophytic and pathogenic species that collectively produce numerous secondary metabolites with diverse structures and biological activities. Fusarium species, particularly pathogenic species, also secrete effectors that have potential to suppress plant defenses. Advances in Artificial Intelligence (AI)/Machine Learning have provided tools that have markedly improved our ability to identify, predict 3D structures, and assess diversity of fungal effectors. Using these tools and an in-house genome sequence database, we identified 2,916 genes encoding putative effectors in 199 species representing the breadth of phylogenetic diversity of Fusarium. Examination of the putative effectors using functional annotation tools and the AI program AlphaFold provided insight into the diversity of 3D structures of the effectors. Expression analysis of 25 of these effectors in the cereal head blight pathogen Fusarium graminearum revealed that seven are highly expressed during wheat head

infection. The predicted 3D structures of effectors, secondary metabolite biosynthetic enzymes, and other proteins from two Fusarium species (F. graminearum and F. verticillioides) can be viewed at https://fusarium.maizegdb.org/protein_structure. Understanding of structural diversity, function, and distribution of effectors has potential to aid in development of control strategies that reduce crop diseases and mycotoxin contamination problems caused by Fusarium.

11:20 Towards gut microbiome-based precision dieting: understanding interindividual variations in resveratrol hydrogenation through a gut bacterial pathway Yanyan Wu, yanyanwu@umass.edu, Fang Li, Hang Xiao. Food Sci., U. of Massachusetts Amherst Resveratrol (RES) is a natural polyphenol compound with a wide range of health-promoting activities, including protective effects against colon cancer and renal disease. Despite numerous examples of interindividual variations in the microbial conversion of diet-derived compounds, an in-depth understanding of the resveratrol metabolism by human gut microbiota is lacking. The objective of this study was to investigate the role of gut bacteria in interindividual differences in resveratrol metabolism. First, our in vivo study using antibiotic-treated mice established RES metabolite-dihyroresveratrol (DHR) is a gut bacteria-derived metabolite, as indicated by their depletion in the urine samples of antibiotic-treated mice measured by liquid chromatography-mass spectrometry detection. Second, our in vitro study identified a gut bacterial strain and candidate genes responsible for metabolizing RES to DHR through the culture-based assay, transcriptomic analysis, and RT-qPCR analysis. Third, our ex vivo study illustrated the interindividual variations in metabolizing RES to DHR by performing fermentation experiments with feces samples from 9 healthy volunteers. Moreover, the hydrogenation rate is positively correlated with the gut bacteria abundance and potential candidate genes' abundance using regression analysis. Together, our findings emphasize the significance of considering interindividual variations when investigating the health benefits of diet-derived components as well as highlighting the contribution of gut bacteria in interindividual variations in metabolism. This work is the bedrock of bringing the field closer to developing gut microbiome-based precision dieting strategies.

11:40 Impact of antibiotic ivermectin on the gut microbial community Lin Liu[1], linshu.liu@usda.gov, Karley Mahalak[1], Adrienne Narrowe[1], Jenni Firrman[1], Johanna M. Lemons[1], Pieter Van den Abbeele[2], Aurélien Baudot[2], Stef Deyaert[2]. (1) Eastern Regional Research Center, USDA, Wyndmoor, Pennsylvania(2) Cryptobiotix SA, Ghent, Belgium Ivermectin (IVM) is a macrocyclic lactone discovered as a fermentation product of the soil microorganism Streptomyces avermitilis. IVM has demonstrated potent activity in combating a broad spectrum of human intestinal helminths, ectoparasites, filarial diseases and for malarial control. It is broadly used in veterinary medicine as an anti-helminthic preparation. Recently, IVM has been investigated for re-purposing applications, with reported testing for cancer therapy and against bacterial, fungal, and viral diseases. As the microbiome is accepted as an important component of host health, the interaction of IVM with the resident microbiome should be considered in evaluating its end use. Long-term dysbiosis would be undesirable, and even short-term IVM administration should not broadly alter the composition of the host microbial community. Here the impact of IVM on the human gut microbiota was tested in vitro. In 2019, three mature gut microbial communities were established in a triple-SHIME for each of three donor fecal samples. The three communities were maintained on standard medium, medium with added soluble fiber, and medium with added insoluble fiber. After stabilization with the fiber treatments, a single 9-mg dose of IVM was administered to evaluate any short-term effects on the microbiome using 16S rRNA sequencing of the bacterial community and fungal ITS sequencing together with measurements of short-chain fatty acids. Overall, any effects of IVM were donor dependent and did not induce dysbiosis. Small changes observed at the time of IVM addition were recovered by the end of the experiment. Fiber amendment may buffer against perturbation and offer a protective effect on the bacterial community as the proportion of dead cells was lower in the fiber-treated communities than in the no-fiber control communities. Fungal communities also displayed donor and site-specific effects with some instances of IVM associated reversals of abundance between the Ascomycota and Basidiomycota.

