Division of Agricultural and Food Chemistry of the ACS Spring 2022

CORNUCOPIA

including the AGFD program and abstracts for the

263rd American Chemical Society (virtual & live) National Meeting on

March 20 - 24, 2022

in

SAN DIEGO

MICHAEL GRANVOGL & LINSHU LIU

Program Chairs

Questions about VIRTUAL PROGRAMMING?

see page 2

Going to San Diego?
Join the AGFD Social Reception (free refreshments!)
held concurrently with the
AGFD Undergraduate Poster Competition
Tuesday March 22 7-9 pm
in the Convention Center

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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

I am grateful to have an opportunity to serve as AGFD Chair of year 2022, a challenge that I can't treat lightly. I am humbled by this responsibility entrusted by AGFD membership, and I plan to use all my ability to serve you.

First, I must express my deepest appreciation to our past Chairs, Lucy and Youngmok and all ExCom members for guiding and helping me to assume this important AGFD assignment. I also thank all symposium organizers, presiders and presenters for the great contributions to AGFD programs in times when we are facing unprecedented challenges. In the past two years, pandemic ravaged, laboratories were partially shut down, travel was limited, and meeting was constrained; the 259th, 260th, and 261st ACS national meetings had to be organized in totally virtual format. The 262nd meeting developed into a hybrid format that allowed those who felt comfortable travelling to do so while also allowing those who were unable to attend in-person to participate remotely. The virtual format was also optimized in such a way that all presentations, whether online or in-person, were delivered live. This design allowed participants to ask questions and network with their peers in a way that pre-recorded presentation format was lacking. The 2022 Spring meeting will continue to use hybrid format. We accepted 226 submissions including 160 oral reports and 66 posters arranged as 10 symposia. These presentations cover the applications of big data, AI, and Nano-technology in agricultural and food chemistry, most recent nutrition and gut microbiome research, as well as food chemistry and safety. Certainly, your genuine creativity and dedication will be appreciated by all attending the forthcoming Spring Meeting.

As Covid-19 pandemic passed the peak and started rapidly decreasing, our colleagues have begun to return to work in-person in laboratories. Thus, I hope that the 2022 Fall ACS Meeting may return to its traditional format. However, we understand the need of keeping all possible options open. Dr. Michael Granvogl will lead the organization of 2022 Chicago and 2023 Indianapolis meetings. If you are interested at participating in these meetings, please show your support by contacting him at michael.granvogl@unit-hohenheim.de

I look forward to welcoming you in Chicago in August.

Best regards,

LinShu Liu
2022 AGFD Chair
Linshu.liu@usda.gov

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VIRTUAL PROGRAMMING – HOW DOES IT WORK ?

See the ACS website links, below, for the San Diego meeting.

Go to **ACS.org, Meetings and Events, ACS Meetings and Expositions,**
Click on **Frequently Asked Questions or** use the link:
https://www.acs.org/content/acs/en/meetings/acs-meetings/registration/faq.html#general

For more info - click on **Meeting Experience** or use the link:
https://www.acs.org/content/acs/en/meetings/acs-meetings/registration/why-attend.html

FUTURE PROGRAMS

CHICAGO August 21-25, 2022

ACS Meeting Theme: Sustainability in a Changing World

Advancement of Application of Agricultural & Food Chemistry Award: Symposium honoring Shengmin Sang LinShu Liu linshu.liu Michael Morello mjmorello226@gmail.com

Advancements in Food and Metabolomics Jessica Cooperstone cooperstone.1@osu.edu Devin Peterson Peterson.892@osu.edu

Advances in Packaging Recycling and Sustainability John Koontz John.Koontz@fda.hhs.gov Yoon Song yoon.song@fda.hhs.gov

Alternative Protein Sources for Human Nutrition (Plant- Based Protein) John Finley jfinley5@lsu.edu Brian Guthrie Brian_Guthrie@cargill.com_ Michael Morello mjmorello226@gmail.com

Artificial Intelligence (AI) Applications for Food and Agriculture Bosoon Park bosoon.park@usda.gov

Biobased Polymers and Applications Jinwen Zhang jwzhang@wsu.edu Raisha Gorshkova gorshkova.raisa@gmail.com LinShu Liu linshu.liu@usda.gov

Breeding for Better Nutrients and Flavor for Freshly Consumed Fruits and Vegetables Xiaofen Du xdu@twu.edu Yun Yin yunyin2@vt.edu

Emerging In-Vitro Gut Models for Understanding Nutrient-Microbiome Interactions Laurel Doherty laurel.a.doherty.civ@mail.mil Ida Pantoja-Feliciano ida.g.pantojafeliciano.civ@mail.mil Karley Mahalak Karley.mahalak@usda.gov

Extraction and Biotechnology: a Natural and Sustainable Future for Flavors Liz Kreger Elizabeth.Kreger@sensient.com Lewis Jones Lewis.Jones@sensient.com

Food Bioactives in Infectious and Autoimmune Diseases Fang Li fl2532@cumc.columbia.edu Hang Ma hang_ma@uri.edu Xian Wu Wux57@miamioh.edu

Food, Food Systems and Precision Nutrition Thomas Wang tom.wang@usda.gov

General Papers (Oral) Michael Granvogl michael.granvogl@uni-hohenheim.de LinShu Liu linshu.liu@usda.gov

General Papers (Poster) Michael Granvogl michael.granvogl@uni-hohenheim.de LinShu Liu linshu.liu@usda.gov

Improving Food for a Changing World Alyson Mitchell aemitchell@ucdavis.edu Akira Murakami akira@shse.u-hyogo.ac.jp

JAFC Research Article of the Year Award & AGFD Young Scientist Award Symposium Michael Granvogl michael.granvogl@uni-hohenheim.de Thomas Hofmann Thomas.hofmann@tum.de

Modification of Agricultural Biomass into Value-Added Products Majher Sarker majher.sarker@usda.gov Helen Ngo helen.ngo@usda.gov Madhav Yadav madhav.yadav@usda.gov

Nanoencapsulation and Delivery of Bioactive Food Ingredients Using Food Biopolymers Qingrong Huang qhuang@sebs.rutgers.edu Qin Wang wangqin@umd.edu

New Insights in Gut Microbiota Health-Benefits Coralia Osorio Roa cosorior@unal.edu.co

Nutraceutical Lipids, Proteins and Biopeptides Fereidoon Shahidi fshahidi@gmail.com and fshahidi@mun.ca

Spencer Award: Symposium in honor of Dr. H.N. Cheng Michael Appell michael.appell@ars.usda.gov Christine Hilbert chilbert@swbell.net Sarah Leibowitz sleibowitz@gmail.com Michael Morello mjmorello226@gmail.com

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Sustainability and Greentech in Agriculture and Food Omowunmi Salik sadik@njit.edu Michael Appell michael.appell@gmail.com

Sustainable Agriceuticals Hyunsook Kim hyunsk15@hanyang.ac.kr LinShu Liu linshu.liu Daxi Ren dxren@zju.edu.cn Wallace Yokoyama wally.yokoyama@ars.usda.gov Liangli (Lucy) Yu lyu5@umd.edu

Utilization of Upcycled Foods in New Product Innovation Xiaofen Du xdu@twu.edu Yixiang Xu yixu@vsu.edu

BEYOND CHICAGO

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

Chemistry of Wine (tentative) Gavin Sacks gls9@cornell.edu Elizabeth Chang eabc@vt.edu Gal Kreitman gal.kreitman@ejgallo.com

Co-sponsor **2024 Spring - New Orleans** Meeting theme: **Many Flavors of Chemistry** Apply for thematic program funds Neil DaCosta neil.dacosta@iff.com

Mid-Atlantic Regional Meeting - looking for someone from AGFD to organize and chair a symposium/technical session on **Food Lipids/Lipid Chemistry** Contact: Wajira S. Ratnayake wajira.ratnayake@ingredion.com

Executive Committee Meeting Minutes

Sunday, August 15, 3:00-6:00 pm EST, via Zoom

Takes place at each ACS National Meeting

Attendance: Alyson Mitchell, Lucy Yu, Keith Cadwallader, LinShu Liu, Bosoon Park, Michael Granvogl, Michael Tunick, Youngmok Kim, Lauren Jackson, Karley Mahalak, Laurel Doherty, Michael Appell, Michael Morello, Xiaofen Du, Majher Sarker, Kathryn Deibler, Fereidoon Shahidi, Steve Toth, Zhichao Zhang, Tianxi Yang, Apratim Jash, Michael Qian, Carl Frey

AGFD Chair Youngmok Kim called the meeting to order at 3:01 PM (EST). The **minutes** of the spring 2021 Executive Committee meeting were approved with no changes and are published in the fall 2021 Cornucopia.

Youngmok Kim summarized the **Special Topics Meeting** and **Business Meeting.** The committee discussed how to increase nominations for AGFD awards. Student representatives have created a new student Listserv and student awards will be advertised through this Listserv as a starting place. ACS members that are faculty members were asked to also disseminate student award information at their institutes. The committee discussed the announcement by ACS leadership August 12, indicating that for Atlanta (and San Diego) at least 50% of the speakers need to be physically present for a "hybrid" meeting and that someone be physically present onsite to preside over each symposium. Virtual symposia can be presided from anywhere. The timing of this announcement precluded efficient conveyance of this message to all symposium organizers. Youngmok Kim and LinShu Liu are working to identify folks to preside over sessions. Organizers for the spring San Diego meetings need to be aware of this policy. The committee also discussed financial support for regional meetings. It was agreed that our Division does not typically offer finical support for regional meetings.

Stephen Toth gave the **Treasurer's Report**. The division spent only $6,280 this year due to virtual meetings, received $8,000 from donations, $8,475 from dues, and $56,186 from the ACS allotment. The net (revenues minus expenses) for the year so far is $67,302 giving AGFD $1,076,730 in the bank and in investments. The division is financially healthy. The **Awards Committee Report** was given by Mike Morello. All award information can be found on the Division website. Mike reviewed the point of contact for each award including: Advancement of Application of Agricultural and Food Chemistry /IFF Award (Mike Morello); Young Industrial Scientist Award (Brian Guthrie); Young Scientist Award (Michael Granvogl); ACS Fellow Award (Fereidoon Shahidi); Student Awards (Kathryn Deibler); Sterling B. Hendricks

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Award (Mike Appell); JAFC Best Article of Year Award (Thomas F. Hofmann); and Distinguished Service Award (Mike Tunick). Current awardees received their plaques via mail. Pictures were taken and will be posted on the AFGD website. Mike identified new challenges for the Awards Committee which includes setting a process for identifying and submitting nominations for the Kavli Emerging Leader Award. The Division was very happy that five of our distinguished members received ACS Fellows awards and include; Keith Cadwallader, Kathryn Deibler, Bosoon Park, Wallace Yokoyama and Liangli (Lucy) Yu. Congratulations were also given to Fereidoon Shahidi who received the Sterling B. Hendricks Memorial Leadership Award; Neil DaCosta recipient of the Distinguished Service Award, Lauren Jackson, LinShu Liu, Coralia Osoria Roa, and Jianping Wu recipients of the AGFD Fellow Award, and Holly Child recipient of the AGFD Roy Teranishi Graduate Fellowship in Food Chemistry. Rickey Yada received the 2021 AGFD Award for Advancement of Application of Agricultural and Food Chemistry and Xiaonan Lu received the 2021Young Scientist Award.

The **Student Committee Report** was given by Zhichao Zhang (UC Davis). Apratim Jash (Cornell University) will be replacing Zhichao after this meeting. They are hosting a social networking Zoom room at the Atlanta meeting and Zhichao will be attending the Poster session to welcome students. They created a new student Listserv and surveyed the students to identify a student-oriented event for the San Diego meeting. The Zoo was chosen.

LinShu Liu gave the **Program Report** for the virtual spring 2021 National Meeting. Overall, it was a good, but small meeting. He reported that many felt disappointed at not being in-person to network. The meeting was smaller than typical and included 290 abstracts given in both oral and poster presentations. In total there were 33 sessions held in 8 symposia. Youngmok Kim indicated that we need to improve and develop programming for upcoming meeting in Indianapolis and San Francisco. Michael Granvogl will contact subdivision leaders to help them organize. Michael Qian indicated that Pacifichem will take place as a hybrid meeting in December 2021 in Hawaii. Most US speakers have elected to attend the meeting in-person whereas most international speakers indicated they will attend virtually. The current ACS policy is if you selected in-person, you will not be able to switch to virtual. Many thought this was a restrictive policy that may need to be more flexible in light of the delta variant of COVID-19. A location for the next International Flavor Conference has not been decided and will depend upon Covid-19.

Steven Toth requested that the **budget** for the San Diego 2022 spring national meeting be set at $40,000. This is slightly lower than previous years as attendance is anticipated to be down due to COVID-19. The budget was passed.

Subdivision Reports were given by Youngmok Kim. The Biotechnology/Bioengineering Subdivision was reorganized and a new slate of officers were selected. The new officers will start their duties in 2022. The previous inactive members have been removed. The Flavor Subdivision is organizing a symposium for spring 2022 entitled *Milking It – Exploring Flavour, Spoilage and Shelf-life of Dairy Products*, and one for fall 2022 entitled *Breath Monitoring for Food Consumption, Drug Intake, Health and Wellbeing*. They are also publishing an ACS Symposium Series book entitled *Dynamic Flavor: Capturing Aroma Release Using Real-time Mass Spectrometry*. The Functional Foods Subdivision will have an upcoming symposium for the fall meeting entitled *Application of Omics Technologies in Food and Medicinal Plants*. The Food Safety Subdivision have two symposia planned for spring. The potential titles of these symposia include *Characterization of Natural Antimicrobials and Antioxidants and Their Applications in Food Preservation,* and *Advancement in the Detection of Food Chemical and Microbiological Hazards*. Prof. Boyan Gao, email: gaoboyan@sjtu.edu.cn will be the new secretary for Food Safety Subdivision beginning in 2022. The Diet and Gut Microbiome Subdivision inaugural programming went well with 22 speakers in 2 sessions. All speakers were invited to contribute manuscripts for a special issue within JAFC. This subdivision is planning two symposia for the spring entitled *Advancements in Nutriomics* and *Gut Reactions*. There also symposia planned for fall 2022 with a session related to *New Insights in Gut Microbiota Health Benefits* and one on *Emerging In Vitro Gut Models for Understanding Nutrient: Microbiome Interactions*. The Chair will be transitioning to Guodong Zhang with Vice-Chair shifting to Karley Mahalak. The Nutrition Subdivision has symposia planned for spring 2022 entitled *Chemistry and Health Benefits of Fermented Foods* and for fall 2021 entitled *Analytical Methods for Health Beneficial Bioactive Components & Hazards in Ethnic Foods*. This division has identified Hae Won Jang at Sukmyeong University and Tom Wang at USDA for secretaries in 2021 and 2022.

The Councilor Reports were given by Lauren Jackson, Alyson Mitchell and Mike Tunick. Council meeting will be held on August 25, 2021 (virtually). The ballot for President Elect of ACS includes Judith Giordan and John Warner. Three elections will be held for the Council Policy Committee, Committee on Committees, and Nominations & Elections. DAC Committee has plenty of money for project innovation grants. Mike pointed out that we should consider applying for a Division Strategic Planning retreat. Lauren Jackson was identified as the point person for this. Lauren indicated that there

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is a decline in the number of industrial members and that ACS is not meeting Diversity, Equality, Inclusion, and Respect (DEIR) goals. A prioritized action plan is now being drawn up as a result. Lauren suggested putting in an IPG grant for developing the Young Industrial Scientist Achievement Award. Membership has been sustained during the pandemic by being more flexible and by offering tiered membership. For those interested, professional employment guidelines for hiring in the chemistry industry exist, and language has been added to be more inclusive. Mike Morello pointed out there is a new initiative for how ACS is developing their strategic plan that is available on line.

The **Nominations Report** was given by Immediate Past Chair Lucy Yu. All subdivisions have leadership lined up through 2022. The Sustainability Subdivision should be included in the Cornucopia in 2022. Liz Kreger was previously identified as a potential candidate and her candidacy was passed at the Business Meeting. There are two Alternative Councilor positions that need to be filled this year. Lucy Yu will form a Nomination Committee with 3-4 members to identify at least 3-4 candidates and these will go out for a vote in September.

Cornucopia editor Carl Frey indicated that the Cornucopia was put together late as the files from ACS were received only 2.5 weeks before the meeting, and were not in any meaningful order. A total of 100 copies were printed for the hybrid meeting. Usually, 200-250 copies are printed for a meeting. AGFD will decide on how many copies to print for San Diego after the fall meeting.

Alyson Mitchell reported that there was no activity in **Hospitality/Public Relations** since we had no in-person meetings.

Membership Chair Michael Qian indicated that ACS did not provide a new membership report after the spring meeting.

Youngmok Kim gave the **Journal Report** for Thomas Hofmann. Dr. Yolanda Gogorcena was hired as an associate editor. The Journal of Agricultural and Food Chemistry grew 26% and the impact factor is now at 5.279 IP. There were 1,500 publications last year and 144,000 citations. *JAFC* will publish a special issue of each fall meeting. The new ACS FST (Food Science and Technology) journal will publish a special issue of the spring ACS meetings. The ACS-FST has published 125 manuscripts in six issues since August 2020 and 87% of authors are from outside of the United States.

In the **Communications Report,** Michael Appell indicated that the website is updated periodically. It is done through Wix.com (<$180/3 years). Mike Morello asked that the number of hits to the website be shared with the Executive Committee. Lauren Jackson indicated that we may want to promote our division better and make our members more visible on the website. Alyson Mitchell suggested to have each member in a leadership role send a bio (50 words or less) and a picture to Michael Appell to post on the website. Michael Appell suggested putting together a committee to keep the website updated and going. This will be managed through the Communications Committee in conjunction with the student representative and interested leadership members (Mike Morello, Alyson Mitchell, Mike Appell and Lauren Jackson). A motion was made and approved for Alyson Mitchell to donate or discard the four outdated conference computers in any way that makes sense.

There was no **Old Business**. In **New Business**, Mike Morello pointed to the need to increase the number and diversity of nominations for our Division awards. It was discussed, and the Executive Committee will begin to review nomination forms in order to identify a more diverse candidate pool. It was also decided that the September newsletter will be dedicated to Student awards and a reminder about the Division awards will be made in the January newsletter.

LinShu Liu discussed the desire of **AGRO** to program next to AGFD at the fall meetings in the convention center, all agreed this would benefit both divisions. AGRO also asked to have a single joint special issue for the fall meeting in the Journal of Agricultural and Food Chemistry. This was discussed. No clear benefit to the division was identified, so AGFD will not pursue this offer.

Mike Morello indicated that DAC committee funds grants through IPG for planning activities. Our division has not had a Strategic Planning meeting since 2016. The committee decided to put forward an IPG for a follow up Strategic Planning retreat. A second **IPG grant** will be put forward for Improving Industry Participation by Youngmok Kim and Brian Guthrie. Mike indicated that there are also grants to enhance international relationships that the Division could apply for.

The meeting adjourned at 5:36 PM (EST). *Submitted by AGFD Secretary Alyson Mitchell*

MILESTONES

Long time AGFD member and past AGFD Chair **Chi-Tang Ho** marked **50 years of ACS of membership** in 2021.