General Papers

8:05 Integrative approaches for identifying bitter-tasting compounds Veronika Somoza, veronika.somoza@univie.ac.at. Leibniz Inst. for Food Systems Biology at the Technical U. of Munich, Freising, Germany Compounds and oral bitter taste receptors (TAS2Rs). Analytical methods for the identification of bitter-tasting compounds targeting TAS2Rs traditionally comprise low throughput sensory procedures, for which safety data and amounts in the milligram range are required. The discovery of TAS2Rs in non-gustatory tissues has initiated various in silico and in vitro approaches for the identification of bitter-tasting compounds. In silico strategies build on structural similarities between in vitro and sensory-evaluated bitter tastants and their TAS2R molecular interaction properties, as already compiled in several databases, e.g. BitterDB (https://bitterdb.agri.huji.ac.il) or FSBI-DB (https://fsbi-db.de/). Although such in silico approaches benefit from independence from human sensory trials, the results are not always in line with sensory perception since chemoinformatic strategies mostly integrate data from individual agonists targeting a given TAS2R. The implementation of cell-based, high-throughput in vitro screenings provides another strategy that is irrespective of the toxicological safety of compounds. With further progress and insights into the taste signaling pathway of mammalian cells, native cell-based assays founded on immortal human cell lines, which endogenously express taste receptor genes from non-taste tissue, have been established. These cell-based assays represent the native transduction signaling pathways and enable the identification of agonists being active on a multi-receptor level, as well as on the native cell context, which may offer relatively close association with sensory results. However, multi-receptor activation has to be taken into account since other chemoreceptors than TAS2Rs might be additionally targeted, thereby contributing to the cellular outcome measure analyzed. To elucidate the contribution of the individual chemoreceptor, either knock-out approaches, such as CRISP-Cas, or over-expression experiments e.g. in HEK-293 cells, should be considered for native cell systems. Overall, to combat the limitations of in silico and in vitro screening approaches in order to resemble sensory perceptions, multi-receptor activation patterns of taste-active food constituents have to be elucidated.

8:25 Structural elucidation, anti-inflammatory activity and intestinal barrier protection of longan pulp polysaccharide Yajuan Bai1,2, xbaizxyq@sina.com. (1) Chinese Academy of Agricultural Sciences Inst. of Food Sci. and Tech., Haidian District, Beijing(2) Hainan Academy of Agricultural Sciences, Haikou, China LPIIa, a purified polysaccharide from longan pulp, was isolated. Its anti-inflammatory activity and intestinal barrier protection were investigated with LPS-treated co-culture model of Caco-2 cells and RAW 264.7 macrophages. The average molecular weight LPIIa was 159.3 kDa. Its detailed structure was shown below. The backbone of LPIIa was composed of (1→3,4)-linked-α-Rhap, (1→4)-linked-β-Galp, (1→6)-linked-β-Galp, and (1→3,6)-linked-β-Galp, with branches at the O-4 of Rha and O-3 of Gal, consisting of side chains

of α-Araf, β-Galp, and α-Glcp. In LPS-induced RAW 264.7 macrophages, LPIIa suppressed the production of inflammatory mediators, including TNF-α, IL-6, NO, and PGE2, and inhibited iNOS and COX-2 gene expression. In addition, LPIIa attenuated intestinal tight-junctional channel protein Claudin-2 expression and increased tight-junctional barrier protein ZO-1 expression in Caco-2 cells. Knowing the structural features and activities of longan polysaccharide gives insights into longan polysaccharide application as an anti-inflammatory agent or adjuvant in curing the intestinal inflammation.

8:45 Predictive Breeding for Wine Quality: From Sensory Traits to Grapevine Genome Ulrich Fischer1, ulrich.fischer@dlr.rlp.de, Jochen Vestner1, Annemarie Siebert1, Florian Schwander2, Franco Röckel2, Tom Heinekamp2, Lena Frenzke3, Stefan Wanke3, Torsten Wenke3, Reinhard Töpfer2. (1) Inst. for Viticulture and Enology, Dienstleistungszentrum landlicher Raum, Neustadt, Rheinland-Pfalz, Germany(2) Julius Kuhn-Institut fur Rebenzuchtung Geilweilerhof, Siebeldingen, Rheinland-Pfalz, Germany(3) Faculty of Biology, Inst. for Botany, Technische U. Dresden, Sachsen, Germany New pathogen resistant varieties require a much reduced use of fungicides. Thus they will strongly contribute to the 50% reduction goal of pesticides in agriculture requested by the EU in the Green Deal manifest. Selection of new pathogen resistant grapevines also requires the quality assessment of the wines produced. This necessity slows down severely the breeding progress. To circumvent this bottleneck, development of predictive models for wine quality traits is essential to considerably improve efficacy and accelerate the breeding process. The centrepiece of our study is a segregating white wine F1 population of 'Calardis Musqué' and 'Villard Blanc' consisting of 150 genotypes with 13 plants per genotype at two locations. A 'Genotyping by Sequencing' approach with a novel bioinformatics pipeline delivered a high-density genetic map of the breeding population. Experimental micro-vinification at 4-liter scale provided authentic wines for sensory evaluation and chemical analysis of major and minor metabolites including aroma compounds such as monoterpenes. Moreover, five annual repetitions at two locations allow robust modelling and an estimation of environmental impact on the phenotypic data. Genetic, metabolic, and sensory data for multiple vintages combine into a comprehensive data base for predictive modelling. Descriptive analysis and quality score cards were adapted to the large number of wines and the broad range of wine qualities resulting from an unselected set of grapevine genotypes. Based on sensory evaluation of all 150 genotypes a set of best and worst wines was differentiated throughout five vintages. Among others, intensity of "floral" attribute played a crucial role for total quality within this population and correlates significantly with linalool and cis-rose oxide concentration in the wines of all vintages measured by SIDA-SPE-GC-MS. In addition, variation in linalool enabled the discovery of several genomic regions. These quantitative trait loci (QTLs) collocate with putative genes associated with terpene biosynthesis. Multi seasonal data allow refinement and validation of models predicting these wine quality traits. Further exploitation of the large data set will provide more insights into genomic regions related to other wine quality traits. Implementation of prediction models will allow an early selection in the year following the crossing of genotypes of promising genetic quality potential versus those yielding poor wine quality.

9:05 Replacing shortening with high oleic soybean oil oleogels in bakery products: Impact on dough properties and quality of baked goods Muxin Zhao, muxin.zhao@ndsu.edu, Bingcan Chen. Plant Sciences, North Dakota State U., Fargo In recent years, there has been growing interest in edible oleogel as a potential replacement or a reducer of solid fats in high-fat food products. Despite extensive research on the effectiveness of oleogels in the final bakery products, their impact on dough quality is still not well-documented. To address this gap, the effects of two oleogels on the properties of bread and cracker doughs as well as baked products were investigated in this study. Two types of oleogels were prepared by mixing expeller-pressed high-oleic soybean oil (EPHOSO) with either monoacylglycerol (MAG) or rice bran wax (RBX) at a 10 wt% concentration. This study used the Rapid Visco Analyzer, Farinograph, and Rheometer to measure dough properties. In both bread and cracker doughs, the MAG oleogel was found to produce a longer peak time and a higher pasting temperature, which suggested that it may have the potential to slow down the gelatinization process. However, the replacement of shortening with either MAG or RBX oleogel did not result in any significant changes in the dough properties, as confirmed by the measurements taken with Farinograph and rheological instruments. The study also revealed that both MAG and RBX oleogels retained the quality of baked bread similar to that prepared with shortening, with MAG oleogel exhibiting a softening effect on bread crumbs. Similarly, oleogels could create crackers with comparable quality to those made with shortening, with MAG oleogel showing a stronger effect on reducing the hardness of the baked crackers. Overall, the results of this study suggest that EPHOSO-based oleogel has a high potential to replace shortening in bread and cracker formulations without compromising the quality of the final baked products. This study emphasizes the significance of oleogels as a promising and sustainable alternative to solid fats in the food industry.

9:25 Chemical composition of pyrolyzed vegetation foliage utilizing a pyro probe coupled to two-dimensional gas chromatography Roderquita K. Moore, roderquita.k.moore@usda.gov. Forest Service, USDA, Madison, Wisconsin Wildland fires are uncontrollable due to fuel on the forest lands. This vegetation is the ignition to forest fires not being contained and extinguished. The degradation of these chemicals can be extremely toxic and cause climate control issues in our environment. The chemicals from vegetation are known to have fire igniters. In this study, we are investigating secondary metabolites through pyrolysis. From this study, we determine the best parameters to identify the metabolites from the pyro probe ignition. A GC/MS and two-dimensional GC was used to characterize the chemicals being released through pyrolysis.

10:00 Conformational Epitope of important peanut allergens Ara h 5 is the dominant epitope triggering allergies Junjuan Wang, wangjunjuan93@163.com, Mengzhen Hao, Qianwei Wang, Huilian Che. China Agricultural U., Beijing Conformational epitopes typically account for 90% of total antibodies bound to an antigen and are associated with the development of food allergic tolerance and the severity of food allergy. Conformational IgE epitopes of Ara h 5 and Ara h 8 were identified. Recombinant Ara h 5 and Ara h 8 protein exhibit binding activity towards the 27 other allergic patients in the Dot-Blot and direct ELISA analysis. Interestingly, under reducing condition (heating + DTT), the IgE-binding capacity of the Ara h 5 protein demonstrated lower than that of the native form. Additionally, heating and roasting reduced the IgE binding capacity of Ara h 5 proteins to peanut and other allergic sera. Compared with Ara h 5 protein, IgE binding capacity of Ara h 8 protein is less variable through structural modification. However, the effect of Ara h 5 protein on the release of β-hexosaminidase from RBL-2H3 cells and inhibition of IgE binding reaction between serum IgE and peanut crude protein in allergic patients was stronger than that of Ara h 8. It was noteworthy that conformational epitope of Ara h 5 protein plays a key role in the IgE binding activity. And the Ara h 5 and Ara h 8 proteins are cross-reactive with other allergens that can cause respiratory reactions. Conformational IgE epitopes of the two

most important peanut allergens, Ara h 5 and Ara h 8, were identified using phage peptide library. Mimotopes were screened for binding by IgE and IgG antibodies raised in mice against both proteins. All the mimotopes mapped to surface patches of Ara h 5 and Ara h 8 by the Pepitope analysis. The results showed that the conformational epitope sequences of Ara h 5 protein were WETIYSR and FHWWYLK. The conformational epitopes of Ara h 8 protein are FPYMKFV, FPYMKFR, SMFARID and SFHWWLF. The results provide a theoretical basis for the production of hypoallergenic peanut protein and the immunotherapy of peanut allergy.

10:20 New LC-HRMS method for the simultaneous determination of 67 phenolic compounds in Canadian prairie berries to introduce them as a potential source of bioactive compounds Chamali Kodikara1,2, chamali.kodikara@agr.gc.ca, Srinivas Sura1, Nandika Bandara3, Thomas Netticadan1,2, Champa Wijekoon1,2,3. (1) Morden Research and Development Centre, Agriculture and Agri-Food Canada, Morden, Manitoba, Canada(2) Canadian Centre for Agri-Food Research in Health and Medicine, Winnipeg, Manitoba, Canada(3) Food & Human Nutritional Sciences, U. of Manitoba, Winnipeg, Canada Prairie berries are cold hardy fruits consumed by Canadians for their perceived health benefits. Phenolic compounds found in plants have various biological activities and are abundant in berries, making their analysis of significant interest. However, analyzing phenolic compounds in berries is challenging due to their structural complexity, low concentration, and diversity. Various methods, including high-performance liquid chromatography coupled with various detectors, such as ultraviolet-visible and fluorescence spectrophotometry, have been developed to analyze phenolics in berries. However, most of these methods have limitations in their sensitivity, selectivity, and resolution, leading to inaccurate and unreliable data on the composition of phenolic compounds. The liquid chromatography high-resolution mass spectrometry (LC-HRMS) technique is one of the methods that have high sensitivity and selectivity due to accurate mass and fragment selection, facilitating the identification of a wide range of phenolic compounds in complex matrices. This study aimed to develop an LC-HRMS method for the comprehensive and simultaneous detection, identification, and quantification of 67 phenolic compounds with optimized sample preparation for 15 varieties of wild berries grown in Canadian prairies, including Vitis riparia (wild grape), Prunus virginiana L (chokecherry), Ribes hirtellum (gooseberry) and Amelanchier alnifolia L (Saskatoon berry). Phenolic compounds were extracted using a novel extraction protocol to achieve maximum recovery for all the analyzed compounds. Wild grapes were rich in phenolic compounds such as resveratrol (4.2±0.02 µg/g), while gooseberries were rich in isoquercetin (84.8±0.08 µg/g) and para-coumaric acid (65.6±0.02 µg/g). Moreover, saskatoon berries were rich in chlorogenic acid and quercetin. Rutin and chlorogenic acid were the most abundant phenolic compounds in chokecherry. This comprehensive analysis helped in the identification of the potential bioactive compounds and metabolite markers unique to each berry. The information from this study will help in finding innovative applications for these different prairie berries in the food, nutraceutical, and pharmaceutical industries.