Peter Schieberle, University Professor (emeritus) Faculty of Chemistry Technical University Munich, celebrated 20 years as **Associate Editor of the Journal of Agricultural and Food Chemistry** and will now step back from his duties. He thanks his colleagues for help in reviewing for the journal and his editorial staff in particular for their cooperation which contributed to significantly increasing the impact factor of JAFC over the years.

AGFD congratulates Chi-Tang and Peter and looks forward to their continued successes and contributions.

Find information about AGFD awards at www.agfoodchem.org Scroll down 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 (Michael Granvogl), AGFD Fellow Award (Fereidoon Shahidi), AGFD Distinguished Service Award (Mike Tunick), Teranishi Fellowship (Liangli [Lucy] Yu), Graduate & Undergraduate Student Symposia (Kathryn Deibler), Service Award (Michael Qian), Sterling B. Hendricks Memorial Lectureship (Michael Appell/Bosoon Park), Spencer Award (Sarah Leibowitz), ACS Fellow Award (Michael Morello, Michael Appell, Carl Frey)

ΦΤΣ
The Honor Society of Food Science and Technology

Membership opportunities with Phi Tau Sigma

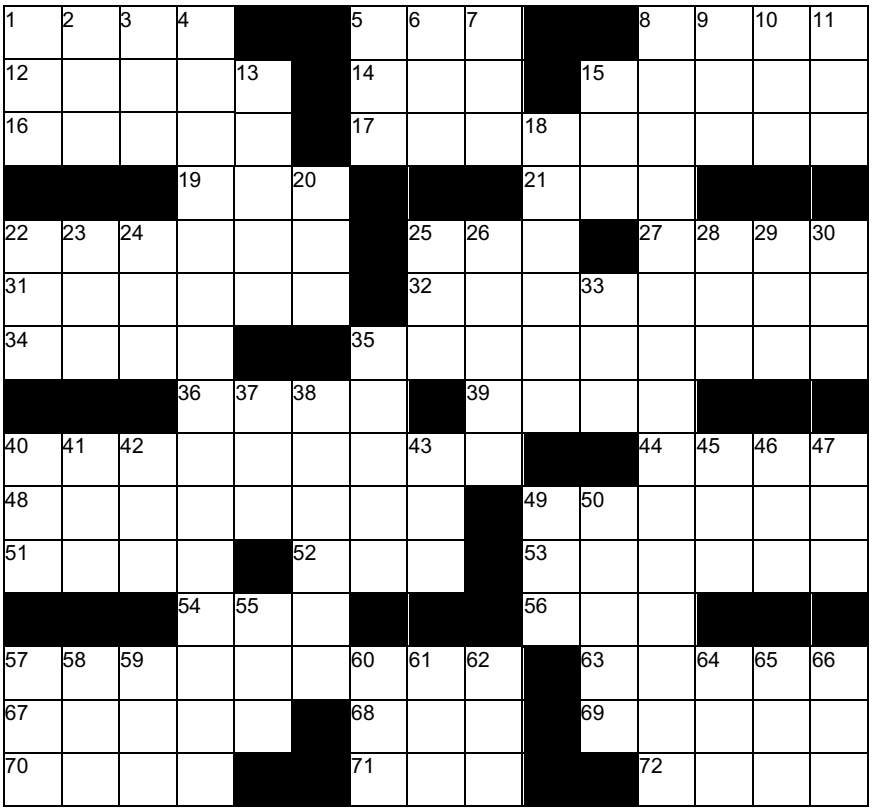
The Honor Society of Food Science and Technology

The mission of Phi Tau Sigma is to raise the stature and recognize scholarly achievements of the Food Science and Technology profession. Phi Tau Sigma encourages outstanding achievement by Food Science students and professionals and enhances the careers of Food Science professionals through its member network. Benefits include recognition, networking, mentoring, student scholarships and leadership, career and educational opportunities.

Phi Tau Sigma goals are:
--Recognize and honor academic and professional achievements of students and professionals within the Food Science/Industry and aligned sciences/industries
--Encourage the application of fundamental scientific principles to all fields of Food Science and Technology
--Stimulate the exchange of scientific knowledge through meetings, lectures, and publications
--Promote leadership in science, service, education, and social programs for the Society membership
--Establish and maintain a network of like-minded professionals
--Promote charitable, scientific, literary and educational programs

Membership nomination forms for the 2023 scholarships, must be submitted **by May 1, 2022**. For membership nomination information and forms please visit http://phitausigma.org/membership/ For questions contact Executive Director, Kathryn Kotula, Ph.D. klkotula@msn.com. (write Phi Tau Sigma Scholarship in the subject line.)

PACIFIC TIME ZONE PUZZLE



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

Congratulations to - Jeremy R. Espano of Vanderbilt U. for the 1st correct solution submission

Kudos also to - Steve Tait of Indiana U. for also submitting a correct solution.

ACROSS

1 Na^{+}, Cl^{-}, Fe^{+++} and Ca^{++}
5 Yosemite --- or Uncle ---
8 Lip
12 Reduces in amplitude
14 Flight schedule approx.
15 Brief film appearance
16 Las Vegas ---- or drag ---
17 Continental drift study
19 Gravestone inscription
21 Computer programming pioneer: --- Lovelace
22 Right triangle quotient: side/hypotenuse
25 Provider of form 1040
27 One billionth prefix
31 Meteor impact aftermath
32 Marching band boomer
34 The Biggest Little City in the World
35 Adorable
36 ---- circus or ---- market
39 Succulent: ---- *vera*
40 DNA transcriber (with 58 Down)
44 Unfortunately!
48 E.g.: boeuf bourguignon
49 Electro-shock weapons
51 To cry weakly. Whimper.
52 Poet's 'before'
53 Contaminate with disease
54 Shared by me and you
56 --- Farrow or --- Hamm
57 Bride's clothes & linens
63 Salivary gland infection prevented by MMR vax.
67 Asian sub-continent
68 Computer screen pop-ups
69 Marry without a big to-do
70 Some college courses are ----/fail
71 Summertime shirt
72 Big, heavy book

DOWN

1 Docs checked by the TSA
2 Quaker ---meal
3 Spectroscopy technique using strong magnets
4 Famous plane built in San Diego by Ryan Airlines
5 Chemistry --- or tea ---
6 Consumed for lunch
7 Popular cheese pairing
8 Big crack 150 miles east of San Diego
9 Parisian friend
10 'Dry' on a champagne label
11 Help!
13 Book title location
15 North Atlantic bottom dwelling fish
18 Mortarboard adornment
20 Middle of 65 Down
22 *Bad Moon Rising* band
23 E.g.: galena or cinnabar
24 --- Francisco or --- Jose
25 Arabic 'son of'
26 Rain detection technology
28 Jackie O's husband
29 Catholic clergy female
30 Texter's 'unbelievable!'
33 World's largest Portuguese speaking city: --- Paulo
35 Can't wait to start
37 Hugo's --- *Miserables*
38 Inputs
40 Scotch Tape maker
41 Wide shoe size designation
42 See 66 Down
43 Female that goes 'baa'
45 Wind to a sailor's back
46 Circle circumference section
47 Concorde or Tupolev Tu-144
49 Web creator: --- Berners-Lee
50 Graphic storybook style
55 Springsteen's *Born in the* ---
57 Iceberg part above waterline
58 See 40 Across
59 Takes too many meds
60 Dinnertime! Sit down and ---
61 Gator---
62 Employ
64 Cow talk
65 One in 1,000,000
66 Playground toy (w/42 Down)

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 >3000 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
LinShu Liu USDA-ARS-ERRC
linshu.liu@ars.usda.gov

Chair-Elect - Serves 1 year. Substitute for the Chair as needed
Michael Granvogl
michael.granvogl@uni-hohenheim.de

Vice-Chair - Serves 1 year. Assist Chair-elect. Develop future technical programs.
Jonathan Beauchamp
Fraunhofer-Institute
Jonathan.beauchamp@ivv.fraunhofer.de

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

Treasurer - Responsible for Division finances.
Stephen Toth
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 members.
Apratim Jash aj623@cornell.edu

Nominations - Develop officer slate. Served by Immediate Past Chair.
Youngmok Kim
youngmok.kim@finlays.net

Public Relations - Publicize Division.
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 - Solicit nominations, oversee awards process.
Chair Michael Morello
mjmorello226@gmail.com
Fellow Awards Fereidoon Shahidi
fshahidi@mun.ca
Young Scientist Award
Michael Granvogl
Michael.Granvogl@uni.hohenheim.de
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
Brian Guthrie
Brian_Guthrie@cargill.com

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AGFD TECHNICAL PROGRAM

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

SUNDAY MORNING Mar. 20
Hilton Bayfront Sapphire A/B
Food Macromolecules: Functionality, Health Benefits, Delivery Systems
Cospons. AGRO
N. Nitin, W. H. Yokoyama, *Organizers*
8:00 Introductory Remarks.
A001 8:05 Industrially-scalable microencapsulation of bioactive ingredients in alginates with controlled-release properties. T. Jeoh, H.B. Scher, Y. Tang, B. Arbaugh, R.M. Kawakita, S. Strobel
A002 8:20 Modulation of gut microbiota of broilers by controlled release of polyphenols and essential oils. H. Bao, S. Nahashon, T. Taylor, F. Chen, A. Kilonzo-Nthenge, H. Zhou, Y. Wu
A003 8:35 Effects of *Pleurotus eryngii* polysaccharide on gut inflammation and microbiota regulation. G. Ma, H. Du, H. Xiao
A004 8:50 Curcumin loaded metal-organic framework delivery systems. P. Ma, Q. Wang
A005 9:05 Ultrasonic encapsulation and delivery of functional foods. M. Ashokkumar
A006 9:20 Development of wet media milled purple sweet potato particle-stabilized Pickering emulsions: the synergistic role of bioactives, starch and cellulose. X. Lu
A007 9:35 Characterizing the role of network structure and filler/matrix interactions for tailored functionality in composite protein gels: Emulsion-filled gelatin as a case study. A.J. Gravelle, A.G. Marangoni
A008 9:50 Simultaneous loading and protection of bioactive compounds using protein-based assemblies. L. Liang
10:05 Intermission.
A009 10:15 Micro and nanoscale core-shell carriers for co-delivery of synergistic bioactives. C. Anandharamakrishnan
A010 10:30 Chitin nanofiber stabilized Pickering emulsions with potential in encapsulation of antibacterial essential oils. Y. Huang, H. Liu, S. Liu, S. Li
A011 10:45 Storage stability and loss of resveratrol in protein particles: loading, antioxidant activity and oxidation sensitivity. X. Yin, L. Liang
A012 11:00 Fabrication of hollow zein composite particles with sodium tripolyphosphate for the encapsulation of quercetin. M.A. Khan, L. Liang
A013 11:15 Rapid visible light-mediated crosslinking of casein-based hydrogels to facilitate wound healing. Q. Zhu, X. Zhou, Z. Hu, W. Cao, K. Yu, T. Ren, D. Ren
A014 11:30 Casein-propylene glycol alginate complexes: Formation, stability, and properties for preparation of high internal phase emulsions. N. Li, Q. Zhong
A015 11:45 High protein content casein-alginate conjugates produced by transacylation reaction as novel emulsifiers. N. Li, Q. Zhong

Virtual Zoom Room 16
Big Data and Artificial Intelligence in Agricultural and Food Chemistry
Cospons. PRES
M. Appell, H. Cheng, B. D. Guthrie, *Organizers, Presiding*
10:00 Introductory Remarks.
A016 10:05 Antibiotic discovery by means of computers. C. de la Fuente
A017 10:35 Experiences in algorithm based chemical process optimization and early attempts towards closed loop automation. S. Bertelsen
A018 11:05 Use of machine learning to navigate the sequence-activity landscape during directed evolution campaigns. O. Alvizo
11:35 Intermission.
A019 11:50 Landscape view: The application of artificial intelligence in agricultural and food chemistry research. Z.J. Baum
A020 12:20 Catalyzing AI-driven research for U.S. agriculture. B. Stucky, D.C. Peters
A021 12:50 Democratizing AI to build solutions for the farms of the future. S.B. Mirsky
1:20 Discussion.

Virtual Zoom Room 1

Human Intervention on Biosynthesis

Cospons. AGRO Maiher Sarker, LinShu Liu, Karley Mahalak, *Organizers, Presiders*

10:00 Introductory Remarks.

A022 10:05 Glucan phosphorylase as useful bio-catalyst for precision synthesis of amylose and its analogs. J. Kadokawa

A023 10:31 Mucorales as promising oleaginous fungi to produce high value of γ linolenic acid and carotenoids. H. Mohamed, Y. Song

A024 10:57 Extraction of soybean polysaccharide using immobilized cellulase. J. Liu, Y. Dong, Z. Rao, K. Tang

A015 11:23 Biotechnological research to enhance the growth and docosahexaenoic acids (DHA) production of marine heterotrophic microalgae, *Aurantiochytrium* sp. Y. Nazir

11:50 Intermission.

A016 12:10 Potential sophorolipid uses in antimicrobial applications. R. Ashby, X. Fan, O. Olanya, M. Ozdener

A027 12:36 Biofunneling and functionalization of agricultural waste polymers to advanced platform chemicals. L.N. Jayakody, K. Anderson, L. Dissanayake, S. Kayastha, D. Perry, L. Ryaan

A028 1:02 Increase in lipid and DHA production by Aurantiochytrium Sp. under the influence of chemical inducers. M. Sarker, S. Hussain

A029 1:28 Construction of medium-chain fatty acids (MCFAs) cell factory via metabolic engineering of Mucor circinelloides. S. Hussain, Y. Song

1:55 Concluding Remarks.

SUNDAY AFTERNOON

Hilton Bayfront Sapphire A/B

Food Macromolecules: Functionality, Health Benefits, Delivery Systems

Cospons. AGRO N. Nitin, F. Zhong, *Organizers*

2:00 Introductory Remarks.

A030 2:05 Bioactive components in parabiotic kefir lactic acid bacteria and obesity. H. Kim, E. Kim, S. Han, K. Seo

A031 2:20 Egg white protein ovotransferrin prevents bone loss in ovariectomized rats. N. Shang, J. Wu

A032 2:35 Improvement of probiotic survivability, persistence and colonization in gut by loading probiotic cells with plant extracts. R. Rai, M. Silva, W.H. Yokoyama, N. Nitin

A033 2:50 Reformulating traditional Mediterranean foods: A functional tomato product. B. Berk, M. Çetin, S. Sumnu, B. Mert, O. Ozarda, M. Oztop

A034 3:05 Bio-based micro and nanostructures for the delivery of bioactive compounds. M. Cerqueira

A035 3:20 *In planta* encapsulation of macro-nutrients for enhanced nutritional functionality. S. Dhital

A036 3:35 Eugenol cyclodextrin inclusion complex encapsulated pullulan nanofibers for potential food packaging applications. A. Celebioglu, T. Uyar

A037 3:50 Salt reduction using food macromolecule carrageenan. Y. Fang, W. Lu, Z. Hu

4:05 Intermission.

A038 4:15 Room temperature encapsulation of functional ingredients vis high-throughput electrohydrodynamic technology. J.M. Lagaron, C. Prieto

S039 4:30 Unraveling the potential of dry bean flour for utilization in the bakery industry. N. Navneet, m. martinez martinez, I. Joye

A040 4:45 Fate of curcumin-nanoemulsion and the bioaccessibility of curcumin during dynamic *in vitro* digesiton within complex dairy matrices. A. Ye

A041 5:00 Eugenol/cyclodextrin inclusion complex encapsulated pullulan nanofibers for potential food packaging applications. T. Uyar, A. Celebioglu

A042 5:15 Electrospun biopolymeric nanofibers as nanocarriers of bioactive compounds. S. Jafari, E. Assadpour

A043 5:30 Microencapsulation using whey protein isolate as wall material: Particle formation behaviour and interactions with core material. N. Fu

Virtual Zoom Room 1

Big Data and Artificial Intelligence in Agricultural and Food Chemistry

Cospons. PRES

M. Appell, H. Cheng, B. D. Guthrie, *Organizers, Presiding*

3:00 Introductory Remarks.

A044 3:05 Using machine learning to predict obesity risk based on genome-wide, epigenome-wide gene-gene, and gene-diet interactions. Y. Lee, J.J. Christensen, L.D. Parnell, C.E. Smith, J. Shao, N.M. McKeown, J.M. Ordovas, C. Lai

A045 3:35 Determining the sex of chicken eggs by machine learning and high-speed volatiles mass spectrometry. A.R. Rivers

A046 4:05 Catch me if you can – tracking volatile compounds as biomarkers of dynamic food processes using direct analysis. J. Beauchamp

4:35 Intermission.

A047 4:50 Big data in food production. R. Weel

A048 5:20 Hypercube big data analytics with artificial intelligence for food safety. B. Park

A049 5:50 Big data and deep learning in agriculture and food chemistry - considerations and practice. Y. Tseng

6:20 Discussion.

SUNDAY EVENING

Virtual Zoom Room

General Poster Session and the Undergraduate Poster Competition

M. Granvogl, L. Liu, *Organizers*

A050 7:00 Green polymers derived from cashew based raw materials. H. Cheng, A. Biswas, R.F. Furtado, C.R. Alves, C. Prieto, J.M. Lagaron

A051 7:00 Quantitative specific gravity analysis of salvia rosmarinus in ethanol solutions. E.M. Zippi, A. Marsalis

A052 7:00 Food grade Limonene can be an effective homemade insect repellent. M. Kakkanat, A. Colesmith, H. Brown

A053 7:00 Adulteration of maple syrup: Molecular vs. luminescence spectroscopic approaches. S. Rathnayake, M. Singh, R. Hanner, M.G. Corradini

A054 7:00 Development of hemp nanocellulose-based bioplastics and their application for food packaging. A. Fleming, X. Lu

A055 7:00 Potential of soil enzyme manganese peroxidase to degrade catechin and related polyphenols. M. Fu, A.E. Hagerman

A056 7:00 Analysis and characterization of west Tennessee honeys. E. Ahmed, B. Barrett, A.H. Shelton

A057 7:00 Potential for release of toxic alkaloid ricinine and for influence of bacterial functional diversity from castor cake after soil application. K. Cheng, C. Liu, F. Shen, Y. Tzou, Y. Chuang

A058 7:00 Changes of volatile compounds in rice-based distilled spirits, *soju* aged in different kinds of containers. W. Kim, S. Lee

A059 7:00 Variability of tannic acid and its role in stabilizing hollow zein nanoparticles. S.Y. Mallikarachchi, A.E. Hagerman

A060 7:00 Improving the functional characteristics of sorghum phenolics. J. Peterson, D. Smolensky, S. Bean, U. Yucel

A061 7:00 Influence of the microelements on anticancer metabolites biosynthesis in basidiomycetes. A. Ostrokhishko, A. Pomytkina, L. Levkina, F.V. Lavrentev

A062 7:00 Effect and mechanism of *Citrus depressa* Hayata peel extract against acetaminophen-induced liver injury in mice. Z. Su, P. Tsai, G. Wei, X. Chen

A063 7:00 Enhancing the stability of fish oil-in-water emulsions using whey protein- kappa carrageenan complexes. H. Khouryieh

A064 7:00 Inhibiting ice recrystallization by cellulose nanocrystals: Influences of sucrose concentration and storage time. M. Li, T. Wu

A065 7:00 Effect of boiling and steaming on the carbohydrates of sweet corns. W. Zhang, B. Zhu, L. Yu, J. Zhao, S. Li, X. Wu

A066 7:00 Detection of *Campylobacter jejuni* in agri-food products using a paper-based microfluidic device based on recombinase polymerase amplification and lateral flow immunoassay. Y. Chen, Y. Hu, X. Lu

A067 7:00 Biocatalytic approaches to valorization of food and agriculture waste streams. Z. Wang, J.M. Goddard

A068 7:00 Non-fouling and antimicrobial polyurethane coatings to prevent cross-contamination in food processing facilities. A. Rudlong, J.M. Goddard

A069 7:00 Phenolic metabolites in plasma and urine of children after blueberry consumption. L. Lavefve, R. Liyanage, L. Howard, K. Ono-Moore, R. Lan, E.C. Diaz

A070 7:00 Tailoring protein chemistry for *in situ* water safety applications: rapid pathogen detection and microplastic degradation. H.S. Zurier, S.R. Nugen, J.M. Goddard

A071 7:00 Evaluation of novel coatings to prevent smoke phenol absorption in Pinot noir grapes. L. Garcia, T. Tran, D.C. Cerrato, M. Penner, Y. Zhao, E. Tomasino

A072 7:00 Electrochemical teardown of a trace pesticide assessment system. V. Dhamu, C. Telang, S. Muthukumar, S. Prasad

A073 7:00 Texture and taste flavor characteristics of pecan kernel and the effect of variety. Z. Yusufali, X. Wang, K. Kubenka, X. Du

A074 7:00 Quantitative variation of taste and texture properties in 165 F2 cucumber progenies. C. Duan, Y. Weng, X. Du

A075 7:00 Black tea polyphenols provide a nutraceutical option for preventing the onset of celiac disease *In vitro*. P. Mathews, C. Van Buiten

A076 7:00 Quality characteristics of restructured goat meat jerky as Influenced by natural preservative properties of raisins. B.B. Lemma, J. Lee

A077 7:00 Comprehensive analysis of aromatic and metabolic compounds in beer brewed by new wild yeast by GC-MS and special databases. Y. Takemori, E. Shimbo, Y. Higashi, H. Kawamitsu, K. Kawamura, E.R. Kuhn, T. Yamamiya, N. Suzuki

A078 7:00 Evaluation of non-alcoholic beverages from hop using GC-MS and HPLC. Y. Takemori, M. Hayakawa, A. Nomura, J. Nagata, E.R. Kuhn, T. Yamamiya, N. Suzuki

A079 7:00 Genotoxicity evaluation of lignin-derivable of six bisguaiacols using in silico, in vitro, and in vivo methods. X. Zhang, J.S. Mahajan, T.H. Epps, L. Korley, C. Wu

A080 7:00 Identification and quantitation of anthocyanins in berries using liquid chromatography and high resolution tandem mass spectrometry. N. Abshiru, D. Randolph, B.V. Nemzer

A081 7:00 Phytonutrient composition and potential anti-inflammatory activities of air-dried purslane (*Portulaca oleracea)*. F. Al-Taher, D. Kalita, B.V. Nemzer

Hilton Bayfront Sapphire A/B

Characterization of Natural Antimicrobials and Antioxidants and Their Applications in Food Preservation

Cospons. AGRO H. Redfearn, G. Sun, *Presiding*

A082 8:00 The evaluation of the fabricated bioactive packaging material using essential oils and natural polymers by electrospray. A. Charles, T. Jin, R. Mu, F. Chen, A. Kilonzo-Nthenge, Y. Wu

A083 8:20 Interfacial chemistry of a bioderived active packaging film dictates its performance in complex matrices. I. Kay, J.M. Goddard, J.E. Herskovitz

A084 8:40 Sorghum DDGS as a renewable source for production of functional packaging films. U. Yucel, V. Trinetta, S. Bean

A085 9:00 Pre-commercial feasibility evaluation of non-equilibrium pulsed discharge for sanitation of whole and cut fresh. G. Fridman

A086 9:20 Amino acids and their derivatives preventing oxidation of frying oil: Promising natural antioxidants. H. Hwang

9:40 Intermission.

A087 9:50 Rapid discovery of novel antimicrobial peptides with machine learning algorithms to improve safety, quality, and shelf-life of clean label food products. C. Xu, Y. Zhou, G. Wang

A088 10:10 Antioxidants and antimicrobials to maintain freshness and minimize *Listeria* contamination of fresh-cut apples. X. Fan

A089 10:30 Grape pomace as a natural antimicrobial and antioxidant and their application in active food packaging. Y. Xu, E. Sismour

A090 10:50 Biobased microcarriers for enhanced antimicrobial delivery to improve food safety and quality. K. Huang

A091 11:10 Potential new antimicrobials/antioxidants from peptides using high voltage field technology. T. Jin

Virtual Zoom Room 1

Gut Reaction

Guodong Zhang, Jason Soares, Karley Mahalak**,** *Organizers, Presiding*

10:00 Introductory Remarks.

A092 10:05 Discovery of a gut bacterial metabolic pathway that drives α-Synuclein aggregation and neurodegeneration. L. Ortiz de Ora, K. Uyeda, E. Bess

A093 10:45 Discovery and characterization of gut microbial enzymes involved in keto-reductive metabolism. L. Qian, H. Ouyang, L. Gordils-Valentin, J. Hong, A. Jayaraman, X. Zhu

A094 11:15 Gut microbial metabolism of aromatic amino acids under dietary and microbiota interventions. C. Chen, Y. Zhou

11:55 Intermission.

A095 12:00 Effect of fructooligosaccharide on the adult human gut microbiome in vitro. K. Mahalak, J. Firrman, L. Liu, W. Hu, K. Bittinger

A096 12:40 Understanding the gut as a human bioreactor. E. Holmes

1:20 Panel Discussion.

1:35 Concluding Remarks.

MONDAY AFTERNOON

Hilton Bayfront Sapphire A/B

Characterization of Natural Antimicrobials and Antioxidants and Their Applications in Food Preservation

Cospons. AGRO Y. Wu, U. Yucel, *Presiding*

A097 2:00 Vitamin derivatives as effective light controlled biocidal agents for food contact surfaces. G. Sun, Z. Zhang, P. Tang, N. Nitin, L. Wang

A098 2:20 Antioxidant behavior of polypropylene-*graft*-maleic anhydride. H. Redfearn, J.M. Goddard

A099 2:40 Combined effect of biodegradable packaging with natural antimicrobials and physical agents for liquid foods preservation. L.J. Bastarrachea

A100 3:00 Fungicidal constituents from phytopathogens. K.M. Meepagala

A101 3:20 Application of natural antimicrobials for the preservation of fresh produce. X. Sun, A. Plotto, J. Bai

3:40 Intermission.

A102 3:50 New ethyl phenolic branched chain fatty acid arginate products with antimicrobial and surfactant properties. H. Ngo, X. Fan

A103 4:10 Antimicrobial activity of defence phytochemicals: Prenylated (iso)flavonoids and isothiocyanates. C. Araya Cloutier, S. Kalli, S. Andini, J. Vincken

A104 4:30 Chemical compositions and antioxidant activities of 36 typical pomegranates grown in China. W. Zheng, Y. Luo, B. Gao, L. Yu

A105 4:50 Ultrasound improves the antibacterial effect of thyme essential oil nanoemulsions against foodborne pathogens in simulated and real food system. M. Guo, Q. He, Z. Yang

Virtual Zoom Room 1

Advancements in Nutriomics

K. Mahalak, G. Zhang, *Organizers* J. P. Karl, *Presiding*

3:00 Introductory Remarks.

A106 3:05 Gut microbiome variation influences host responses to diet. F. Rey

A107 3:35 Mechanistic implications of the synergistic effect of diabetes drug metformin with the lactate dehydrogenase inhibitor sodium oxamate. B. Dayal, M.A. Lea

A108 3:55 Metabolic interplay between gut microbiome and host FGF21during dietary protein

restriction. G. Ecklu-Mensah, A. Martin, C. Ha, G. Hendrick, D. Layman, J. Gilbert, S. Devkota
4:25 Intermission.
A109 4:40 Novel combinations of prebiotics and polyphenols and their effects upon gut and cognitive health in active military personnel. B. Sayers, G.R. Gibson, A. Wijeyesekera
A110 5:10 Effects of supplementation with polyphenols and fiber on gut microbiota form and function during parallel batch fermentation. J. Whitman, L.A. Doherty, I. Pantoja-Feliciano, J.P. Karl, K. Racicot, S. Hussain, J.W. Soares
A111 5:30 Lactose as a modifier of the gut microbiota. J. Firrman, L. Liu, K. Mahalak, j. lemons, P. Tomasula, W. Hu, K. Bittinger
6:00 Discussion.
6:30 Concluding Remarks.

MONDAY EVENING
Convention Center In-Person & Zoom Room
Sci-Mix
M. Granvogl, L. Liu, *Organizers*
A112 8:00 Effects of *Pleurotus eryngii* polysaccharide on gut inflammation and microbiota regulation. G. Ma, H. Du, H. Xiao
A113 8:00 Antioxidant behavior of polypropylene-*graft*-maleic anhydride. H. Redfearn, J.M. Goddard
A114 8:00 Rapid wort color analysis of malts. N.O. Flynn
A115 8:00 Quantification of capsaicin and dihydrocapsaicin concentration in potentially the hottest beer using HPLC analysis. V. Ebenki, R. Parrish, S. Smith
A116 8:00 Investigating protein adsorption on nanoparticle-based sensors and delivery vehicles in plants. E. Voke, R.L. Pinals, N. Goh, M. Landry
A117 8:00 Gut microbial metabolism of aromatic amino acids under dietary and microbiota interventions. C. Chen, Y. Zhou
A118 8:00 Sensomics-assisted insights into flavor changes of functional food arising by implementing plant-based proteins as fat-replacer. F. Utz, J. Kreissl, T.D. Stark, C. Schmid, C. Tanger, U. Kulozik, T. Hofmann, C. Dawid
A119 8:00 Creation of flavor compounds in cheese. M.H. Tunick
A120 8:00 Rapid methods for detecting the presence of nitrite contamination in food and drink. A. Nikolaidis
A121 8:00 Detecting adulteration of red rice yeast dietary supplements by distinguishing between lovastatin and monacolin K. K. Hannon, J. Sabala, K. Kubachka, M. Mantha, L. Lorenz, J. Roetting, M. Perini, S. Pianezze
A122 8:00 “This fish smells okay, but is it still good?” Using biogenic amines to distinguish seafood species under several stages of decomposition. M.P. Matos, S. Genualdi
A123 8:00 Non-fouling and antimicrobial polyurethane coatings to prevent cross-contamination in food processing facilities. A. Rudlong, J.M. Goddard
A124 8:00 Fermenting beer with maltose negative yeast: The fate of sugars, alcohol, and volatile flavor compounds in nonalcoholic and low alcohol beers. L. Benedict, S.J. White, C.J. Riley, T.L. Chamberlain, H.N. Nguyen, O. McElearney
A125 8:00 Evaluation of non-alcoholic beverages from hop using GC-MS and HPLC. Y. Takemori, M. Hayakawa, A. Nomura, J. Nagata, E.R. Kuhn, T. Yamamiya, N. Suzuki
A126 8:00 Salt reduction using food macromolecule carrageenan. Y. Fang, W. Lu, Z. Hu
A127 8:00 Bioactive components in parabiotic kefir lactic acid bacteria and obesity. H. Kim, E. Kim, S. Han, K. Seo
A128 8:00 Potential sophorolipid uses in antimicrobial applications. R. Ashby, X. Fan, O. Olanya, M. Ozdener
A129 8:00 Protecting the integrity of plant-based sweeteners: Updating the FCC standard for Steviol Glycosides. T. Xu
A130 8:00 Gas chromatography-based metabolomics to characterize the differences between atypical and dark-cutting beef. R. Ramanathan, F. Kiyimba, J. Habiger, G.G. Mafi
A131 8:00 Synthesis and sensory characterization of novel umami enhancing and kokumi peptide glycoconjugates. J. Zhang, H. Wang, G. Su, M. Zhao, C. Ho
A132 8:00 Influence of the microelements on anticancer metabolites biosynthesis in basidiomycetes. A. Ostrokhishko, A. Pomytkina, L. Levkina, F.V. Lavrentev
A133 8:00 Evaluation of non-alcoholic beverages from hop using GC-MS and HPLC. Y. Takemori, M. Hayakawa, A. Nomura, J. Nagata, E.R. Kuhn, T. Yamamiya, N. Suzuki

TUESDAY MORNING Mar. 22
Hilton Bayfront Sapphire A/B
Chemistry of Alcoholic Beverages
Cospons. AGRO Nick Flynn, *Organizer, Presiding*
A134 8:00 Introduction: Chemistry of alcoholic beverages. N.O. Flynn
A135 8:10 Rapid wort color analysis of malts. N.O. Flynn
A136 8:30 Dry-hopping as a general tool to influence the concentrations of key odorants in beer as well as to optimize the overall aroma of alcohol-free beer. M. Granvogl, T. Hofmann, S. Brendel
A137 8:50 Quantification of capsaicin and dihydrocapsaicin concentration in potentially the

hottest beer using HPLC analysis. V. Ebenki, R. Parrish, S. Smith
A138 9:10 Unveiling the chemistry of sake. E.R. Kuhn
9:30 Intermission.
A139 9:45 Comprehensive aroma characterization of unaged (blanco) tequila. X. Huang, K.R. Cadwallader
A140 10:05 Investigating extraction and reutilization of oak products in model beverage systems. J. Belew, J. Beaver
A141 10:25 Using Raman spectroscopy for classification of alcohol products. S. Shidler, L. Grainger, T. Prusnick
A142 10:45 Elucidating reproducibility of site contributions to composition of Pinot noir wines over multiple vintages: Elemental profile and organic acids characterization. M. M. M. Lima, D. Hernandez, R. Runnebaum
A143 11:05 Determination of histamine, agmatine, and putrescine in wine by ion chromatography single quadrupole mass spectroscopy. T.T. Christison, J. Rohrer
A144 11:25 Incorporation of ^{13}C as a chemical label for smoke fuel used for smoke affected wine studies. D.C. Cerrato, L. Garcia, M. Penner, E. Tomasino
11:40 Panel Discussion.

Virtual Zoom Room 1
General Papers
Cospons. AGRO
M. Granvogl, L. Liu, *Organizers, Presiding*
10:00 Introductory Remarks.
A145 10:15 Simultaneous quantification of 24 aldehydes and ketones in oysters (*Crassostrea gigas*) with different thermal processing procedures by HPLC-electrospray tandem mass spectrometry. G. Zhao
A146 10:35 PAM free loop mediated isothermal amplification coupled with CRISPR/FnCas12a cleavage for on-spot detection of three rice pathogens. z. zhu, L. Yang
A147 10:55 Coin operated water vending machines: Bacterial contamination analysis. S. Asenjo, R. Gerona, M. Miñoza, C. Flores, G. Sildora
A148 11:15 Ovalbumin-specific peptide aptamer selected in the *In vitro S*election process using *E. coli* extract. S. Kim, A. Yumoto, N. Minagawa, Y. Heo, K. Son, Y. Ito, T. Uzawa
A149 11:35 The use of mustard bioherbicide in organic potato production: weed control, soil health, and crop quality. D. Temmen, J. Randall, I.E. Popova
11:55 Intermission.
A150 12:15 Rapid screening of glycosyltransferases in plants using a linear DNA expression template based cell-free transcription-translation system. X. Shi, S. Guo, M. Wang
A151 12:35 Analytical performance of a portable gluten sensor for celiac disease patients. A. Maric, K. Scherf
A152 12:55 Challenges of detecting an evolving prion disease, chronic wasting disease (CWD). C.J. Silva
A153 1:15 Gas chromatography-based metabolomics to characterize the differences between atypical and dark-cutting beef. R. Ramanathan, F. Kiyimba, J. Habiger, G.G. Mafi
A154 1:35 Selective dietary plant extract as inhibitors of cyclooxygenase -1 and cyclooxygenase-2 activities. D. Kalita, B.V. Nemzer
1:55 Concluding Remarks.

TUESDAY AFTERNOON
Virtual Zoom Room 1
Advances in Nanomaterials for Food and Agricultural Applications
Cospons. AGRO
S. Chang, B. Park, *Organizers, Presiding*
3:00 Intermission.
A155 3:00 Sustained release of hydrogen sulfide from poly (lactic acid) micro particles containing a dithiophosphate to enhance plant growth. N. Ranasinghe Arachchige, E.M. Brown, N.B. Bowden
A156 3:20 Investigating protein adsorption on nanoparticle-based sensors and delivery vehicles in plants. E. Voke, R.L. Pinals, N. Goh, M. Landry
A157 3:40 Electrostatic interactions of carbon dots with plant model and native cell walls. S. Jeon, P. Hu, K. Kim, C. Castillo, J.A. Pedersen, J. Giraldo
A158 4:00 Eco-friendly targeted pest control using nanomaze lure: Application in agricultural nanotechnology. K. Kaur, D.V. Kumar
4:20 Intermission.
A159 4:35 Fabrication of electrospun polyacrylonitrile carbon nanofibers with functionalized multi-walled carbon nanotube for electrochemical biosensing applications. R. Wang, R. Wang
A160 4:55 Nanoscale biomaterial for developing next-generation agrochemicals. R. Raliya
A161 5:15 Chemically tailored nanomaterials to improve material properties of renewable canola protein-based packaging materials. N. Bandara, T. Dissanayake, B. Chang, T. Mekonnen, C. Narvaez-Bravo, S. Ranadheera
A162 5:35 Tobacco mild green mosaic virus as a multifunctional platform for efficient pesticide delivery. I. Gonzalez Gamboa, A. Caparco, N.F. Steinmetz
5:55 Concluding Remarks.

Virtual Zoom Room 17
General Papers
Cospons. AGRO
M. Granvogl, L. Liu, *Organizers, Presiding*
3:00 Introductory Remarks.

A163 3:05 Nutrient compositions of two varieties of tomatoes harvested from single-layer and double-layer high tunnels. A. Odediran, N. Mikiashvili, J. Yu, P.L. Coffey, S. Gu
A164 3:29 Identification of odorants in American pawpaw fruit, *Asimina triloba*. S. Warner, J.P. Munafo
A165 3:53 Identification of odorants in chardonnay marc seeds. S. Warner, J.P. Munafo
A166 4:17 Characterization of odorants from southern mountain mint, *Pycnanthemum pycnanthemoides*. M. Dein, J.P. Munafo
A167 4:41 Synthesis and sensory characterization of novel umami enhancing and kokumi peptide glycoconjugates. J. Zhang, H. Wang, G. Su, M. Zhao, C. Ho
5:05 Intermission.
A168 5:20 Does ultrasound-assisted extraction on berries improve phenolic compounds content in juices?. A.A. Watrelot, L. Bouska
A169 5:44 Characterization of an exopolysaccharide (EPS-3A) produced by *Streptococcus thermophilus* ZJUIDS-2-01 isolated from traditional yak yogurt. F. Cao, M. Liang, J. Liu, P.X. Qi, D. Ren
A170 6:08 Determining the distributions of antioxidants from tea extract in oil-in-water emulsions and exploring the effect of chemical structures on the distributions. L. Cheng, Q. Huang
A171 6:32 “This fish smells okay, but is it still good?” Using biogenic amines to distinguish seafood species under several stages of decomposition. M.P. Matos, S. Genualdi
6:56 Concluding Remarks.