10:40 Flavor elucidation and simultaneous quantitation of key tastants and odorants of sourdough bread crumb Laura S. Eckrich, laura.amann@tum.de, Oliver Frank, Corinna Dawid, Thomas Hofmann. Chair of Food Chemistry and Molecular Sensory Science, School of Life Sciences, Technische U. Munchen, Bayern, Germany Sourdough bread is highly appreciated for its unique taste and aroma. As a scientific basis, it is essential to identify the key compounds that contribute significantly to the flavor of bread crumb in order to investigate the influence of different ingredients and production parameters. By means of the sensomics approach, ten tastants and eleven odorants were identified as the key flavor compounds of sourdough bread crumb and verified by recombination and omission experiments. Based on this, a sensitive, high-throughput ultra-high-performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS) method using stable isotope dilution analysis (SIDA) was developed, validated, and applied. By derivatization with 3-nitrophenylhydrazine (3-NPH), this method allows the simultaneous quantification of both non-volatile key tastants as well as volatile key odorants in bread crumb. The knowledge obtained about the key taste and aroma compounds and the quantitation method can be utilized to control and optimize the flavor of bread and to acquire objective and independent information about the flavor quality of breads.

11:00 Mechanochemical extraction of protein from moor grass Olusegun Olalere, oao94@bath.ac.uk, Hannah Leese, Chris Chuck, Bernardo Castro Dominguez. Chemical Engineering, U. of Bath, Claverton Down, United Kingdom Mechanochemical assisted extraction (MAE), named as one of the top ten sustainable technologies by IUPAC that will ‘change the world’ is an efficient method that leverages the mechanical force in ball mills to enable the breakdown of lignocellulosic structures and removal of other bioactive compounds. The extensive rapid micro heating at the point of the ball contact driven by the friction between the balls and the biomass allows reactions to proceed when the system is operated without additional heating thus decreasing extraction time, energy usage, and affording simple scale up. This work explores the effect of MA E coupled with additives (e.g., salts, water, etc) to enhance protein extraction from underutilised moor grass . Using a planetary stainless steel ball mill, we studied the effect of salt assisted grinding on protein extraction. Using a Taguchi array, a ball mill parametric assessment was implemented to understand the effect of milling time , milling speed , grass concentration, salt content, etc. The results showed that MAE yielded a higher protein extraction rate (>20%) using salt-assisted grinding compared to 19% and 13% obtained through conventional alkaline extraction and water assisted ball milling. The purity and functionality of the extracted proteins was analysed using various characterization techniques to elucidate the mechanisms behind MAE extraction and determine its critical process parameters (CPPs), namely: the molar ratio of salt content, initial particle size of grass, and milling speed. This work shows the potential of MAE as a sustainable and efficient alternative for protein extraction from plant sources.

11:20 Preservation of food by isochoric (Constant volume) freezing Cristina Bilbao-Sainz1, cristina.bilbao@usda.gov, Bor-Sen Chiou1, Tara McHugh1, Boris Rubinsky2, Vivian Wu1. (1) USDA ARS Western Regional Research Center, Albany, California(2) U. of California Berkeley Isochoric freezing is a pressurized freezing technique that allows storage of foods at subfreezing temperatures without ice formation inside the food products. Isochoric freezing occurs in a constant volume chamber when the temperature of an aqueous system is reduced below the freezing temperature. Under these conditions, ice begins to form in the aqueous system and expands to generate hydrostatic pressure inside the rigid chamber. This pressure then depresses the freezing point of the aqueous solution and ice will form until the effective freezing point of the system is equal to the surrounding temperature. At this point, there are two phases coexisting at the constant subfreezing temperature: a solid ice phase and a liquid phase. Food products can then be stored in the space occupied by the liquid phase at subfreezing temperatures without any internal ice formation. This protects food from ice formation damages that occur during conventional freezing at atmospheric pressure, while retaining the benefits of storage at

temperatures below the freezing point of water. Studies on spinach, tomato and potato indicated that isochoric freezing produces foods with higher quality and nutritional value than conventional freezing. Microbiological studies also showed that isochoric freezing of liquids at -15 °C reduced Salmonella Typhimurium and Listeria monocytogenes from an initial concentration of 7 log cfu/ml to unrecoverable levels in 12 hours. In addition, fundamental thermodynamics showed that freezing in an isochoric system to a given temperature was significantly less energy intensive than freezing in a traditional system. This was attributed to two physical effects: the reduction in total frozen mass and the temperature dependence of water's latent heat of fusion. In conclusion, preservation of foods by isochoric freezing can improve their quality, nutrition and safety while also saving energy.