TUESDAY EVENING
Convention Center In-Person Room
General Poster Session and the Undergraduate Poster Competition
M. Granvogl, L. Liu, *Organizers*
A172 7:00 Providing context for chemical effects through compound structure similarity. B.T. Cook, J. Abedini, S. Bell, J. Rooney, E. McAfee, J. Phillips, D. Allen, N. Kleinstreuer
A173 7:00 Soy whey protein containing trypsin inhibitors improves the texture of surimi-like gels made with protein recovered from catfish by-products. Y. Zhang, S.K. Chang
A174 7:00 Data study of the effect of biochar application on greenhouse gas emissions from agricultural soils. C. Chan, S. Li
A175 7:00 Automated identification of potential pesticides residues in fruit samples using HRMS data. E. Ortega, I. Zamora, R. Lopez-Ruiz, A. Garrido Frenich, R. Romero-Gonzalez
A176 7:00 Phytochemical characterization of ninety-two Rosinweed (*Silphium integrifolium*) Genotypes: GC-MS profiles and their chemometric analysis. A. Chitrakar, Y. Zhang, B. Johnson, E. Murrell, E. Chérémond, M. Brasuel
A177 7:00 Earthworms increase the potential for enzymatic bioactivation of biochars made from co-pyrolyzing animal manures and plastic wastes. J. Sanchez-Hernandez, K. Ro, A.A. Szogi, S. Chang, B. Park
A178 7:00 Modeling beer ratings with machine learning. C.N. Vialva, E. Frondarina, G. Fogel, D.A. Hecht
A179 7:00 Peanut allergen isolation using ligand bound magnetic nanoparticles. R. Arena, G. Nagorite, A.I. Omoike
A180 7:00 Chemical and electrochemical ion intercalation on cobalt hydroxide: Selective phase transformation and application to electrocatalytic reactions. O.O. Onawumi, P.B. Ayoola, O.A. Adewusi
A181 7:00 Improving the extraction and recovery of organic acids from root exudates by WAX-SPE. N.P. Rosario, P. Larsen, G. Barding
A182 7:00 Sensitive and visual detection of *Salmonella* spp. using CRISPR-Cas12a assisted lateral flow assay. S. San, J. Chen
A183 7:00 Sucrose treatment improves phytochemical levels and bioactivities of mung bean sprouts. J. Lee, H. Heo, H. Lee
A184 7:00 Antioxidant and anti-hypertensive effects of sinapic acid via activation of Nrf2/HO-1 pathway in EA.hy926 endothelial cells. H. Lee, H. Kim, J. Lee
A185 7:00 Effects of various pre-treatment and cooking on the levels of biogenic amines in mackerel. H. Ahn, Y. Kim, K.G. Lee
A186 7:00 Correlation analysis between volatile compounds and α-dicarbonyl compounds in various beans as responses to different roasting conditions. S. Do, J. Park, G. Lee, K.G. Lee
A187 7:00 Effect of ultraviolet light exposure and compost tea supplementation on growth and nutrient profile of hydroponically grown mustard greens. R. Castro, D. Pentico, S. Lu, S. Dinh, J.J. Love, D. Larom, R. Pérez, C. Liu
A188 7:00 Fluorosulfurylation of amino acid-based sweeteners towards novel high intensity artificial sweeteners
. S. Khasnavis, N.D. Ball
A189 7:00 Determination of quaternary amine polar pesticides using improved cation-exchange separation technology combined with suppressed conductivity and tandem mass spectrometry detection. T.T. Christison, J.E. Madden, J. Rohrer
A190 7:00 Effect of infrared drying method on chemical and microbial stability of cold-hardy grape pomaces. Z. Shad, C. Venkitasamy, E. Kuelbs, A.A. Watrelot
A191 7:00 Use of 1H NMR spectroscopy to identify fraud in commercial honey samples. V. Kizirian, R. Hellberg

A192 7:00 Development of novel antioxidant, antibiofilm and hydrophobic cinnamic acid and cinnamic acid derivatives based cellulose nanofibrils (CNF) films for food packaging applications. S. LakshmiBalasubramaniam, D. Skonberg, M. Tajvidi, C. Howell
A193 7:00 Oxygen functionalized MWCNTs decorated with silica-coated spinel ferrite–A nanocomposite for potentially rapid and efficient decolorization of the aquatic environment. Z.A. Al Othman, S. Wabaidur
A194 7:00 Anti-bacterial, anti-inflammatory activities of lactic acid bacteria-bioconversioned indica rice (Oryza sativa L.) extract. H. Ahn, H. Kwon, K.G. Lee
A195 7:00 Improvement of Robusta coffee aroma with L-leucine powder. H. Park, A. Cho, K.G. Lee
A196 7:00 Reduction of sulfur containing volatiles from antioxidative onion skin extract. J. Hong, M. Kim, J. Lee
A197 7:00 PVA hydrogel film containing lemongrass essential oil emulsion for smart food packaging. H. Kim, U. Park, C. Ban, S. Lim
A198 7:00 Zn^{2+} and Ag^{+} doped oyster shell waste as a natural antimicrobial agent for active packaging. P. Kitae, S. Jongchul
A199 7:00 Quantification of “smoke taint” compounds in grapes and wine by SPME-GCMS. E.R. Kuhn, A. Sandy, A. Owens, D. Gruszecka
A200 7:00 Fermenting beer with maltose negative yeast: The fate of sugars, alcohol, and volatile flavor compounds in nonalcoholic and low alcohol beers. L. Benedict, S.J. White, C.J. Riley, T.L. Chamberlain, H.N. Nguyen, O. McElearney
A201 7:00 Analysis of accelerating the whiskey aging process. S. Walker, R. Dixon
A202 7:00 Hop (Humulus lupulus) acid and metabolite profiles as a function of growth region by HPLC and GC-MS analysis. C. Paoletta, C. Balog, D.V. Liskin, A. Higgs, A. Brehm, R.A. Quinlan
A203 7:00 Characterization of aroma and taste profiles as a function of malt growth region in craft brewing by HPLC and GC-MS. C. Balog, C. Paoletta, A. Higgs, D.V. Liskin, A. Brehm, R.A. Quinlan
A204 7:00 Structures and binding sites of human bitter taste receptors complexed with G protein and agonists. M. Yang, S. Kim, W.A. Goddard, B.D. Guthrie, S.B. Liggett
A205 7:00 Response of metal oxide semiconductor E-nose on aroma compounds and its application in Chinese baijiu. Y. Li, K. Yang, D. Zhao, J. Zheng, M.C. Qian

ACS Integration Testing - Poster
Spons. ACS, Cospons. AGFD

WEDNESDAY MORNING Mar. 23

Virtual Zoom Room 19
Advances in Nanomaterials for Food and Agricultural Applications
Cospons. AGRO
S. Chang, B. Park, *Organizers, Presiding*
10:00 Introductory Remarks.
A206 10:05 Modified hydroxyapatite nano seed coating for the seedling stage enhancement of *Zea Mays*. L. Abeywardana, M. de Silva, C. Sandaruwan, D. Dahanayake, G. Priyadarshana, S. Chathurika, V. Karunaratne, N. Kottegoda
A207 10:25 Smart cellulose nanocrystal-based materials for intelligent packaging. Z. Yu, X. Lu
A208 10:45 Material degradation inside and out: Contributions to the deterioration of electrospun matrices with encapsulated corn oil. L. Colaruotolo, S.S. Singh, L. Lim, S. Dobson, A. Sadat, I. Joye, M.G. Corradini
A209 11:05 Advances in nanomaterials for food and agricultural applications. I.Z. Zareen Ahmad
11:25 Intermission.
A210 11:40 Effect of zein and carboxyl-methyl chitosan coated resveratrol nanoparticles on chicken embryonic development as endocrine disruptors. J. Zhang, X. Zhang, Q. Wang, C. Wu
A211 12:00 Compressible nanobubbles induced self-assembly of 7S globulins isolated from pea (*Pisum Sativum L.*). T. Yan, D. Liu
A212 12:20 Hierarchical assembly of safe, pragmatic biocatalytic materials. E. Moreno Reyes, J.M. Goddard
A213 12:40 Synthesis, stability and kinetics of hydrogen sulfide release of dithiophosphates. N. Ranasinghe Arachchige, E.M. Brown, A. Paudel, N.B. Bowden
1:00 Concluding Remarks.

Virtual Zoom Room 1
General Papers
Cospons. AGRO
M. Granvogl, L. Liu, *Organizers, Presiding*
10:00 Introductory Remarks.
A214 10:05 Resistance mechanism of salmonella typhimurium at low water activity against heat treatment and added trans-cinnamaldehyde or eugenol. Q. Ding, C. Ge, R.C. Baker, R.L. Buchanan, R.V. Tikekar
A215 10:29 Analytical and carbohydrate chemistries of contemporary waterpipe tobaccos. J.H. Lauterbach
A216 10:53 Characterization of hydroxypropyl methylcellulose bio-composite structures with microcrystalline cellulose-containing natural anthocyanin for developing pH sensing indicator. A. Boonsiriwit, Y. Lee
A217 11:17 Scalable functional cationic swabs for improved pathogenic microbes sampling from food

contact surfaces. A. El-Moghazy, N. Wisuthiphaet, N. Nitin
A218 11:41 Ecofriendly extraction of polyphenolic compounds from *Vaccinium meridionale* fruit by-product with natural deep eutectic solvent (NADES). G.A. Garzon, C.E. Gonzalez, D. Gonzalez, C.D. Mendieta, V. Monroy
12:05 Intermission.
A219 12:20 Identification of polymers, additives, and contaminants in food contact articles using rapid, direct - high resolution mass spectrometry. K.L. Reese, J. Rusko, I. Perkons, L.K. Ackerman
A220 12:44 Raman imaging of plant metabolite crystals. S. Shidler, L. Grainger, T. Prusnick, A. Lewandowska
A221 1:08 Gossypol effects on mammalian cell growth and gene expression. H. Cao, K. Sethumadhavan
A222 1:32 Changes in cell wall composition of cool-season pasture grasses over the growing season. S. Newhuis, I.A. Kagan, B. Harlow, M. Flythe, R.R. Schendel
1:56 Concluding Remarks.

WEDNESDAY AFTERNOON
Virtual Zoom Room 2
Tackling Food Fraud Through Innovative Methodologies: Opportunities and Challenges
Q. Rao, Z. Xie, *Organizers, Presiding*
3:00 Introductory Remarks.
A223 3:05 Using ingredient standards to protect food integrity and combat economically motivated adulteration. Z. Xie
A224 3:25 Use of amino acid fingerprinting in authenticity verification of nonfat dry milk and skim milk powders. S.D. Bhandari, Z. Xie
A225 3:45 Development of a LC-QTOF-MS based method for the classification of honeys with different quality attributes. L. Tian, C. Akiki, L. Liu, S. Bilamjian, T. Anumol, D. Cuthbertson, S. Bayen
A226 4:05 Protecting the integrity of plant-based sweeteners: Updating the FCC standard for Steviol Glycosides. T. Xu
4:25 Intermission.
A227 4:40 Exploration of nanobody based immunoassays for the tracing of food fraud. D. Li, C. Morisseau, Y. Ying, B.D. Hammock
A228 5:00 Immunoassays for the detection of meat adulterants. Q. Rao, X. Jiang
A229 5:20 Rapid methods for detecting the presence of nitrite contamination in food and drink. A. Nikolaidis
A230 5:40 Detecting adulteration of red rice yeast dietary supplements by distinguishing between lovastatin and monacolin K. K. Hannon, J. Sabala, K. Kubachka, M. Mantha, L. Lorenz, J. Roetting, M. Perini, S. Pianezze

Virtual Zoom Room 1
Milking It: Exploring Flavor, Spoilage and Shelf-Life of Dairy Products
Cospons. AGRO
Jonathan Beauchamp, Yu Wang, *Organizers, Presiding*
A231 3:00 Creation of flavor compounds in cheese. M.H. Tunick
A232 3:20 Evolution of volatile compounds during cheddar cheese ripening and discovery of the key flavour compounds related to predetermined cheese qualities. Y. Chen, C. Ayed, Q. Yang, T. Foster, N. Yang
A233 3:40 Multivariate methods in dairy spoilage characterization. L. Kuuliala, J. Beauchamp, B. DeBaets, F. Devlieghere
A234 4:00 Real-time monitoring of VOCs associated with kefir *versus* kefir-like (plant-based) fermentation induced inoculating diverse microbial resources. V. Capozzi, M. Fragasso, I. Khomenko, P. Silcock, F. Biasioli
A235 4:20 Non-targeted high-resolution mass spectrometry study for evaluation of milk freshness. M. Suman, C. Loffi, D. Cavanna, G. Sammarco, D. Catellani, C. Dallasta
A236 4:40 Shelf life of packed UHT milk: Storage test and mathematical modelling. M. Reinelt
5:00 Intermission.
A237 5:20 Sensomics-assisted insights into flavor changes of functional food arising by implementing plant-based proteins as fat-replacer. F. Utz, J. Kreissl, T.D. Stark, C. Schmid, C. Tanger, U. Kulozik, T. Hofmann, C. Dawid
A238 5:40 Influence of volatile compounds on consumer acceptability of infant formula. G. Eyres, P. Silcock, S. Gallier, L. Tolenaars, S. Then
A239 6:00 Photooxidation of milk. P.J. Bremer, M. Asaduzzaman, P. Silcock, E. Zardin, J. Beauchamp
A240 6:20 Understanding microbially induced flavor quality changes in milk. M. Alothman, P. Silcock, K. Lusk, P.J. Bremer
A240 6:40 Exploring volatile spoilage markers and sensory defects of UHT milk in accelerated shelf-life tests. A. Krempl, B. Handwerker, A. Strube, K. Rieblinger, J. Beauchamp

THURSDAY EVENING Mar. 24
ACS Integration Testing - Poster
Sponsored by ACS, Cospons. AGRO

ABSTRACTS for AGFD SPRING 2022 TECHNICAL PROGRAM

A001 Industrially-scalable microencapsulation of bioactive ingredients in alginates with controlled-release properties Tina Jeoh1, tjeoh@ucdavis.edu, Herbert B. Scher1, Yuting Tang1, Benjamin Arbaugh1, Ryan M. Kawakita1,2, Scott Strobel1,3. (1) Biological and Agricultural Engineering, Univ. of California Davis (2) Provivi, Inc., Santa Monica, California (3) PivotBio, Inc., Emeryville, California Alginates are naturally-occurring, Generally Regarded As Safe (GRAS), anionic polysaccharides, that have long been known for its potential to microencapsulate food ingredients. Alginates rapidly gel under benign, ambient conditions, resulting in matrices that have enteric release properties. Commonly crosslinked with calcium, alginates incorporate the food ingredient in the alginate matrix, that can be triggered to fully release the payload with the addition of strong chelating agents. Alginates also form complex coacervation matrices with protein, forming matrix-microcapsules with pH-responsive gelation properties. Microencapsulation in alginates is easily executable at the lab bench scale, but the many steps and processes can be cost prohibitive to scale-up for commercial-scale production. This talk will describe industrially-scalable spray-drying and fluid-bed coating processes to microencapsulate bioactive ingredients in crosslinked alginates and complex coacervated alginate-protein matrices. Several examples of successes and challenges in the encapsulation of protein, peptides, oil emulsions, including volatile ingredients will be described.

A002 Modulation of gut microbiota of broilers by controlled release of polyphenols and essential oils Haona Bao1, Samuel Nahashon1, Thyneice Taylor1, Fur-Chi Chen1, Agnes Kilonzo-Nthenge1, Huaijun Zhou2, Ying Wu1, ywu@tnstate.edu. (1) Tennessee State Univ., Nashville, (2) Univ. of California Davis In the current study, polyphenols from grape pomace and essential oils, namely thymol and carvacrol, were encapsulated by water soluble yellow mustard mucilage (WSM), maltodextrin and gum Arabic at various ratios. The effect of wall materials on the controlled release of the bioactive core compounds were tested in vitro using simulated poultry intestinal digestion system. The optimal formula was further tested in vivo on broilers by evaluating the effects on intestinal microbiota and growth performance. The encapsulated compounds were mixed with the bird's diet as feed additives and compared with antibiotic diet and control basal diet. The intestinal content was collected and ilium and cecal microbiota were analyzed using16S rRNA sequencing test. The in vitro study showed that the addition of the novel wall material WSM has significantly modified the releasing pattern of the bioactive compounds under gastrointestinal environment, where over 73% of bioactive compounds were delivered to the lower intestinal tract where most infectious bacteria are preferably located, while the particles without WSM had 49% available bioactive compounds left after exposed to the acidic gastro environment. The in vivo study has revealed that the incorporation of the encapsulated compounds has significantly modified the microbiota after 3 weeks of continuous ingestion, where the population of the infectious bacteria like Escherichia coli, Listeria monocytogenes, Staphylococcus aureus has significantly decreased, and bacterial diversity and the population of some representative probiotic bacteria like Lactobacillus have significantly increased ($P< 0.05$). Additionally the supplementation of encapsulated particles has significantly decreased the feed conversion rate ($P<0.05$) and increased the carcass weight. In conclusion, the encapsulated compounds were successfully delivered to the target location at lower intestinal tract thus improved poultry gut health and growth performance.

A003 Effects of Pleurotus eryngii polysaccharide on gut inflammation and microbiota regulation Gaoxing Ma1,2, Hengjun Du2, Hang Xiao2, hangxiao@gmail.com. (1) College of Food Sci. and Eng., Nanjing Univ. of Finance and Economics, Nanjing, Jiangsu, China (2) Dept. of Food Science, Univ. of Massachusetts Amherst Pleurotus eryngii is a widely consumed edible mushroom with high nutritional value, from which the P. eryngii polysaccharide (PEP) has been considered to contribute multiple heal-promoting effects. As research focuses on the relationship between gut microbiota and host health level, the biological activities of PEP through its interaction with gut microbiota have not been adequately studied. Hence, correlations between the health benefits and gut microbiota alteration induced by PEP were carried out in the present study. Firstly, PEP was isolated and chemically characterized. Simulated digestion and fermentation models were utilized and revealed that PEP was not decomposed during digestion in the stomach or small intestine but was degraded and utilized by colonic microbiota to produce a variety of short-chain fatty acids (SCFAs). Moreover, two newly identified PEP named WPEP and NPEP were purified from PEP, from which both these two polysaccharides could significantly inhibit LPS-induced inflammatory responses through the blocking of the activation of MAPK and NF-κB pathways. The inhibiting effects and the potential underlying mechanisms of WPEP were investigated. Results showed that WPEP significantly alleviated colitis symptoms and gut microbiota dysbiosis, such as decreased abundance of Akkermansia muciniphila and Clostridium cocleatum and increased abundance of Bifidobacterium pseudolongum, Lactobacillus reuteri, Lactobacillus salivarius, and Ruminococcus bromii. In summary, our results demonstrated the anti-inflammatory potential of PEP and the related mechanisms, indicating that PEP could be utilized as a functional food component in colitis management as well as a potential prebiotic agent to treat inflammation-related disorders.

A004 Curcumin loaded metal-organic framework delivery systems peihua ma, peihua@umd.edu, Qin Wang. Nutrition and Food Science, Univ. of Maryland at College Park Metal-organic frameworks (MOFs), a group of cutting-edge designable porous scaffolding materials attracted attention in reticular chemistry, which has potentials to satisfy fundamental demands for delivery systems. Here, three types of curcumin-loaded UiO-66 (representative high biocompatibility and water-stable MOFs) delivery systems, curcumin-loaded UiO-66, curcumin-loaded UiO-66 high internal-phase Pickering emulsions (HIPPE) and curcumin loaded UiO-66 functional film were prepared, named as curcmin@UiO-66, curcumin@UiO-66 HIPPE, and curcumin@UiO-66/Chitosan, respectively. The loading capacity for these three delivery systems was reached 3.45% w/w, 7.33%, and 26.18%, respectively. All systems were characterized using X-ray diffraction (XRD), physisorption analyzer, scanning electron microscopy (SEM), and energy-dispersive X-ray spectrometer (EDS), for crystallography, morphology, physicochemical properties, with computer assistant optimization with DFT and GCMC simulation for maximum loading capacity. The result showed that these systems all exhibit extremely high surface area and porosity, as well as strong thermal stability as evidenced by TGA results, which demonstrated great potentials for application as a food delivery system. These novel MOF nanoparticle

stabilized delivery systems are expected to be useful for other bioactive components and antimicrobial agents, which would find applications in functional food, food safety, and biomedical areas in the future.

A005 Ultrasonic encapsulation and delivery of functional foods Muthupandian Ashokkumar, masho@unimelb.edu.au. The Univ. of Melbourne, Victoria, Australia The interaction between sound waves and microbubbles in solutions generates acoustic cavitation, the growth and collapse of bubbles, under certain experimental conditions. The near adiabatic collapse of microbubbles during acoustic cavitation generates extreme reaction conditions in liquids. Application of ultrasound in food and bioprocessing has attracted significant attention from food scientists and food industries. Ultrasonic encapsulation of nutrients and functional foods in a biopolymeric shell has been developed recently. The physical forces generated during acoustic cavitation process help to emulsify hydrophobic and hydrophilic nutrients and functional foods, stabilized by biopolymers. The oxidative radicals generated within cavitation bubbles are then used to crosslink the biopolymers forming a thin shell around the functional core. For example, the images of ultrasonically synthesized chitosan microspheres are shown. A non-polar liquid nutrient, ultrasonically encapsulated in the core of chitosan-shelled microspheres, can be seen in one of these images. The image of a hollow microsphere can be seen in the 2nd image. Such an encapsulation process results in protecting the core materials from degradation by oxygen and light during storage. This approach has generated the possibility of delivering nutrients using a variety of food matrix (example, yoghurt, fruit juice, milk, etc.). The fundamental aspects of ultrasonics and sonochemistry and their application for the encapsulation and delivery of functional foods will be discussed.

A006 Development of wet media milled purple sweet potato particle-stabilized Pickering emulsions: the synergistic role of bioactives, starch and cellulose Xuanxuan Lu, luxuanxuan2@jnu.edu.cn. Food Sci. and Eng., Jinan Univ., Guangzhou, Guangdong, China Most food-grade Pickering particles nowadays are prepared using purified single-compound substances as starting materials. However, to obtain these substances, complex extraction and purification procedures are often needed. Meanwhile, natural bioactive compounds existing in raw materials are lost. Herein, it is essential to develop a new strategy which could effectively fabricate sustainable and multifunctional particles directly from raw biomass materials. Purple sweet potatoes, rich in bioactive compounds, were used to produce purple sweet potato particles (PSPPs) via wet media milling. The effect of milling time on particle size, morphology, the content and antioxidative activity of bioactive compounds in PSPPs were investigated. Wet media milling could effectively decrease the particle size of PSPPs from 3371 ± 109.98 nm to 312 ± 18.4 nm after 240 min of milling. And significant amounts of bioactive compounds and their antioxidative activity were retained. Pickering emulsions (PSPP-Es) were successfully formed using PSPPs as Pickering stabilizers. The resulting PSPP-Es exhibited good freeze-thaw and heating stability. Low pH (3-6) and strong ionic strength (150 mM-600 mM) conditions contributed to smaller droplet size (10-12 μm) and better storage stability of PSPP-Es due to better complexation between phenolics and major components in PSPPs. Besides, PSPP-Es possessed better lipid oxidative stability than Tween 80-stabilized emulsion due to the presence of intrinsic antioxidants. This work would facilitate the development of Pickering stabilizers with outstanding emulsifying ability and functional properties directly from whole grain materials, and wide application of whole grain particle-stabilized Pickering emulsions in food, cosmetics and pharmaceutical industry.

A007 Characterizing the role of network structure and filler/matrix interactions for tailored functionality in composite protein gels: Emulsion-filled gelatin as a case study Andrew J. Gravelle1, agravelle@ucdavis.edu, Alejandro G. Marangoni2. (1) Dept. of Food Sci. and Tech., Univ. of California Davis (2) Dept. of Food Science, Univ. of Guelph, Ontario, Canada Many food matrices can be viewed as emulsion-filled protein hydrogel composites, including various cheeses, comminuted meats, and yogurts. The functional and textural attributes of such products are strongly impacted by the properties of the embedded droplets, their distribution in space, and their interaction with the continuous protein matrix. This work addresses the effect of network microstructure, lipid physical state, and filler/matrix electrostatic interactions on the linear elastic properties of a model composite food system; emulsion-filled gelatin gels. Solid fat- and liquid oil-based whey protein isolate-stabilized emulsion droplets were used as filler particles (average droplet size 1-2 μm). The gels were prepared with varying pH, either above (pH 6; Gel-6) or below (pH 4; Gel-4) the isoelectric point of whey protein. Confocal micrographs demonstrated the emulsion droplets were homogeneously distributed throughout the Gel-6 composites, whereas the Gel-4 gels were dominated by heterogeneously distributed droplet-rich, protein-dense domains. For both systems, the elastic modulus increased with filler loading, with fat having a greater effect than oil; however, the reinforcement was substantially more pronounced in the heterogeneous Gel-4 composites. Increasing gelatin content (2-8wt% protein) reduced the extent of filler-induced reinforcement in both the fat- and oil-filled Gel-4 composites. This behaviour is not expected for rigid fillers, but could be rationalized based on stress-translation through the heterogeneous network. In contrast, the relative reinforcement of the Gel-6 gels was independent of gelatin content, which was attributed to site-specific filler/matrix interactions. We have proposed a micromechanistic model which more accurately describes the experimentally observed reinforcement in emulsion-filled gels than traditional particle-reinforcement theories. This model provides an intuitive, mechanistic reasoning for the observed mechanical response. Further developing these relationships will be critical for using structural design approaches to modify and design functional food systems, and understanding the role of filler/matrix interactions will be advantageous for adapting new and emerging protein sources.

A008 Simultaneous loading and protection of bioactive compounds using protein-based assemblies Li Liang1,2, liliang@jiangnan.edu.cn. (1) State Key Lab of Food Sci. and Tech., Jiangnan Univ., Wuxi, Jiangsu, China (2) School of Food Sci. and Tech., Jiangnan Univ., Wuxi, Jiangsu, China Bioactive compounds (BCs) possess health benefits, but they are not stable upon exposure to sensitive environments. It is thus necessary to encapsulate and protect BCs for their application in functional foods. There appear to be interesting market opportunities for functional foods fortified with a range of BCs and offering multiple health benefits. Co-administering different BCs may produce synergistic effect on their bioactivity and improved stability. These provide motivation to develop the carrier systems that can simultaneously load a plurality of BCs. BCs with different solubility were simultaneously bound to ligand-binding proteins, since the proteins have multiple binding sites. The co-loaded BCs were more stable than the single-loaded bioactive compound. Furthermore, BCs were co-encapsulated at the oil-water interface of emulsions and in the protein matrix in emulsion gels. In addition, it was also found that the BCs with different solubility could be co-loaded in protein-based homogenous particles, due to the smart partition of BCs. Food proteins were used as wall materials to encapsulate and protect multiple BCs, and the effects were improved by their combination with polysaccharides.

A009 Micro and nanoscale core-shell carriers for co-delivery of synergistic bioactives C Anandharamakrishnan, anandharamakrishnan@iifpt.edu.in. National Inst. of Food Tech., Entrepreneurship and Management (NIFTEM) - Thanjavur, Thanjavur, Tamil Nadu, India In recent years, the approach towards health and food has drastically changed with an enormous gain of knowledge about nutrition and medicine. The growing demand for customized functional foods and dietary supplements drives the market size for nutraceutical products which is poised to grow at a CAGR of 8.9% from 2020 to 2028. Nutraceutical compounds are nature-derived and are valued for their ability to promote quality of life, health, and longevity. Interestingly, the combination of certain nutraceuticals gives synergistic benefit for bioavailability enhancement, and to reduce the outset of inflammation and oxidation. The development of co-delivery carriers for these synergistic nutraceuticals is important to enhance their stability, processability, and bioavailability. Co-delivery carriers can be designed to alter the release profile of individual nutraceuticals to derive specific health benefits from synergism. The novel encapsulation approaches at scalable operations for co-delivery of synergistic compounds at micro and nanoscale is the demand for both and nutraceutical and pharma industry. Also, encapsulation approaches like matrix, multi-compartment, and core-shell structure are important to alter the release profile and stability of encapsulated bioactives. This talk will provide insight on micro and nanoscale core-shell carrier development using food macromolecules for two potent synergistic nutraceuticals (curcumin and resveratrol). Core-shell alginate microparticles of ~ 8µm using three fluid nozzle spray drying approach and zein-PEG and Zein-ethyl cellulose core-shell nanoparticles (~300 nm) by the electrohydrodynamic operation were developed. The characteristics of core-shell encapsulate to alter the properties of encapsulated bioactives, release profile, bioavailability enhancement and the scalability of the process will be discussed. These particles enhanced the intestinal permeability of resveratrol by 2.2-fold and curcumin by 3.5-fold, compared to its native form. Moreover, customization of these nutraceuticals carriers in a 3D printed food matrix for personalized delivery of synergistic nutraceuticals will be presented.

A010 Chitin nanofiber stabilized Pickering emulsions with potential in encapsulation of antibacterial essential oils Yao Huang1, huangyao@cug.edu.cn, Hui Liu1, Shan Liu1, Sheng Li2. (1) China Univ. of Geosciences, Wuhan, China (2) Hubei Gedian Humanwell Pharmaceutical Excipients Co., Ltd, Ezhou, China With increasing consumption demand on products with lower synthetic contents and less environmental risk, novel preservation techniques utilizing natural antimicrobials have become the new trend in the food industry. In the present work, surfactant-free essential oil o/w emulsions were successfully fabricated from Cinnamon cassia oil with partially deacetylated chitin nanofiber (ChNF) adopted as a Pickering stabilizer. The emulsions displayed high stability against coalescence during a storage period of 90 days. The possible mechanisms for the emulsion stabilization were suggested to be the ChNF adsorption at the oil-water interfaces and the subsequent formation of an inter-droplet network by self-assembly of ChNF in the continuous phase, which was further strengthened by the formation of imine bond by the reaction between aldehyde groups from the cinnamon oil and amino groups on ChNF. Furthermore, the in vitro experiment confirmed the antimicrobial performance of the emulsions against E. coli. Although the addition of ChNF seemed to reduce the bactericidal kinetics of the emulsion, enhanced diffusion efficiency of the emulsions were observed on agar disc when compared to that of the pure cassia oil, which would be beneficial for its application in aqueous medium. Meanwhile, controllable release of the cassia oil with extended shelf time was also achieved through the ChNF encapsulation. The present work evidences the potential of biopolymer nanoparticles as both emulsion stabilizers and encapsulation materials for essential oil delivery, which might find their application in food preservation, drug delivery and related field.

A011 Storage stability and loss of resveratrol in protein particles: loading, antioxidant activity and oxidation sensitivity Xin Yin, 445724684@qq.com, Li Liang. Jiangnan Univ. School of Food Sci. and Tech., Wuxi, Jiangsu, China Whey protein isolate (WPI), sodium caseinate (SC) and soy protein isolate (SPI) were used as model carriers to complex with resveratrol in the form of nanoparticles. Their effects on the storage stability of resveratrol were studied in terms of antioxidant activity, polyphenol loading capacity and protein oxidation. The antioxidant activity of proteins and load efficiency of resveratrol ranked in the order of SC>SPI>WPI, which were inconsistent with their impact on the polyphenol storage stability. The effect of proteins on the storage stability of resveratrol was mainly dependent on their oxidation. The oxidation degree of proteins ranked in order SPI>SC>WPI. The co-oxidation of resveratrol with SPI and SC occurred during storage. The oxidation of WPI was the least and not affected by resveratrol. WPI improved the storage stability resveratrol, but SPI accelerated the loss of resveratrol, while the impact of SC on resveratrol stability basically changed from protective to harmful effect. The data gathered here should help guide the design of protein-based carriers for the protection of polyphenols.

A012 Fabrication of hollow zein composite particles with sodium tripolyphosphate for the encapsulation of quercetin Muhammad Aslam . Khan2,1, 8202001246@jiangnan.edu.cn, Li Liang2,1, liliang@jiangnan.edu.cn. (1) School of Food Sci. and Tech., Jiangnan Univ., Wuxi, Jiangsu, China (2) State Key Laboratory of Food Sci. and Tech., Jiangnan Univ., Wuxi, Jiangsu, China Hollow zein particles emerged as an alternative to solid particles for the encapsulation and delivery of food bioactives due to the remarkable encapsulation and sustained release capabilities of bioactives. To date, hollow zein particles were fabricated with sodium carbonate templet and employed to encapsulate and deliver bioactives, which are more resistant to degradation in the high alkaline condition caused by the disintegrated sodium carbonate templet. Therefore, there is an urgent need to explore an alternative to sodium carbonate templet. Herein, we proposed sodium tripolyphosphate (STP) as a sacrificial templet to fabricate bare and composite hollow zein particles. TEM micrograph showed a distinct lighter hollow core with a darker shell. The size of hollow zein particles developed using STP was concentration-dependent, and the particles having the smallest diameter of 105 nm were obtained at 1.5 mg/mL of STP with a ζ-potential of -27 mV compared to solid particles with 172 nm and -35 mV prepared under identical conditions. Upon coating with casein/chitosan complex, the size of both hollow and solid particles increased to 142 and 196 nm, with a reversal of ζ-potential to 43 and 40 mV, respectively. The encapsulation efficiency of quercetin in bare and coated hollow zein particles was about 29 and 24% higher than that of solid ones. Moreover, the loading capacity of quercetin in hollow and solid zein particles was 3.8 and 2.5 %, respectively. These findings suggest that the hollow zein particles fabricated employing novel sacrificial templet expand their application as carriers for the encapsulation and delivery of delicate bioactive compounds in functional foods.

A013 Rapid visible light-mediated crosslinking of casein-based hydrogels to facilitate wound healing Qinchao Zhu1, 1285307720@qq.com, Xuhao Zhou3, Ziyi Hu1, Wangbei Cao2, Kang Yu2, Tanchen Ren3, Daxi Ren1. (1) Inst. of Dairy Science, Zhejiang Univ., Hangzhou, Zhejiang, China (2) Zhejiang Univ., Hangzhou, China (3) Dept. of Cardiology of The Second Affiliated Hospital of Zhejiang Univ. School of Medicine, Hangzhou, China

At present, wound infection is a crucial health problem for people. Wound infection can not only hinder healing but also result in serious complications. Hydrogel dressings normally provide an appropriate and humid environment to expedite cell thriving and wound healing, while the wound can still keep active and exudation can be exhausted. In this study, casein, which was be biocompatible, biodegradable, renewable, readily available, inexpensive and non-toxic, was chosen as the raw material for the synthesis of hydrogel. The di-tyrosine bond was formed in casein to synthesize hydrogels by a visible light-mediated photoredox system. The physicochemical properties of the casein-based hydrogels were investigated by gelation kinetics, scanning electron microscopy (SEM) observation, infrared spectra analysis, mechanics analysis, adhesion test and swelling ratio test. This photomediated system rapidly crosslinks casein (<1 min), allowing 3D printing of constructs with high resolution features, in the range of 50-100 μm. The results showed that the hydrogels can quickly stanch after short tail and shorten the wound healing time of skin defect in mice. This demonstrates that the hydrogels hold potential for hemostasis and wound healing therapy.

A014 Casein-propylene glycol alginate complexes: Formation, stability, and properties for preparation of high internal phase emulsions Nan Li, nli20@vols.utk.edu, Qixin Zhong. Dept. of Food Science, UT AgResearch, Knoxville, Tennessee Protein-polysaccharide nanocomplexes are commonly studied to improve the acidic stability and have recently been studied for formation of high internal phase emulsions with an oil volume fraction of higher than 73%. In the present paper, we present recent studies on casein-propylene glycol alginate (PGA) complexes formed with both non-covalent and covalent interactions. A pH-cycle method was used to prepare casein- PGA complexes by first increasing pH to 11-12, followed by acidification to pH 7.0 or 4.5, near pH 4.6 - the isoelectric point of caseins. At alkaline pH, hydrolysis of ester bonds of PGA led to formation of alginate and covalent casein-alginate conjugates via the transacylation reaction. The covalent conjugate and remainder casein and alginate formed nanocomplexes, and the properties of nanocomplexes were a function of the casein:PGA mass ratio studied from 4:1 to 1:2. At 1% w/v casein, a greater extent of conjugation was observed at a higher content of PGA, and the increased dispersion clarity was observed at both pH 7.0 and 4.5. The hydrodynamic diameter at pH 7.0 was smaller at a lower content of PGA, whereas the hydrodynamic diameter at pH 4.5 was the smallest when the casein:PGA mass ratio was 2:1. Morphology analysis further suggested the importance of particle mass density to dispersion clarity. Molecular force analyses suggested that both covalent and non-covalent (mainly electrostatic and hydrophobic) interactions contributed to complex formation and dispersion stability. The complexes formed with casein:PGA mass ratio of 2:1 were capable of stabilizing emulsions with 80% (v/v) soybean oil without macroscopic phase separation during 7-d storage at room temperature. The high internal phase emulsion had the gel-like structure visually which was supported by rheological and microscopy data. Casein-PGA complexes may find unique applications in protein beverages and emulsion products such as mayonnaises.

A015 High protein content casein-alginate conjugates produced by transacylation reaction as novel emulsifiers Nan Li, nli20@vols.utk.edu, Qixin Zhong. UT AgResearch, Knoxville, Tennessee Polypeptide-containing polysaccharides such as gum arabic are emulsifiers but have the limited polypeptide content (typically <10%). Although Maillard-type conjugates with a relatively high content of proteins have shown the improved emulsifying properties, Maillard reaction is time-consuming and produces numerous undesirable byproducts, even after the conjugation. In our work, covalent casein-alginate conjugates were synthesized by the transacylation reaction, and the purified conjugates had exceptional properties emulsifying and stabilizing corn oil. Conjugation was done by mixing 1% w/v propylene glycol alginate (PGA) and different amounts of sodium caseinate (NaCas) for 2 h at pH 11.0. After dialysis to remove free molecules, NaCas-alginate conjugates with 52.8%, 66.2%, and 76.5% NaCas were prepared at NaCas:PGA mass ratios of 1:2, 1:1, and 2:1, respectively. The purified conjugates were capable of emulsifying corn oil at a low surfactant-to-oil ratio (SOR) of 0.75:100 (w:v), and the emulsions were stable at a wide range of pH and ionic strength, as well as after thermal pasteurization. A higher content of NaCas in the conjugate resulted in smaller oil droplets, whereas the alginate content was critical to the stability of oil droplets through electrostatic and steric mechanisms. To further illustrate structure-function correlations, individual α-, β-, and κ-caseins were conjugated with alginate, corresponding to protein content of 39.17%, 37.78%, and 23.14%, respectively. Similar to the NaCas conjugates, emulsions with a low SOR of 1:100 (w:v) were stabilized by individual casein conjugates, with smaller droplets at a higher protein content of conjugates. The emulsions had much lower SORs than those utilizing Maillard-type conjugates (SOR = 1:21-1:4) and did not have the undesirable color. Since the transacylation reaction is fast, is easy to scale-up, and does not produce byproducts, the casein-alginate conjugates have the potential for use as novel emulsifiers with tunable properties.