11:40 Electrochemical lab-on-kitchen approach towards combinatorial testing for food contaminants Durgasha Poudyal1, durgasha.poudyal@utdallas.edu, Vikram Narayanan Dhamu1, Manish Samson1, Sriram Muthukumar2, Shalini Prasad1. (1) Bioengineering, The U. of Texas at Dallas, Richardson(2) EnLiSense LLC, Allen, Texas With the growing population and rise of the food demand supply, there is an immense interest on-demand information about food quality prior to consumption. On an average, 50% or above in thousands of imported and domestic grown foods tested by the U.S. FDA (food and drug administration) were reported to be found with at least one pesticide in detectable levels. The gold standard method to detect pesticides or GMOs residues in food is complex and is not amenable to rapid consumer usage. In this work, we demonstrate the feasibility of an electrochemical portable sensing approach for the simultaneous direct detection of spiked pesticides and GMOs protein in real food matrix. The immunoassay based multiplex plex sensing platform was fabricated using respective antibodies associated with the target pesticides/ GMOs protein. A simple lab-on-kitchen level matrix preparation has been demonstrated and sensor response was tested using non-faradaic electrochemical impedance spectroscopy (EIS), tested for a linear range of concentrations from 0.3 ng/mL to 243 ng/mL with limit of detection (LOD) of 0.3 ng /mL for both the target antigens (pesticides and GMOs) respectively. The calibrates dose response were tested in real sample matrix (both high and low fate) and the spiked and recovery test results fall within ± 20% error in real sample matrix which demonstrates the performance of our platform with maximum residue limit (MRL) for the given targets. Hence, electrochemical portable tool extended to multi-analyte direct sensing with simple matrix processing protocol can be a future commercial field-testing tool for use at everyday consumer end.

Virtual Session - General Papers

10:05 Molecular assessment of metabolome alterations in Lotus japonicus roots induced by arbuscular mycorrhiza Josef Ranner[1], josef-ranner@web.de, Michael Paries[3], Georg Stabl[2,3], Caroline Gutjahr[2,3], Timo D. Stark[1], Corinna Dawid[1]. (1)Chair of Food Chemistry and Molecular Sensory Science, Technische U. Munchen, Bayern, Germany(2) Max-Planck-Institut fur molekulare Pflanzenphysiologie, Potsdam, Brandenburg, Germany(3) Plant Genetics, Technische U. Munchen, Bayern, Germany Agricultural crop plants can experience enhanced growth, stress tolerance, and yield when engaging in an arbuscular mycorrhiza symbiosis with Glomeromycota fungi. This interaction involves the fungus absorbing mineral nutrients from the soil and exchanging them for hexoses and lipids from the plant through so-called arbuscules, which are tree-like fungal structures formed within root cortex cells. Arbuscule formation and degradation result in extensive cell reprogramming, which is well understood, but little is known about how arbuscular mycorrhiza affects the host root metabolome. To examine the impact of arbuscular mycorrhizal symbiosis on the root metabolome of the model legume Lotus japonicus, we employed an untargeted metabolomics approach. We analyzed methanolic extracts of mycorrhizal (myc) and non-mycorrhizal roots (mock) using ultra-high-performance liquid chromatography–electrospray ionization–time-of-flight–ion mobility–mass spectrometry (UPLC–ESI–ToF–IM–MS) and identified up-regulated marker metabolites through principal components analysis (PCA) and orthogonal partial least squares–discriminant analysis (OPLS–DA) highlighted as S-plots. We characterized these marker metabolites by co-chromatography with authentic standards or by isolation from L. japonicus roots using preparative HPLC and one- and two-dimensional nuclear magnetic resonance (NMR) spectroscopy experiments. We discovered three previously unknown mycorrhizal marker polyphenols in L. japonicus roots, including one coumaronochromone, one pterocarp-6a-ene, and one aryl benzofuran carbaldehyde. Moreover, we detected three further coumaronochromones, three flavonoids, three isoflavonoids, and one coumestan in mycorrhizal L. japonicus roots.

10:25 Nutrients characteristics of the leaf, stem and root of Eclipta prostrata (L) Oluwayemi O. Onawumi[1], Abiodun Sodamade[1,2], sodamade1@gmail.com, Olufisayo A. Onawumi[3], Dupe L. Abiona[1,4]. (1) Pure and Applied Chemistry,, Ladoke Akintola U. of Technology, Ogbomoso, Oyo, Nigeria(2) Chemistry, Emmanuel Alayande College of Education, Oyo, Nigeria(3) Bioscience, Federal research Inst. of Nigeria, Ibadan, Oyo(4) Chemistry, The Polytechnic Ibadan, Oyo, Nigeria Eclipta prostrata (L) is one of the plant samples used locally in the south western part of Nigeria in preparation of herbs for treatment of some ailments, diseases and hormonal disorder. The sample was purchased, and authenticated with a view to evaluate its nutritional composition by determining the proximate composition, mineral content, and amino acid profile using standard analytical methods. The proximate analysis revealed; the moisture content for the root to be the highest followed by the stem, while the leaf has the least value. The ash content and protein values respectively are (7.54±0.00)g/100g, 12.48±0.03g/100g for the root and the highest followed by the stem (7.54±0.23)g/100g; (11.36±0.47)g/100g and the leaf has the least values. More crude fat and crude fiber are found in the root followed by the stem. The leaf has the highest value of nitrogen free extractive; while the root has the least. The dietary mineral revealed highest concentration of Na, K, Ca, Mg, Zn and Fe in the root than other parts. Other minerals that were detected in the three parts of the plants samples in trace amount are: Cu, Mn, P, and Cd. Lead was not detected in the samples but the stem showed trace amount of selenium. The amino acid profile revealed significant proportion of both essential and non-essential amino acid. The amino acid values are higher in the stem than the leaf and the root of the plant samples. The consumption and pharmaceutical use of the whole part of the plant are therefore encouraged. The plants could serve as raw material to produce essential supplements needed by man.