A016 Antibiotic discovery by means of computers Cesar de la Fuente, cfuente@pennmedicine.upenn.edu. Psychiatry, Univ. of Pennsylvania Perelman School of Medicine, Philadelphia Machines have the potential to outperform humans and revolutionize our world. In this talk, I will describe our efforts using machines to develop computational approaches for antibiotic discovery. Computers can already be programmed for superhuman pattern recognition of images and text. In order for machines to discover novel antibiotics, they have to first be trained to sort through the many characteristics of molecules and determine which properties should be retained, suppressed, or enhanced to optimize antimicrobial activity. Said differently, machines need to be able to understand, read, write, and eventually create new molecules. I will discuss how we trained a computer to execute a fitness function following a Darwinian algorithm of evolution to select for molecular structures that interact with bacterial membranes, yielding the first artificial antimicrobials that kill bacteria both in vitro and in relevant animal models. My lab has also developed pattern recognition algorithms to mine the human proteome, identifying throughout the body thousands of antibiotics encoded in proteins with unrelated biological function, and has applied computational tools to successfully reprogram venoms into novel antimicrobials. Computer-generated designs and innovations at the intersection between machines and biology may help to replenish our arsenal of effective drugs, providing much-needed solutions to global health problems caused by infectious diseases.

A017 Experiences in algorithm based chemical process optimization and early attempts towards closed loop automation Søren Bertelsen, sorenbertelsen@gmail.com. Advanced Analytics, Novo Nordisk A/S, Malov, Denmark Chemists from Novo Nordisk A/S have initiated several optimisation projects using machine learning tools and robotics as alternatives to traditional design of experiments (DoE) methodologies and hands-on experiments. The reasoning is a pursuit to find better optima using fewer resources. Specifically, we have successfully applied Bayesian Optimization (BO) to a number of process optimizations in various areas such as synthetic chemistry, analysis development, stem-cell research, microbial cultivation, formulation development and others. BO is an iterative process optimization technique in which no prior data is required to get started. In essence, BO helps ensure that the experimentalists are performing the experiment from which we can learn the most (or

which has the highest likelihood of being the optimal setting). We will present a few use cases including a chemical setup but also highlight the applicability of the code in other domains by showing the optimization of a recipe for an American brownie (a popular cake). Perspectives are drawn to our development of self-thinking robots that are able to autonomously optimize enzymatic transformations given a set of constraints and objectives. We are building an easy-to-use interface to Bayesian Optimization that will empower the domain experts to apply advanced machine learning while having little or no prior knowledge in coding. The code and user-interface are open-source.

A018 Use of machine learning to navigate the sequence-activity landscape during directed evolution campaigns Oscar Alvizo, oscar.alvizo@codexis.com. Computational Biology, Codexis, Redwood City, California Directed evolution has proven to be a powerful tool in the engineering of proteins, and in particular enzymes. It is often the case that dozens of genetic mutations are required to optimize an enzyme's performance for a specific application. With most mutations being deleterious, the incorporation of so many modifications require a guided approach to traverse sequence space to ensure that only the most promising mutations are included. Machine learning techniques can play a key role in navigating through the multi-dimensional landscape of sequence-activity space. The power of software will be highlighted in the development of successful programs that have led to commercially relevant enzymes in the in the food, pharmaceutical and biotherapeutic fields.

A019 Landscape view: The application of artificial intelligence in agricultural and food chemistry research Zachary J. Baum, ZBaum@cas.org. Chemical Abstracts Service, 2540 Olentangy River Road, Columbus, Ohio Artificial intelligence (AI) shows promise for optimizing agricultural strategies to promote sustainable development in a rapidly changing environment. Even as AI is being applied in agricultural and food chemistry (AGFD) alongside virtually all other chemical disciplines, the most prevalent use cases may not be apparent to many who are focused on their respective research interests. Here, the CAS content collection, covering chemistry from over 50,000 journals, 64 patent authorities, and many other sources, is analyzed as a corpus of literature to reveal current trends and future opportunities for AI in AGFD. We contextualize the current research landscape of AI in AGFD by classifying and quantifying all AI-related publications from 2000 to 2021, allowing comparisons to other areas of chemistry. AI applications in various AGFD research focuses, their prevalence, and their connections to non-agriculturally focused chemistry are discussed. Our work may assist researchers working in AI-amenable AGFD to identify growth opportunities, potential collaborations, and emerging work in underdeveloped areas.

A020 Catalyzing AI-driven research for U.S. agriculture Brian Stucky, brian.stucky@usda.gov, Debra C. Peters. SCINet Big Data Program, Office of National Programs, USDA Agricultural Research Service, Beltsville, Maryland Recent advances in artificial intelligence (AI) are finding increasing application in a wide range of agricultural research, including in agricultural and food chemistry. New, agency-wide initiatives in the USDA's Agricultural Research Service (ARS) are accelerating AI-driven research by expanding access to high-performance computing, AI expertise, and relevant training resources. In this presentation, I will discuss these initiatives by first presenting a high-level, computationally oriented overview of modern AI methods. Next, I will describe key AI-related efforts currently underway at the ARS. I will conclude by sharing several concrete examples of how AI methods are helping transform ARS research, in agricultural and food chemistry and beyond.

A021 Democratizing AI to build solutions for the farms of the future Steven B. Mirsky, steven.mirsky@usda.gov. Sustainable Agricultural Systems Laboratory, US Dept. of Agriculture, Beltsville, Maryland The Farm of the Future will need to have improved productivity, efficiency, and be regenerative. Researchers and farmers will increasingly rely on technology to accomplish these goals, the former through highly coordinated transdisciplinary research teams and the latter through increased precision and automation of all aspects of food production from farm to fork. The Precision Sustainable Agriculture (PSA) team provides a good framework for how to conduct coordinated national on-farm and on-station research, extension, and education. This team is quantifying how climate, soil, management, genetic and social factors interact, and provide site-specific solutions to growers. The site-specific solutions come in the form of decision support tools that provide growers with near real-time decision making and for long-term planning. This has been accomplished through the development of automated data acquisition, aggregation, analytics (AI and machine learning), and visualization. Integration of IoT sensing systems (internet of things) has been central to this enterprise. This symposium presentation will review key aspects of PSA and how it uses technology to build solutions for the farm of the future.

A022 Glucan phosphorylase as useful bio-catalyst for precision synthesis of amylose and its analogs Jun-Ichi Kadokawa, kadokawa@eng.kagoshima-u.ac.jp. Dept. of Chemistry and Biotechnology, Kagoshima Daigaku, Japan Amylose is one of representative natural polysaccharides as a component of starch, which is composed of α(1→4)-linked glucose repeating units. Amylose with well-defined structure is synthesized by glucan phosphorylase (GP)-catalyzed enzymatic polymerization of α-D-glucose 1-phosphate (Glc-1-P) monomer. The polymerization occurs from the chain end of maltooligosaccharide as a primer with liberating inorganic phosphate. The resulting amylose is readily precipitated in aqueous reaction media, owing to the formation of double helical assembly. As complete separation of amylose from the other component, amylopectin, in natural starch is difficult, the GP-catalyzed polymerization is a very useful method to obtain a pure amylose sample. As GP shows weak specificity for the recognition of substrates, furthermore, the author has found that the enzyme isolated from thermophilic bacteria (Aquifex aeolicus VF5) catalyzes the enzymatic polymerization of analog substrates of Glc-1-P as monomers, which are composed of different monosaccharide residues, to produce unnatural polysaccharides (amylose analog polysaccharides) comprising the corresponding α(1→4)-linked monosaccharide units (Scheme 1). For example, the GP catalyzes the enzymatic polymerization of α-D-glucosamine 1-phosphate (GlcN-1-P) monomer to produce an aminopolysaccharide composed of α(1→4)-linked GlcN repeating units. The new amylose analog aminopolysaccharide has been named 'amylosaime'. Amylosamine is water-soluble polysaccharide, different from amylose, but has formed a water-insoluble double helical assembly with an anionic polysaccharide, amylouronic acid, having carboxylate groups.

A023 Mucorales as promising oleaginous fungi to produce high value of γ linolenic acid and carotenoids Hassan Mohamed1,2, hassanmohamed85@azhar.edu.eg, Yuanda Song1. (1) Agriculture Engineering and Food Science, Shandong Univ. of Technology, Zibo, Shandong, China (2) Botany and Microbiology, Al-Azhar Univ. - Assiut Branch, Assiut, Assiut, Egypt γ-linolenic acid (GLA) and carotenoids, have attracted much interest due to their nutraceutical and pharmaceutical importance. Mucoromycota, typical oleaginous filamentous fungi, are known for their production of valuable essential fatty acids and carotenoids. In the present study, 81 fungal strains were isolated from different Egyptian localities, out of which

11 Mucoromycota were selected for further GLA and carotenoid investigation. Comparative analysis of total lipids by GC of selected isolates showed that GLA content was the highest in Rhizomucor pusillus AUMC 11616.A, Mucor circinelloides AUMC 6696.A, and M. hiemalis AUMC 6031 that represented 0.213, 0.211 and 0.20% of CDW, respectively. Carotenoid analysis of selected isolates by spectrophotometer demonstrated that the highest yield of total carotenoids (640 μg/g) was exhibited by M. hemalis AUMC 6031 and M. hemalis AUMC 6695 and these isolates were found to have a similar carotenoid profile with, β-carotene 65%, zeaxanthin 34 %, astaxanthin, and canthaxanthin 5 % of total carotenoids. The total fatty acids of all tested isolates showed moderate antimicrobial activity against Staphylococcus aureus and Salmonella Typhi, and Penicillium chrysogenum. To the best of our knowledge, this is the first report on the highest yield of total lipid accumulation (51.74% CDW) by a new oleaginous fungal isolate R. pusillus AUMC 11616.A. A new scope for further study on this strain will be established to optimize and improve its total lipids with high GLA production. So, R. pusillus AUMC 11616.A might be a potential candidate for industrial application.

A024 Extraction of soybean polysaccharide using immobilized cellulase Jie Liu, liujie@zzu.edu.cn, Yitong Dong, Zhilu Rao, Keyong Tang. Zhengzhou Univ., China Soluble soybean polysaccharide (SSPS), a polysaccharide extracted from soy cotyledons, has great potential for applications in food industry. The major component of SSPS composed of short-chain homogalacturonan and long-chain rhamnogalacturonan backbones with a number of branches, including sugar chains of β-1,4-galactans and α-1,3- or α-1,5-arabinans. SSPS has excellent physico-chemical properties. It has been used to stabilize acid milk dispersions and oil emulsions as additives, and to pack food products as thin films. The present study aimed to analyze the effect of immobilized cellulase on the quality and property of the extracted SSPS. The immobilized cellulase was capable to increase the extraction rate of SSPS under optimized conditions. The physical properties of the films made from the extracted SSPS were investigated.

A025 Biotechnological research to enhance the growth and docosahexaenoic acids (DHA) production of marine heterotrophic microalgae, Aurantiochytrium sp. Yusuf Nazir, yusufnazir91@yahoo.com. Dept. of Food Sciences, Univ. Kebangsaan Malaysia, Bangi Lipid derived from microalgae has attracted considerable interest worldwide as a promising alternative source to fish oil especially for the production of polyunsaturated fatty acids (PUFAs), such as DHA; an important omega-3 PUFAs that has been recognized to play a vital role in human health and development. Aurantiochytrium sp., a marine heterotrophic microalga that can produce a substantial amount of DHA is shown to be an ideal candidate to be developed and exploited for the industrial-scaled production of DHA. Nevertheless, there are two major challenges in developing this microalga based DHA at the industrial level:1) low production yield, 2) exorbitant production cost primarily due to the costly substrate. Hence, several biotechnological approaches have been developed to address these issues including screening and optimization of key cultivation parameters, strategic exogenous addition of phytohormones, utilization of low-cost, safe, and extensively abundant fruit extracts (FEs) as alternative carbon sources as well as the development of mutants with superior oxidative defence, growth and DHA biosynthetic capacity by plasma mutagenesis. The combination of these parameters coupled with feeding of key nutrients and strategic shift of dissolved oxygen (DO) levels in 5L scale production has resulted in a 21-fold increment of DHA production with a lower production cost as compared to prior of the study, indicating that these biotechnological approaches can be a prototype to the production of DHA by Aurantiochytrium sp at industrial level.

A026 Potential sophorolipid uses in antimicrobial applications Richard Ashby1, rick.ashby@ars.usda.gov, Xuetong Fan1, Ocen Olanya1, Mehmet Ozdener2. (1) USDA Agricultural Research Service, Wyndmoor, Pennsylvania (2) Monell Chemical Senses Center, Philadelphia, Pennsylvania Widespread use of antibiotics has resulted in an increasing issue associated with microbial resistance. As such, efforts are underway to discover new antimicrobial products that are not currently related to the resistance phenomena. Sophorolipids (SL) are microbially produced glycolipids that have been documented to possess antimicrobial properties. The antimicrobial nature of these molecules is primarily centered against Gram+ bacteria but at sufficient concentrations can also inhibit Gram- bacteria. In addition, recent work has demonstrated that SL can also block the bitter taste response in the mammalian tongue. In this presentation, SL use as an antimicrobial agent will be discussed as it pertains to its effects on the bacterial strains associated with some of the more common food-borne and dermal ailments as well as the implication of blocking the bitter taste response for use in oral applications.

A027 Biofunneling and functionalization of agricultural waste polymers to advanced platform chemicals Lahiru N. Jayakody1,2, lahiru.jayakody@siu.edu, Ken Anderson3, Lakshika Dissanayake1, Sandipty Kayastha1, Derek Perry3, Ligon Ryaan1. (1) School of Biological Sceinces, Southern Illinois Univ. Carbondale (2) Fermentation Science Inst., Southern Illinois Univ. Carbondale (3) School of Earth Systems and Sustainability, Southern Illinois Univ. Carbondale Advanced bio-based, biodegradable polymers are vital to a circular material economy for the agriculture system, while also minimizing global plastic pollution, high energy consumption, and greenhouse gas emissions associated with synthetic polymer production via petroleum-based feedstocks. Many studies bio-based polymers also exhibit superior performance relative to petroleum-based equivalents. We have developed an innovative thermo-biochemical approach to produce biofunctionalized advanced platform chemicals by leveraging oxidative hydrothermal dissolution (OHD) and engineered microbes. First, we developed an OHD process to depolymerize biomass and synthetic polymers into simple aliphatic and aromatic compounds without using expensive catalysts or harsh solvents. For instance, we are able to solubilize >90% of carbon in corn stover and polyethylene terephthalate into microbially accessible substrates. Next, we engineered the robust none-model microbial host P. putida EM42 and the novel catabolic powerhouse, E. aphidicola LJJL01, to biofunnel the heterogeneous organics present in the OHD streams into high-value platform chemicals. We metabolically engineered the strains to expand substrate utilization, enhance chemical toxicity tolerance, and produce tailored advanced platform chemicals such as cis,cis-muconate, β-keto adipate, and 2,3 butanediol from OHD-derived substrates. The developed novel Thermo-bio hybrid process enables the efficient valorization of waste carbon generated in the agricultural system and enables a circular material economy with profound environmental, energy, and economic impacts.

A028 Increase in lipid and DHA production by Aurantiochytrium Sp. under the influence of chemical inducers Majher Sarker, majher01@yahoo.com, Syed Hussain. USDA ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania Aurantiochytrium sp ATCC PRA-276 strain is known to produce lipid and docosahexaenoic acid (DHA) in bio-synthetic process. In this study, five different chemicals; 2-phenylacetic acid (PAA), humic acid, spermidine, 1 methylcyclopropene, and ferric were evaluated for their influences on Aurantiochytrium sp to increase it's production of lipid

and DHA. After 120 h of cultivation, the individual supplementation of PAA, HA, and FC, increased the biomass, total lipid and DHA production of Aurantiochytrium PRA-276 by 32%–76%, 23%-34%, and 53%–86% in comparison to the control, respectively. The highest biomass and DHA productivities were observed with the supplementation of PAA and FC achieving 76% and 67% and 86% and 66%, compared to the control, respectively. This study suggests that the introduction of aforementioned bio-stimulants can increase the productivity of Aurantiochytrium sp to obtain better yields of lipid and DHA which will lead to economic-feasibility for large scale production.

A029 Construction of medium-chain fatty acids (MCFAs) cell factory via metabolic engineering of Mucor circinelloides Syed Hussain, ammarshah88@yahoo.com, Yuanda Song. School of Agriculture Engineering and Food Science, Shandong Univ. of Technology, Zibo, China Concerns about global warming, fossil-fuel depletion, food security, and human health have promoted metabolic engineers to develop tools/strategies to overproduce microbial functional oils directly from renewable resources. Medium-chain fatty acids (MCFAs, C8–C12) have been shown to be important sources due to their diverse biotechnological importance, providing benefits ranging from functional lipids to uses in bio-fuel production. However, oleaginous microbes do not carry native pathways for the production of MCFAs, and therefore, diverse approaches have been adapted to compensate for the requirements of industrial demand. Mucor circinelloides is a promising organism for lipid production (15–36% cell dry weight; CDW) and the investigation of mechanisms of lipid accumulation; however, it mostly produces long-chain fatty acids (LCFAs). To address this challenge, we genetically modified strain M. circinelloides MU758, first by integrating heterologous acyl-ACP thioesterase (TE) into fatty acid synthase (FAS) complex and subsequently by modifying the β-oxidation pathway by disrupting the acyl-CoA oxidase (ACOX) and/or acyl-CoA thioesterase (ACOT) genes with a preference for medium-chain acyl-CoAs, to elevate the yield of MCFAs. The resultant mutant strains (M-1, M-2, and M-3, respectively) showed a significant increase in lipid production in comparison to the wild-type strain (WT). MCFAs in M-1 (47.45%) was sharply increased compared to the wild type strain (2.25%), and it was further increased in M-2 (60.09%) suggesting a negative role of ACOX in MCFAs production. However, MCFAs in M-3 were much decreased compared to M-1, suggesting a positive role of ACOT in MCFAs production. The M-2 strain showed maximum lipid productivity (~1800 milligram per liter per day or mg/L.d) and MCFAs productivity (~1100 mg/L.d). Taken together, this study elaborates on how the combination of two multidimensional approaches, TE gene over-expression and modification of the β-oxidation pathway via substantial knockout of specific ACOX gene, significantly increased the production of MCFAs. This synergistic approach ultimately offers a novel opportunity for synthetic/industrial biologists to increase the content of MCFAs.

A030 Bioactive components in parabiotic kefir lactic acid bacteria and obesity Hyunsook Kim1, hyunsk15@hanyang.ac.kr, Eseul Kim1, Sanghoon Han1, Kun Ho Seo2. (1) Hanyang Univ., Seongdong-gu, Seoul, Korea (the Republic of) (2) Konkuk Univ., Gwangjin-gu, Seoul, Korea (the Republic of) Anti-obesity action of nonviable probiotic lactic acid bacteria (PLAB) may be attributed to bacterial cellular components recognized by host cells. Anti-inflammation and anti-obesity properties of surface layer proteins (SLPs) that are cellular components isolated from kefir PLAB were determined in macrophage RAW 264.7 cells and obese mice. Kefir SLPs significantly decreased secretion of IL-6 and production of NF-kB p65 protein by LPS-stimulated RAW 264.7 cells in a dose-response manner. C57BL/6J mice were fed a high-fat (HF) diet with oral administration of either saline (CON) or kefir SLPs for six weeks. SLPs significantly reduced HF-induced weight gain and adipose tissue weight, plasma triglyceride concentrations, and insulin resistance. Profiling of adipocyte gene expression showed that anti-obesity effect was significantly related to expression of genes associated with adipogenesis, autophagy, and inflammatory/immune response, and fatty acid oxidation. Taken together, SLPs are a novel bioactive component in kefir PLABs to target obesity and obesity-related disorders.

A031 Egg white protein ovotransferrin prevents bone loss in ovariectomized rats Nan Shang, Jianping Wu, jwu3@ualberta.ca. Univ. of Alberta, Edmonton, Canada Ovotransferrin, an iron-binding glycoprotein, accounting for ~12% of egg white protein, is a member of transferrin family. As a component of innate immunity, ovotransferrin was reported to have antimicrobial, anti-viral, anti-oxidant, and immunomodulatory activities. Using mouse preosteoblast MC3T3-E1 cells, our previously study showed that ovotransferrin 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. Furthermore, ovotransferrin significantly inhibited osteoclastogenesis. The in vivo effects of egg white ovotransferrin on preventing menopausal-induced osteoporosis were investigated using ovariectomized (OVX) rats. The objectives of this work were 1) to evaluate the effects of ovotransferrin treatment on osteoporosis prevention by measuring bone mineral density and micro-architecture; 2) to investigate the regulatory role of ovotransferrin on bone metabolism by measuring the expression of bone formation/resorption biomarkers (representing the bone remodeling process), and the production of osteoclastogenesis associated cytokines. Oral administration of ovotransferrin did not affect body weight, food intake and organ weight. After 12-week treatment, rats supplemented with 1% w/w and 0.2% w/w of ovotransferrin 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 for bone health.

0A32 Improvement of probiotic survivability, persistence and colonization in gut by loading probiotic cells with plant extracts Rewa Rai2, rewarai.iitd@gmail.com, Marluci Silva2, Wallace H. Yokoyama1, Nitin Nitin2. (1) Western Regional Research Center, USDA Agricultural Research Service, Albany, California (2) Dept. of Food Sci. and Tech., Univ. of California Davis Evolutionary bi-directional relationship between gut microbes and plant phenolic bioactives have significantly benefited human health. Despite significant health beneficial impact, delivery of probiotic bacteria and phenolic bioactives to the gut and their ability to persist and interact with the gut microflora is a key constraint that limits their potential. This study focused on the vacuum infusion of phenolic bioactives derived from fruit skin extracts or in purified form into live probiotic bacteria to provide a novel approach to address the challenges of enhancing delivery of both probiotics and plant phenolics to the gut. The phenolic bioactives isolated from the skins of a tropical fruit (jabuticaba) and purified phenolic compound (Catechin) were infused in probiotic cells using our patented vacuum infusion process. The survivability of three different strains of lactobacillus cells with infused isolated and purified phenolics was evaluated during the simulated gastrointestinal digestion. The metabolic activity and the

antagonistic effect of the bacteria with infused probiotics were evaluated using resazurin assay and an agar spot method. Further, the persistence and colonization of catechin infused Lactobacillus Casei strain were evaluated using mouse model. Results demonstrated approximately 103 folds improvement in survivability of probiotic cells with infused phenolics after the simulated gastric and intestinal digestions. Infusion of phenolics in cells did not significantly influence the metabolic activity of the bacteria as well as their ability to suppress the growth of pathogenic organisms. In-vivo results demonstrated significant (90% (1 log) or more) enhancement in persistence of catechin infused cells compared to the control bacteria without infused phenolic compound. Overall, this study validates the unique food grade composition developed by the infusion of phenolic bioactives in probiotic cells to enhance their resistance against gastro-intestinal conditions and persistence and colonization in the gut.

0A33 Reformulating traditional Mediterranean foods: A functional tomato product Berkay Berk, Melis Çetin, S. Gulum Sumnu, Behic Mert, Ozlem Ozarda, Mecit Oztop, mecit@metu.edu.tr. Dept. of Food Eng., Orta Dogu Teknik Universitesi Muhendislik Fakultesi, Ankara, Ankara, Turkey Mediterranean Diet (MedD) is one of the cultural heritages of UNESCO. However, for the young generation, adherence to MedDiet has decreased significantly. To reattract these consumers, reformulating traditional Med food is considered as a strategy. One of the main contributors to the MedD is definitely tomato. Tomatoes and their derived products are known to have strong antioxidant, anti-inflammatory, and anticancer activities. According to the 2019 statistics of Mediterranean International Association of the Processing Tomato (AMITOM)7, ~38 % of world tomato production took place in Mediterranean countries. Another important feature of the MedD is the olive oil. Although it is mostly consumed in the form of oil; the fruit itself is also very nutritive. The phenolics present in the olive are perfect ingredients to design functional foods. In this study, a functional food with Med ingredients have been designed. A salty tomato bar enriched with a specialized olive powder have been produced and characterized. Olive powder has been prepared by using high pressure homogenization followed by microwave vacuum drying. The snack bar was dried using a microwave vacuum dryer at different processing conditions. Antioxidant capacity, phenolic content of the olive powder and the snack bar was determined. In addition, lycopene content of the final samples was determined. Rheological and textural analysis were performed as well. Time Domain NMR, Magnetic Resonance Imaging were used to investigate the water absorption behavior of the formulated foods for shelf life analysis.

034 Bio-based micro and nanostructures for the delivery of bioactive compounds Miguel Cerqueira, miguel.cerqueira@inl.int. International Iberian Nanotechnology Laboratory, Braga, Portugal Micro- and nanoencapsulation using new and innovative technologies have emerged in the last ten years and have been explored for the protection and control release of bioactive compounds in foods. Electrohydrodynamic processing, nanospray dryer and ultrasounds are some technologies that can be used to produce structures with different shapes and sizes. Among the food industry, the use of bio-based materials such as polysaccharides, proteins and lipids are the most interesting, thus maintaining their food-grade status. The developed structures can be used as carriers and used to deliver and control release bioactive compounds. They can also be used to stabilize these compounds during food processing, decreasing the possible changes in their bioactivity. This work overviews some strategies for the encapsulation of bioactive compounds (e.g. vitamins, pro-vitamins, curcumin, caffeine, iron and quercetin) using well-known and innovative encapsulation technologies and food-grade materials (e.g., whey protein, corn zein, lactoferrin, hydroxypropyl methylcellulose, rhamnolipids). Microparticles, nanoparticles, nanofibers, nanohydrogels, lipid-based and multilayer nanosystems are presented being their main properties (size, polydispersity and zeta potential) disclosed and related with their behaviour under different environments (pH and temperature). Furthermore, it is explored how a reverse engineering approach, through two main steps, can be used to design structures for the encapsulation of bioactive compounds.

A035 In planta encapsulation of macro-nutrients for enhanced nutritional functionality Sushil Dhital, sushil.dhital@monash.edu. Chemical and Biological Engineering, Monash Univ., Clayton, Victoria, Australia Food macro-molecules in planta are enclosed within cells encapsulated by cellulosic and pectic cell walls. The intactness of these “natural capsules” modulates the metabolic responses, digestion and fermentation in the GI tract. The structure of the capsule, however, depends on physical and thermal processing. Using this lowest structural level, “intact plant cell”, we demonstrated how the alteration of cellular structure could affect the in-vitro digestion of starch and protein, change in the rate of fermentation, production of metabolites (e.g. short-chain fatty acids) and alteration in gut-microbial population. Intact pulse cells were isolated and subjected to physical force (shearing) to completely destroy the barrier and thermal processing at varying temperatures for a controlled increase in the cell wall porosity. The physically altered cells were subjected to standard in-vitro digestion and faecal fermentation using human faeces as the inoculum. The rate of digestion of starch, protein, rate of fermentation, generation of metabolites (short-chain fatty acids) and shift in the microbial population (phylum, genus and species) were investigated. The cell wall provided a strong barrier for enzyme diffusion during in-vitro digestion. Thus the rate and extent of starch and protein digestion were significantly higher for broken cells compared to intact cells. The effect, however, was more pronounced for starch compared to proteins, suggesting the slow protease action on less denatured proteins. With the increase in cell porosity using the thermal process, the rate of fermentation, production of SCFA and microbial diversity increased. Most noticeably, a significant rise in Bifidobacterium was observed with an increase in porosity of pulse cells, consistent with increased SCFA production. The result shows that the cell wall provides a barrier for intestinal digestion and colonic fermentation, and increased porosity induces catalysis of macro-nutrients due to more accessible substrate. Thus, desired glycaemic response and colonic fermentation profiles can be achieved with the controlled processing of whole foods for enhanced metabolic and gut health

0A36 Eugenol cyclodextrin inclusion complex encapsulated pullulan nanofibers for potential food packaging applications Asli Celebioglu, ac2873@cornell.edu, Tamer Uyar. Fiber Science and Apparel Design, Cornell Univ., Ithaca, New York Electrospinning is a feasible technique in order to develop a free-standing encapsulation and carrying matrix for the active compounds which are widely used in the food industry. This technique allows producing nanofibers from a large range of materials including the biopolymer of polysaccharides and their composites with other components. So, electrospinning enables to obtain sustainable materials by eliminating the environmental and health loadings originating from the use of synthetic products. On the one part, natural and non-toxic cyclodextrin molecules enable the improvement of the stability and solubility of the concerned active compounds by forming inclusion complexes. Thus, the integration of the phenomenon of electrospinning and cyclodextrin paves the way to form promising materials having the advantages parts of both electrospun nanofibers and cyclodextrin molecules. In our study, the inclusion complexes of eugenol-gamma cyclodextrin (γCD) were incorporated in pullulan nanofibers using the electrospinning technique. As a control sample, the pristine eugenol contained pullulan nanofibers were electrospun,

as well. The nanofibrous web of pullulan/eugenol-γCD nanofibers could preserve ~93% of this volatile essential oil compound due to inclusion complexation. On the other hand, only ~23% of eugenol was preserved in the case of pullulan/eugenol nanofibers. The inclusion complexation also provided enhanced thermal stability for eugenol and its volatilization shifted from ~50-190 °C to ~125–300 °C in case of pullulan/eugenol-γCD nanofibers. For the antioxidant performance, pullulan/eugenol-γCD and pullulan/eugenol indicated ~100% and ~58% radical scavenging activity for the same nanofiber concentration. Moreover, pullulan/eugenol-γCD nanofibers maintained the antioxidant activity even after 3-months storage at room temperature (~98%) and heat-treatment performed at 175 °C for 1 h (~93%). The time-dependent release test indicated that pullulan/eugenol-γCD nanofibers have a release profile in a relatively controlled manner compared to pullulan/eugenol nanofibers under the same experimental conditions. Briefly, pullulan/eugenol-γCD nanofibers can be quite a promising encapsulation and carrying matrix for the essential oils which are widely used in both food-related areas.

0A37 Salt reduction using food macromolecule carrageenan Yapeng Fang, ypfang@sjtu.edu.cn, Wei Lu, Zining Hu. Shanghai Jiao Tong Univ., Shanghai, China Hypertension and stroke caused by a high-sodium diet have overtaken cancer as the leading cause of death. Salt reduction has become an urgent problem in our food industry. Among different salt reduction strategies, potassium chloride-based salt substitute is an ideal one. However, potassium chloride has obvious metallic bitter taste, which seriously affects consumers' sensory experience and greatly limits its addition in salt. When the content of potassium chloride in salt is more than 20wt%, it will produce an obvious irritating bitter taste. How to cover the bitter taste without affecting the overall saltiness has become a bottleneck restricting the development of potassium chloride-based salt substitute. In this study, the specific binding of natural seaweed polysaccharides with potassium ions was skillfully utilized to successfully mask the bitter taste of potassium chloride-based salt substituted, and the overall saltiness was basically not affected. The maximum salt reduction could be achieved by 50wt%. Our subsequent in-vivo test confirmed that the salt substitute containing carrageenan can significantly increase potassium intake and reduce calcium loss while decrease sodium intake in mice. This salt substitute can also reduce the catecholamine and creatinine levels in blood, potentially leading to a decreased risk of hypertension and renal injury. In addition, we found this low sodium salt formula can notably improve hypertension induced by high-salt diet in rats and the level of hypertension-related serum biochemical indices. Furthermore, several kinds of liquid and solid foods prepared using the salt substitute showed similar saltiness and even higher sensory acceptability as compared with pure salt group. The results preliminarily verify the good prospect of the salt substitute in practical application.

A038 Room temperature encapsulation of functional ingredients vis high-throughput electrohydrodynamic technology Jose M. Lagaron, lagaron@iata.csic.es, Cristina Prieto. Novel Materials and Nanotechnologies Laboratory, Inst. of Agrochemistry and Food Technology, Paterna, Spain A novel high-throughput technology, termed as electrospraying assisted by pressurized gas (EAPG) is presented here. It is based on the atomization of the polymer solution by a pneumatic injector using compressed air that nebulizes within a high electric field. During this process, the solvent is evaporated at room temperature in an evaporating chamber and the encapsulated material is collected as a free-flowing powder. This technology is a versatile technique that presents multiple advantages compared to conventional encapsulation processes. For instance, it is carried out at room temperature, which reduces the denaturation of bioactive compounds, produces particles with high encapsulation efficiency, results in a reduced particle size with narrow size distribution, does not require a subsequent step to separate the particles from the medium, and it is highly versatile in terms of the encapsulating materials and bioactive compounds that can be processed. In this sense, this technology was first proven for the encapsulation of omega-3 rich oils in different natural biopolymeric matrices, being further proved for the encapsulation of polyphenols and probiotics. In addition, this technology allows achieving the production volumes required by commodity food applications. The current presentation will present this novel technology and highlight some case-studies for the stabilization and shelf-life extension of different functional ingredients using natural biopolymers as encapsulating matrices.

A039 Unraveling the potential of dry bean flour for utilization in the bakery industry Navneet Navneet, nnavneet@uoguelph.ca, mario martinez martinez, Iris Joye. Dept. of Food Science, Univ. of Guelph, Ontario, Canada Most beans in Canada end up in grocery stores and households as dry whole seeds, soups and canned beans. The utilization of dry bean flour is very limited due to its limited functionality and the off-flavours associated with its use. These problems can be tackled by processing bean flours using different physical or chemical treatments. Therefore, in this project, we aim to process whole navy beans into a functional flour using three processing technologies: high hydrostatic pressure (HPP), dry heat (DH), and extrusion technology. The effect of processing on the properties of bean flour was analyzed by compositional analysis, colour studies, molecular spectral data analysis and the determination of water absorption capacity, thermal properties, and rheological properties (aqueous slurries) of unprocessed and processed bean flour. Processing did not alter, as expected, the total ash, starch, and protein content of the bean flours. However, the processing of bean flour did not only result in significant colour variations, but also the molecular spectral data, water absorption capacity, thermal properties, and rheological properties of unprocessed, HPP, DH, and extruded flours were different, implying that flour processing led to changes in the protein/starch matrix. The molecular spectral data showed that flour processing modified the crystalline order in bean starch and the intensity of the amide group associated to bean protein. The water absorption capacity and thermal properties of unprocessed flour were different from that of processed flour. The rheological properties of flour showed a significant change in the elastic and viscous modulus and the gel strength. The processing of flour is expected to modify the major components of flour – starch and protein - thus, ultimately creating opportunities for using it in, e.g., the
bakery industry.

A040 Fate of curcumin-nanoemulsion and the bioaccessibility of curcumin during dynamic in vitro digestion within complex dairy matrices Aiqian Ye, a.m.ye@massey.ac.nz. Massey Univ. Riddet Inst., Palmerston North, Manawatu-Wanganui, New Zealand Nanoemulsions have been regarded as an excellent strategy to effectively deliver hydrophobic bioactive compounds, such as curcumin, in food products as well as improving bio-accessibility during digestion. However, relatively little research is available on the gastrointestinal behavior of these delivery systems within a complex food matrix. This presentation introduces the impact of gastric digestion behaviour of milk and two dairy gels containing curcumin nanoemulsion on intestinal lipid digestion and the bioaccessibility of curcumin. The gastric emptying and the release of oil droplets containing solubilized curcumin into intestinal digestion were influenced by the gel structure and the curd structure formed by milk during gastric digestion. The rennet gel restructured and became denser because of the action of pepsin and the low pH, thus slowing the outflow of both protein and oil droplets from the gel. In contrast,

the acid gel experienced rapid protein disintegration under gastric conditions, faster gastric emptying. All the milk systems formed a curd under dynamic in vitro gastric conditions induced by pepsin, but distinct characteristics of their curds induced by different preheat treatment influenced the gastric emptying of protein and entrapped emulsified nano oil droplets loading curcumin. The release rate of free fatty acid and the concentration of curcumin during intestinal digestion were linked with the compositional profile of the gastric digesta, while the bioaccessibility of curcumin was influenced by the gel structure and the gastric disintegration of the gels. This work highlights how various food matrix can govern the fate of added health promoting compounds, which significantly affect the functionality and application of these bioactive compounds.

A041 Eugenol/cyclodextrin inclusion complex encapsulated pullulan nanofibers for potential food packaging applications Tamer Uyar, tamer@unam.bilkent.edu.tr, Asli Celebioglu. Dept. of Human Ecology, Cornell Univ., Ithaca, New York Nanoemulsions have been regarded as an excellent strategy to effectively deliver hydrophobic bioactive compounds, such as curcumin, in food products as well as improving bio-accessibility during digestion. However, relatively little research is available on the gastrointestinal behavior of these delivery systems within a complex food matrix. This presentation introduces the impact of gastric digestion behaviour of milk and two dairy gels containing curcumin nanoemulsion on intestinal lipid digestion and the bioaccessibility of curcumin. The gastric emptying and the release of oil droplets containing solubilized curcumin into intestinal digestion were influenced by the gel structure and the curd structure formed by milk during gastric digestion. The rennet gel restructured and became denser because of the action of pepsin and the low pH, thus slowing the outflow of both protein and oil droplets from the gel. In contrast, the acid gel experienced rapid protein disintegration under gastric conditions, faster gastric emptying. All the milk systems formed a curd under dynamic in vitro gastric conditions induced by pepsin, but distinct characteristics of their curds induced by different preheat treatment influenced the gastric emptying of protein and entrapped emulsified nano oil droplets loading curcumin. The release rate of free fatty acid and the concentration of curcumin during intestinal digestion were linked with the compositional profile of the gastric digesta, while the bioaccessibility of curcumin was influenced by the gel structure and the gastric disintegration of the gels. This work highlights how various food matrix can govern the fate of added health promoting compounds, which significantly affect the functionality and application of these bioactive compounds.