10:45 Evaluation of the light stability of anthocyanins extracted from blackberry (Rubus spp) using a natural, deep eutectic solvent Oscar Zannou1,2, zannouoscar@gmail.com, Ilkay Koca2, Salam A. Ibrahim3. (1) Faculty of Agricultural Sciences, U. d'Abomey-Calavi, Cotonou, Littoral, Benin(2) Dept. of Food Engineering, Ondokuz Mayis Universitesi, Samsun, Turkey(3) Food and Nutritional Sciences Program, North Carolina Agricultural and Technical State U., Greensboro Natural, deep eutectic solvents are promising green solvents for the extraction and stabilization of bioactive compounds from plant materials. In the present study, anthocyanins were extracted from blackberry fruit with a deep eutectic solvent that was obtained using choline chloride as a hydrogen bond acceptor and glycerol as a hydrogen bond donor. The extracts were exposed under

a daylight lamp over a 28-day period. The light degradation of cyanidin-3-glucoside, cyanidin-3-rutinoside, pelargonidin-3-glucoside and cyanidin chloride was slowed with CHGLY while the aqueous extracts tumbled after one week. Over a 28-day period, the cyanidin-3-glucoside was reduced to 31.22±0.00% and 0.08±0.00% in CHGLY and aqueous extract, respectively. The cyanidin-3-rutinoside, pelargonidin-3-glucoside and cyanidin chloride reduced to 45.38±0.30, 19,34±2.19 and 39,64±0.12 in CHGLY while 5.89±0.38, 0.50±0.03 and 6.50±0.53 in the aqueous extract, respectively. The degradation constant rate (k) of cyanidin-3-glucoside was four-fold less in NADES than in aqueous solutions while the k value of cyanidin-3-rutinoside was two-fold less in NADES than in the aqueous extracts. In addition, k values of pelargonidin-3-glucoside and cyanidin chloride were two times less in NADES than in water. The t1/2 values were 283.59±19.58-589.49±4.97 h and 65.79±0.02-170.42±5.07 h for NADES and water, respectively. The results thus suggest that the cyanidin-3-rutinoside, pelargonidin-3-glucoside and cyanidin chloride were more stable and protected in NADES. Consequently, Choline chloride and glycerol-based NADES is adequate for the extraction and stabilization of anthocyanins from plant materials.

11:05 Fatty acids and derivatives inhibit the spore germination of the barley pathogen Drechslera teres : An activity-guided search for natural pathogen resistance Karina M. Hille1, Karina.hille@tum.de, Timo D. Stark1, Arber Rexhaj1, Peter Gläser1, Felix Hohenender2, Hans Hausladen3, A. Corina Vlot4,5, Thomas Hofmann1, Ralph Hückelhoven2, Corinna Dawid1. (1) Chair of Food chemistry and molecular sensory science, Technische U. Munchen, Freising, Bayern, Germany(2) Chair of Phytopathology, Technische U. Munchen, Freising, Bayern, Germany(3) Plant Technology Center, Technische U. Munchen, Freising, Bayern, Germany(4) Inst. for Biochemical Plantpathologie, Helmholtz Zentrum Munchen Deutsches Forschungszentrum fur Gesundheit und Umwelt, Neuherberg, Bayern, Germany(5) Chair of Crop Plant Genetics, U. Bayreuth, Bayern, Germany Net blotch – caused in barley by infection with the fungus Pyrenophora teres Drechsler [anamorphic Drechslera teres (Sacc.) Shoem] – leads to losses of up to 40% of barley crop yields worldwide. In the absence of fully resistant genotypes on the market, the only way currently available to control the disease is the use of synthetic fungicides. In order to create a basis for more environmentally friendly agriculture in the long term and to gain a better understanding of the plant disease, metabolome changes in barley induced by Drechslera teres infections were characterized. In an activity-guided approach, barley extracts were tested in a spore germination assay for their activity against D. teres. This approach led to the identification and structural elucidation experiments of naturally occurring substances by means of MS and NMR, which show an inhibitory effect on spore germination. These substances were identified as fatty acids and fatty acid oxidation products, which were then also tested for their single substance activity as well as for combinatorial effects and concentration-dependent inhibition of spore germination. To determine the influence of fatty acids and fatty acid oxidation products on variations in the natural resistance of different genotypes, selected genotypes of the Halle Exotic Barley population were infected with D. teres spores under controlled greenhouse conditions. For this purpose, leaves of infected and control plants were sampled at several different points in time and disease symptoms were scored. The concentrations of fatty acids and fatty acid oxidation products within the sampled barley leaves were determined and compared with a focus on genotype, sampling time, and treatment.
Using the disease rating and quantification data, assumptions can be made about the possible course of a D. teres infection and natural resistance in wild barley types. The knowledge gained within the framework of this project adds to the metabolomic basis, which might play a significant role in the selection of barley genotypes resistant to net blotch, especially when combined with the nested association mapping and QTL data of the HEB-population.

11:25 Investigation of allergy prevalence and cross-sensitization in China: a survey based on self-reported and clinical testing data Wenwen Xiong, 948548043@qq.com, Huilian Che, chehuilian@cau.edu.cn, Mengqi Zhang, sxzmq0730@163.com, Tingyun Meng, mengtingyun0111@163.com, Yali Liu, liuyali0099@163.com. China Agricultural U., Beijing Objective: Food allergy has become a serious public health and food safety concern. However, in China, with epidemiological investigations rarely reported, the prevalence of food allergy is unclear. Therefore, the main aim of this study is to estimate the prevalence of food allergies in Chinese and establish a list of food allergens. Methods: An electronic questionnaire inquiring about demographic data, gender, age, and history of allergy was administered through the internet between January and March 2023. Moreover, allergy test reports were collected in cooperation with hospitals to analyze the correlation between the occurrence of allergies. Results: Data was obtained from 12505 participants, comprising 44% males and 56% females. Most people (66.09%) were aged between 18 and 44. The prevalence rate of food allergy in China was about 21.88%. The top eight allergens were crustaceans, mango, milk, egg, fish, bee pupa, cicada pupa, and peanut. A total of 2708 diagnostic reports were collected, and correlation analysis results showed there was a correlation between the occurrence of multiple groups of food allergies, among which the wheat-buckwheat, peanut-soybean, egg-milk, and beef-milk combinations had high Pearson correlation coefficients.
Conclusions: Crustaceans were the most common allergen in China. Fruit allergy also accounted for a certain proportion. Wheat-buckwheat, peanut-soybean, egg-milk and beef-milk allergy correlated, indicating that there may be cross allergens in them. These findings provide a baseline for future studies to obtain more in-depth results.

12:00 Formation of amino acid derivatives during wine fermentation Cemile Yilmaz, cemileyilmaz@hacettepe.edu.tr, Vural Gökmen. Food Engineering Department, Hacettepe U., Ankara, Turkey Fermented foods have been an important part of the human diet for years. Fermentation results in the synthesis of microbially formed neuroactive compounds in foods, which increases the importance of the effect of fermented foods on human health and mood. Although Saccharomyces cerevisiae and lactic acid bacteria are the main members in wine fermentation, there is a growing interest in using non-Saccharomyces yeasts in simultaneous or sequential fermentation with Saccharomyces yeasts. The aim of this study was to investigate the formation of amino acid derivatives, some of which have neuroactive properties, during the fermentation of white and red wines. The effects of non-Saccharomyces yeasts in alcoholic fermentation and Oenococcus oeni in malolactic fermentation on the formation of neuroactive compounds were also addressed. Three different white wines were produced using various yeasts including S. cerevisiae, Metschnikowia pulcherrima, Torulaspora delbrueckii and Kluyveromyces thermotolerans. After alcoholic fermentation with S. cerevisiae, red wines were produced by performing natural malolactic fermentation and O. oeni malolactic fermentation. Liquid chromatography tandem mass spectrometry was used for the analysis of tryptophan derivatives in the melatonin/serotonin pathway and kynurenine pathway, tyrosine derivatives, and bioactive amines in wines. The changes in the neuroactive compounds were mainly observed for the tryptophan derivatives in the kynurenine pathway in wine samples. White wine fermented with T. delbrueckii, K. thermotolerans and S. cerevisiae

simultaneously contained the highest concentrations of kynurenic (65 µg/L), picolinic (70 µg/L), and quinolinic acid (307 µg/L). Moreover, tryptophan ethyl ester levels in all white and red wines increased during alcoholic fermentation. Using non-Saccharomyces yeasts and O. oeni during wine fermentation and different fermentation stages were found to be effective for the formation of amino acid derivatives. The results of this study can be significant for the production of wine rich in neuroactive compounds in the future.

12:20 Saltiness enhancement in commercial soups and sauces using pyroglutamyl peptides Oshin Sahni, foshin@vols.utk.edu, John P. Munafo. Food Sci., The U. of Tennessee Knoxville Hypertension, also known as high blood pressure, is one of the major contributors to cardiovascular conditions including heart disease and stroke, which are the leading causes of death worldwide. Numerous studies have shown that consuming excess sodium is strongly associated with an increased risk of high blood pressure. However, decreasing the sodium content in food can lead to decreased consumer acceptance due to a less desirable flavor. Alternatives to table salt, such as non-sodium salt substitutes like potassium chloride, have been used as one method to replace sodium in foods, but excess use of these salt substitutes can also decrease the sensory acceptability of the food. Thus, increasing the perceived saltiness of low-sodium foods while maintaining their sensory qualities is essential for a sodium reduction strategy to be effective. The objective of this study was to apply saltiness-enhancing pyroglutamyl peptides isolated from mushrooms and other natural products to commercial soups and sauces and determine their effectiveness as saltiness enhancers in these matrices. Previously, we determined the detection thresholds of selected pyroglutamyl peptides in a model broth containing sodium chloride (NaCl), monosodium glutamate (MSG), and guanosine 5'-monophosphate GMP). In this study, we evaluated the potential of these peptides as a solution for reducing the sodium content in commercial soups and sauces by determining their acceptability to a panel of consumers. First, we conducted a triangle test for each product to determine the maximum percent of salt that can be reduced without the consumer panel perceiving a difference in taste. Then, we introduced peptides to the products and conducted additional triangle testing to determine how much further the salt content could be decreased while still maintaining consumer acceptability. The application of these pyroglutamyl peptides in commercial soups and sauces will serve as a foundation for further investigation into their potential use in reducing sodium content in various other food products.

12:40 Predicting the baking quality of wheat using protein analytical and functional parameters Clemens Schuster2, Julien Huen3, Katharina Scherf1, katharina.scherf@kit.edu. (1) Karlsruher Institut fur Technologie, Baden-Württemberg, Germany(2) Leibniz-Institut fur Lebensmittel-Systembiologie an der Technischen Universitat Munchen, Freising, Bayern, Germany(3) The content and composition of proteins and especially gluten are important for the baking quality of wheat flours. Our aim was to carry out a comprehensive characterization of 82 German winter wheat flours in order to analyze the influence of protein composition on rheological and baking quality parameters. Of all flours, the protein and gluten content, the protein and gluten composition, the starch gelatinization behavior as well as rheological parameters (microfarinograph, gluten aggregation, extensibility) and the bread volume were determined in the microbaking test based on 10 g flour. The correlation matrix showed no significant correlations between gluten composition and bread volume. The parameters of the gluten aggregation test allowed prediction of gluten, gliadin and glutenin content with an absolute mean square error of cross-validation of 7.5 mg/g, 6.0 mg/g and 3.2 mg/g, respectively, using partial least squares regression. The gelatinization temperature of the starch also had an effect on gluten aggregation. The gluten aggregation test was thus suitable to predict the gluten, gliadin and glutenin content. The lack of correlations between protein composition and bread volume suggests that baking quality is the result of a complex combination of different parameters that cannot be reliably predicted by single indicators. Moreover, flour blends can achieve excellent baking quality even if quality indicators such as crude protein or extensibility are comparatively low. Further investigations with baking trials on a pilot scale will show whether the results from the microbaking trial can be transferred to technologically relevant processes.

1:00 Characterization of odorants in dried and rehydrated lobster mushrooms Thien Nguyen, huuthien.ng@gmail.com, John P. Munafo. Food Sci., The U. of Tennessee Knoxville The lobster mushroom is a mycorrhizal mushroom with a prominent seafood-like flavor that is commonly found growing in the temperate forests of North America. Due to a recent surge in the popularity of edible mushrooms among food enthusiasts, the lobster mushroom has garnered increased interest in the culinary world due to its unique flavor and texture, making it an attractive seafood alternative. Interestingly, the mushroom is not a single fungal species, but is the result of the colonization of Russula or Lactarius mushroom hosts, by the ascomycete fungus Hypomyces lactifluorum. Since lobster mushrooms are harvested only during a relatively narrow timeframe during the warmer months, they are generally sold year-round as a dried product that is rehydrated prior to cooking. The seafood-like aroma produced by lobster mushrooms increases during cooking, suggesting that thermal treatment enhances the aroma. The odorants responsible for the mushroom's seafood-like aroma have not been previously characterized. To gain the first insights into the aroma chemistry, a preliminary experiment was conducted to characterize the odorants present in the dried and rehydrated mushrooms. In this study, the odorants of dried and rehydrated lobster mushrooms were isolated by solvent assisted flavor evaporation (SAFE) and identified using gas chromatography-olfactometry (GC-O) and gas chromatography-mass spectrometry (GC-MS). A comparative aroma extract dilution analysis (cAEDA) was conducted to determine the differences in flavor dilution (FD) factors of the odorants in the samples. Some notably odorants included 1-oceten-3-ol (mushroom), 1-octen-3-one (mushroom), hexanal (green, fatty), and a series of rancid smelling organic acids. The relative differences between the odorants in the dried and rehydrated mushrooms will be highlighted in the talk. This work provides the foundation for identification and quantitative studies aimed at determining the key odorants responsible for the lobster mushroom's thermally generated seafood-like aroma.

1:20 Substantial equivalence of tobacco products: are all tobacco products of the same type substantially equivalent? Examples of equivalence and nonequivalence among waterpipe tobaccos John H. Lauterbach, john@lauterbachandassociates.net. Chemistry & Toxicology, Lauterbach Associates, LLC, Deland, Florida Many adults are unaware of differences among tobacco products within a given type such as conventional combustible cigarettes and among other types such as cigars, pipe tobaccos, and oral tobacco products. The advent of electrically heated products such as e-cigarettes and other heated tobacco products such as heat-not-burn cigarettes have further confused both the public and the regulatory community particularly in regard to introductions of new products. Substantial equivalence (SE) is an important regulatory concept as it reduces the cost of introducing a new product if the new product is not substantially different from an existing product. For example, most combustible cigarettes on the US market are essentially equivalent, although they differ in dimensions or in other aspects and this

equivalence has been supported through numerous scientific studies on the cigarette products and emissions. However, determining SE for other types of tobacco is much more challenging because there is less of scientific knowledge about the products; and there is a lack of consensus standards for characterizing the products. Waterpipe tobacco (WPT) is one such product type. Waterpipe tobaccos are mixtures of glycerol, sugar syrups, tobacco, and flavors. Tobacco is < 30% and nicotine is < 0.2% by weight. The remainder is glycerol, sugar syrups, and flavors. While HPLC techniques exist for glycerol and the sugars, techniques for flavors and blend composition have yet to be established, and thus determining SE has not been possible. We have found that the same 75/25 acetonitrile/water extract that we have used for the HPLC analyses of glycols and sugars in WPT can also be used for added flavors and polyphenols in the tobacco (used for estimation of blend components) using other columns in place of the Phenomenex Luna Omega Sugar column that is used for sugars and glycols. Other columns used include Cogent Bidentate C18, and Phenyl Hydride as well as Zorbax SB-C3. Since some popular flavors include compounds without strong UV chromophores, residues after evaporation of WPT extracts were treated with benzoyl chloride to form benzoate esters. With these techniques, it is possible to profile WPT's with respect to blend, addition of glycerol and sugars, as well as flavors

1:40 Development and validation of a food frequency questionnaire for adults in Fiji to estimate nitrate and nitrite intake Adrian A. Chetty1,2,3, adrian.chetty@fnu.ac.fj, Joslin Lal2, Surendra Prasad2. (1) Chemistry, Fiji National U., Nasinu(2) Chemistry, The U. of the South Pacific, Suva, Rewa, Fiji(3) Nutri. and Food Sci. U. do Porto, Portugal Food frequency questionnaires are frequently used to survey the food consumption patterns in the population. They are a useful epidemiological tool that can assess the link between disease patterns and food consumption. The present study reports the development of a food frequency questionnaire (FFQ) for the purpose of estimating nitrate and nitrite intake for the adult population in Fiji. The developed FFQ is a 162-food item, semi-quantitative, google form-based questionnaire that looks at the commonly consumed foods and beverages in Fiji. The food items have been categorized into 9 groups. The study population (n = 250) comprised Fijian adults between the age range of 18 – 65. The developed FFQ has been validated by a 24-hr diet recall study (n = 70). The estimated, nitrate and nitrite, dietary daily intake (EDI) was compared to existing tolerable daily intakes (PTWI/ADI) for these analytes. The developed and validated FFQ can be used in future epidemiological surveys in Fiji and the pacific.

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Schedule of Technical, Business and Social Meetings (all Pacific Daylight Time)

Sun. August 13	noon-1:00pm	Special Topic Meeting	Moscone Ctr. West Level 3 Overlook 4
Sun. August 13	7:00pm-9:00pm	Poster Session & Reception	Moscone Ctr. South Gen. Exhibit Hall F
Mon. August 14	noon-1:00pm	Future Programs	Moscone Ctr. West Level 3 Overlook 4
Mon. August 14	5:00pm-8:00pm	Executive Committee	Moscone Ctr. West Room 2024
Tues. August 15	6:00pm-8:30pm	Awards Banquet	Fogo de Chao (see cover for more info)
Wed. August 16	noon-1:00pm	Business Meeting	Moscone Ctr. West Room 2024