A042 Electrospun biopolymeric nanofibers as nanocarriers of bioactive compounds Seid Mahdi Jafari1, smjafari@gau.ac.ir, Elham Assadpour2. (1) Gorgan Univ. of Agricultural Sciences and Natural Resources, Gorgan, Golestan, Iran (the Islamic Republic of) (2) Univ. de Vigo Facultad de Biologia, Vigo, Galicia, Spain Natural bioactive ingredients possess several features and functions; however, their stability, solubility, and bioavailability in food and drug systems and within the gastrointestinal tract is low, requiring encapsulation. The application of electrospinning processes to encapsulate and protect bioactive compounds with different biopolymers is considered as a promising and emerging method, which has attracted the attention of many researchers in recent years. Easy incorporation of bioactive compounds, being cost-effective, and the lack of heat are some important advantages. Thus, the main purpose of this study is investigating the efficacy of electrospinning to encapsulate natural bioactive compounds within nanofibers by application of various food biopolymers. Also, some information about the impact of biopolymers (proteins and carbohydrates) as wall materials employed in electrospinning methods have been discussed.

A043 Microencapsulation using whey protein isolate as wall material: Particle formation behaviour and interactions with core material Nan Fu, nan.fu@suda.edu.cn. Soochow Univ. College of Chemistry Chemical Engineering and Materials Science, Jiangsu, China Whey protein isolate (WPI) is a common wall material in the microencapsulation of bioactive substances through spray drying. As a kind of globule protein with remarkable amphipathic property, the capability of WPI to bind hydrophobic compounds and the adsorption of WPI molecules at oil/water and water/air interfaces have been extensively studied. During spray drying, the particle formation process of WPI, alone or as influenced by other wall and core materials, is also a crucial factor that affects the property and functionality of the spray-dried microparticles. In addition, in the microencapsulation of live microorganisms such as probiotics, the interactions between WPI and the core material may not be limited to common chemical interactions, since the cellular response of the viable cells toward the wall material should also be taken into account. In this work, WPI was used in combination with other wall materials to encapsulate a variety of bioactive substances, including both lipophilic materials and a probiotic strain, Lactobacillus rhamnosus GG (LGG). The microencapsulation was carried out with a Micro-Fluidic Jet Spray Dryer, which was capable of producing monodisperse microparticles with uniform morphology and property. By comparing particle morphology between microcapsules with varying formulation, the particle formation process of WPI, as well as how it was influenced by different wall and core materials, was discussed. It was further correlated with the formation of the property and functionality of the powdered microcapsules. We also showed that the contact of LGG with WPI impacted on its metabolic activity and the stability of cellular surface charge, which likely affected the retention of LGG viability after spray drying. Besides the chemical property of WPI, its particle formation behaviour and compatibility with core material are also of great importance for the development of microencapsulated powders with excellent property.

A044 Using machine learning to predict obesity risk based on genome-wide, epigenome-wide gene-gene, and gene-diet interactions Yu-Chi Lee1, yuchi.lee@usda.gov, Jacob J. Christensen2, Laurence D. Parnell1, Caren E. Smith3, Jonathan Shao4, Nicola M. McKeown5,6, Jose M. Ordovas3,7,8, Chao-Qiang Lai1, chaoqiang.lai@usda.gov. (1) USDA ARS, Nutrition and Genomics Laboratory, JM-USDA Human Nutrition Research Center on Aging at Tufts Univ., Boston, Massachusetts (2) Norwegian National Advisory Unit on FH, Oslo Univ. Hospital; Dept. of Nutrition, Univ. of Oslo, Norway (3) Nutrition and Genomics Laboratory, JM-USDA Human Nutrition Research Center on Aging at Tufts Univ., Boston, Massachusetts (4) USDA-ARS, Statistical and Bioinformatics Group, Northeast Area, Beltsville, Maryland (5) Nutritional Epidemiology Laboratory, JM-USDA Human Nutrition Research Center on Aging at Tufts Univ., Boston, Massachusetts (6) Friedman School of Nutrition Science and Policy, Tufts Univ., Boston, Massachusetts (7) IMDEA Food Inst., CEI UAM + CSIC, Madrid, Spain (8) Centro Nacional de Investigaciones Cardiovasculares (CNIC), Madrid, Spain Obesity is associated with multiple chronic diseases that hamper healthy aging. Obesity risk is defined by genetic, epigenetic, environmental factors, and their complex interactions. This study aimed to gain a more comprehensive understanding of these relations and interactions, focusing on diet-related factors. Such knowledge will guide future research towards the development of more precise prevention and treatment strategies. For this purpose, we conducted a combined genome-wide and epigenome-wide scan for main effects and up to three-way interactions among 402,793 single nucleotide polymorphisms (SNPs), 415,202 DNA methylation sites (DMS), and 397 dietary and lifestyle factors using the Generalized Multifactor Dimensionality Reduction (GMDR) method in a training set consisting of 1,573 participants in exam 8 of the Framingham

Offspring Study (FOS) cohort. After identifying relevant genetic, epigenetic, and dietary factors, we then applied machine learning (ML) algorithms to predict participants' obesity status in the testing set consisting of a subset of independent samples (n=394) from the same cohort. The quality of prediction models was evaluated using Area Under the Receiver Operating Characteristic Curve (ROC-AUC) and accuracy. The GMDR method identified 213 SNPs, 530 DMS, and 49 dietary and lifestyle factors that were significant predictors of obesity. Comparing several ML algorithms, we found that the stochastic gradient boosting model provided the best prediction accuracy for obesity in the training set and overall accuracy of 70% and ROC-AUC of 0.72 in the test set samples. Top predictors of the best-fit model were 21 SNPs, 230 DMS in genes such as CPT1A, ABCG1, SLC7A11, RNF145, and SREBF1, and 26 diet-related factors, including processed meat, diet soda, french fries, high-fat dairy, artificial sweeteners, alcohol intake and specific nutrients and food components, such as calcium, sugar and flavonols. Further studies will be needed to define the roles of these top predictors. In conclusion, we developed an integrated approach with ML to predict obesity using omics and dietary data. This extends our knowledge of the drivers of obesity. Such knowledge can inform precision nutrition strategies for the prevention and treatment of obesity.

A045 Determining the sex of chicken eggs by machine learning and high-speed volatiles mass spectrometry Adam R. Rivers, adam.rivers@usda.gov. Agricultural Research Service, Gainesville, Florida The egg-laying industry culls billions of day-old male chicks annually. The practice has economic and animal welfare implications. Many European Union countries are moving to ban the practice. The industry needs a non-invasive method to rapidly and accurately determine the sex of eggs by day 7 of development so that male eggs can be diverted to other uses before the embryo becomes sentient. Eggs emit a complex mixture of volatile compounds through the shell during development with no single biomarker of sex. Initial work with gas chromatography-mass spectrometry (GC/MS) identified predictive compounds that can be used to train a regularized logistic regression with accuracies of 95%. GC/MS is too slow for hatchery use so we began developing a protocol using a real-time proton transfer reaction mass spectrometer (PTR-MS) which can take up 10 measurements per second. To measure volatiles headspace gas needs to be collected about for 5 minutes. Parallel headspace collection devices were designed, that were compatible with industry-standard egg tray formats. Feature engineering was required to control for differences in the headspace, egg shape, and gestation times. Engineered features were essentially normalized log ratios of compounds selected by univariate feature selection. These features were combined with PCR-based sex determinations on training eggs to train L1 regularized logistic regression models. In production, these models could be improved or refined for specific sites using unlabeled data for semi-supervised learning.

A046 Catch me if you can – tracking volatile compounds as biomarkers of dynamic food processes using direct analysis Jonathan Beauchamp, jonathan.beauchamp@ivv.fraunhofer.de. Dept. of Sensory Analytics and Technologies, Fraunhofer Inst. for Process Engineering and Packaging IVV, Freising, Germany All foods contain a rich mixture of volatile substances, including odor-active aroma compounds that, together with non-volatile taste components, play a key role in imparting flavor. When the food matrix is altered, either by active manipulation, e.g., heat treatment or mechanical processing, or through natural processes, e.g., maturation or fermentation, the composition of its volatile constituents – its volatilome – changes. This shift in the volatilome can be desirable, affording the food a characteristic flavor, or it can be unwanted, resulting in an unpalatable product. Moreover, individual volatile organic compounds, VOCs, can give clues about the status or quality of foods. This aspect can be exploited through chemical analysis of the food, often complemented with sensory evaluations, to characterize the (changing) volatilome and offer insights into the nature of the changes occurring. While the analysis of volatile food constituents by conventional gas chromatography-mass spectrometry, GC-MS, delivers a comprehensive snapshot of the volatilome, direct analysis by real-time analytical technologies, such as direct injection mass spectrometry, DIMS, can track these temporal changes and provide data on the associated dynamic processes. The latter approach can be employed in diverse applications to determine the condition of a food, from food process monitoring to observe and modulate parameters to achieve desirable flavors, e.g., during coffee bean roasting, to shelf-life studies to ascertain the degree of spoilage and aid in use-by date predictions, e.g., storage of milk. This talk will examine how biomarkers within the food volatilome can inform on product quality, and will present technologies and approaches that enable the capture and analysis of these fleeting food constituents.

A047 Big data in food production Rieke Weel, rieke.weel@imec.nl. OnePlanet Research Center, IMEC, Wageningen Campus, Netherlands In the food industry there is an increased focus on sustainable production of healthy food products. Novel real time sensing techniques play an important role in understanding and improving food production processes resulting in more optimal use of resources and reduction of waste streams. While in the past mainly physical parameters such as temperature, pressure and pH were monitored, novel sensing techniques allow for inline sensing of product composition. On the farm sensing will be used to reduce resources, to improve the crop yield and ripeness, to monitor pests and to reduce the environmental impact. Fast detection of microorganisms in product streams or on the surface of ingredients and food products will increase food safety and will speed up batch release of food products. Additionally, sensors are available to understand the behavior of food products in the human body, allowing for the design of more healthy products. All these novel sensors provide novel large data streams that will for the input for the development of a digital twin aiming to optimize product quality and to reduce valuable resources by feedback and feedforward process control. This presentation will discuss how OnePlanet Research Center's newly developed sensing techniques and data analysis can be applied to optimize the food production chain.

A048 Hypercube big data analytics with artificial intelligence for food safety Bosoon Park, bosoon.park@ars.usda.gov. US National Poultry Research Center, USDA Agricultural Research Service, Athens, Georgia Big data and artificial intelligence (AI) will play an important role in the future of agri-food systems, especially food safety with imaging spectroscopy and data fusion. Since a series of foodborne outbreaks often threaten the public, early and rapid detection technology is essential. A hyperspectral microscope imaging (HMI) technique is good candidate to identify and classify foodborne pathogens, because it generates hyperspectral big data both in spatial and spectral domains from bacteria samples at the cellular level. However, conventional machine learning methods are limited to analyze such a big data. In this presentation, two different HMI platforms based on acousto-optic tunable filter (AOTF) and Fabry-Perot interferometer (FPI) are introduced to obtain hypercube. For data analytics, AI classifiers including long-short term memory (LSTM) network as well as convolutional neural networks (CNN) are proposed for automated classification of foodborne bacteria. Compared to classifiers such as latent discriminant analysis, k-nearest neighborhood, and support vector machine based on principal components, which performed between 66% and 85% accuracy for classification, the AI-based classifier achieved the accuracy up to 92.9%. Furthermore, AI-assisted analytics was able to identify

foodborne pathogens instantly by eliminating complicated two-step multivariate feature analysis. This presentation expands advanced hyperspectral imaging technology with integration of microscopy and deep learning algorithms for food safety.

A049 Big data and deep learning in agriculture and food chemistry - considerations and practice Y. Jane Tseng1,2,3, yjtseng@csie.ntu.edu.tw. (1) Graduate Inst. of Biomedical Engineering and Bioinformatics, National Taiwan Univ., Taipei (2) Dept. of Computer Science and Information Engineering, National Taiwan Univ., Taipei (3) Drug Research Center, No.3, Linsen S. Rd., Zhongzheng Dist., Taipei City, Taiwan Big data and deep learning are buzz words for science in recent years. The applications of big data and deep learning techniques have been widely used in various fields. However, the practice of such techniques and the range of data are not carefully examined in the field of Agriculture and Food Chemistry. This talk will focus on practical considerations such as how big is considered big in Agriculture and Food Chemistry, what if our food safety is just not big enough, which neural network to go after, and other issues. It should be a quick review and guideline for scientists in this field for such applications.

A050 Green polymers derived from cashew based raw materials H.N. Cheng1, hncheng100@gmail.com, Atanu Biswas2, Roselayne F. Furtado3, Carlucio R. Alves4, Cristina Prieto5, Jose M. Lagaron5. (1) Southern Regional Research Center, USDA Agricultural Research Service, New Orleans, Louisiana (2) National Center for Agricultural Utilization Research, USDA Agricultural Research Service, Peoria, Illinois, Food Packaging Laboratory, EMBRAPA Agroindustrial Tropical, Fortaleza, Brazil (4) Science and Technology Center, Univ. Estadual do Ceara, Fortaleza, Brazil (5) Novel Materials and Nanotechnology Group, IATA-CSIC, Paterna, Spain Agricultural production is a critically important economic activity, which generates foods, fuels, fibers, and raw materials. Many of the agro-based raw materials are byproducts with relatively low value. One emphasis of our research efforts is to convert some of these agricultural materials into potentially value-added products. A recent collaborative approach is to use byproducts of cashew nut production as the agro-based raw materials. Thus, cardanol from the cashew nutshell liquid has been converted to polymers in two different reaction pathways, generating products with interesting properties. Cashew gum, obtained from the bark of the cashew tree, has been converted to carboxymethyl cashew gum and hydrophobically modified polymers. Blends of cashew gum and gelatin have been used for packaging applications and for microencapsulation. Electrosprayed cashew gum microparticles have been found to be useful for the encapsulation of highly sensitive bioactive materials. An overview of these and other applications will be given in this presentation.

A051 Quantitative specific gravity analysis of salvia rosmarinus in ethanol solutions Elizabeth M. Zippi, lizippi@bellsouth.net, Anna Marsalis. Chemisty and Physics, Louisiana State Univ., Shreveport, Louisiana Specific gravity is a comparative ratio of the density of a given substance divided by the density of a reference substance, usually water. In this project, a quantitative specific gravity analysis of rosemary/ethanol solutions of increasing concentration has been investigated. Ten rosemary essential oil solutions were prepared in ethanol, and the specific gravity of each was determined. An extract of fresh rosemary in ethanol was then prepared, and the specific gravity of 5 different samples of this tincture, as it became more concentrated over time, was measured. Using a plot of specific gravity vs. concentration of the essential oil/ethanol solutions, the concentrations of the extract samples have been approximated. Since there currently is no well-established conversion from rosemary oil to extract, as there is in the case of other herbs, a goal of this project is to propose an acceptable conversion.

A052 Food grade Limonene can be an effective homemade insect repellent Manav Kakkanat1, blueflight1@gmail.com, Alex Colesmith2, Henry Brown2. (1) Chemical Engineering, Univ. College London, United Kingdom (2) Judd School, Tonbridge, Kent, United Kingdom Introduction and aims: Biopesticides can address some of the limitations of synthetic pesticides. Over the COVID-19 pandemic supply chain disruptions were an additional challenge and so we aimed to devise a homemade, biodegradable and non-toxic alternative to synthetic pesticides from easily available kitchen ingredients namely D-Limonene from orange oil and Vanillin. Methods: We compared the repellent and insecticidal effects of orange oil (19% limonene), 2 % vanillin and neutral controls on Drosophila melanogaster (n=136) in a choice chamber. 2ml each of the two test solutions were added to separate yeast fortified test tubes. Unscented yeast served as a neutral control in a third test tube. Cold anaesthetised flies were transferred to the choice chamber and the apparatus was kept in a temperature-controlled fume cupboard. The study was terminated at the end of 48 hours and surviving flies were identified by observed locomotion. The study was performed in triplicate and the results are presented as a whole. Results: Of the flies, 5 % (n=7) were uncommitted, 43 % (n=58) were attracted to unscented yeast, 37% (n=51) to vanillin and the other 15 % (n=20) to limonene ($p=0.002$ in favour of an avoidant response to limonene in D.melanogaster). All flies exposed to limonene died within 48 hours ($p < 0.0001$, compared with unscented yeast). Of the flies exposed to vanillin, 99% survived the 48 hours of observation ($p=0.0005$ compared with unscented yeast). Analysis and conclusions: The findings suggest that commercially available food grade citrus oil extract has a repellent effect on a standardised population of adult Drosophila in a laboratory environment. There is also an apparent insecticidal effect on D. melanogaster at the 19 % concentrations studied in this experiment. Our data on the comparison of Drosophila preferences between limonene and vanillin is new and not previously investigated. They seem to show that vanillin when combined with limonene has the potential to reduce its efficacy as an insect repellent. Such combinations are often considered useful in reducing the volatility of limonene in commercial preparations and may reduce efficacy. The results are promising and suggest limonene in the form of commercial food-grade orange extract may be an easily available, homemade, environmentally friendly alternative to available insect repellents.

A053 Adulteration of maple syrup: Molecular vs. luminescence spectroscopic approaches Sujani Rathnayake3, Maleeka Singh1, Robert Hanner3, Maria G. Corradini1,2, mariagcorradini@gmail.com. (1) Food Science, Univ. of Guelph Ontario Agricultural College, Canada (2) Arrell Food Inst., Univ. of Guelph Ontario Agricultural College, Canada (3) Integrative Biology, Univ. of Guelph, Ontario, Canada Maple syrup is an iconic product that contributes hundreds of millions of dollars annually to the Canadian and USA economies. Due to its high demand, maple syrup is prone to adulteration through dilution with other sugar syrups, undermining brand reputation and product value. The use of molecular approaches based on DNA barcoding and high-throughput sequencing methods has proven valuable for detecting adulteration and contamination in other food commodities. However, the extensive processing methods involved in converting maple sap to syrup lead to degradation of the genetic material, which subsequently lowers molecular approaches' efficacy in detecting possible instances of adulteration. Spectroscopic techniques and their potential to detect maple syrup adulteration have been described in the literature, but it has not been fully explored. This study aims to evaluate the discriminatory power of molecular and photophysical approaches to

assess maple syrup adulteration. Pure maple syrup and its admixtures with commonly reported adulterants (ranging from 1 to 50%), namely beet, corn, and rice syrups, were tested using molecular and luminescence spectroscopic techniques. Physicochemical characteristics of all samples (e.g., pH, water activity, refractive index, and density) were also obtained using standard protocols. Excitation and emission matrices, EMMs, (λexc=250-500 nm, slit=3 nm and λem=280-650 nm, slit=3 nm) were collected using a Duetta Fluorescence and Absorbance Spectrometer (Horiba Scientific, Inc, NJ, USA) to pinpoint differences between samples. Polymerase Chain Reaction (PCR) amplification using mini-rbcL and beet-, corn-, and rice-specific primers did not yield amplifiable bands in a 1% agarose gel and could not be barcoded. The fluorescence fingerprints (EEMs) of the samples allowed identifying excitation-emission combinations with valuable discriminatory information. The efficacy of the ratio of the emission intensities at λem= 350 and 425 nm (I425/I350) when the sample was excited within the UV range (i.e., λexc=290 nm) allowed for easy discrimination of the spiked samples (86% correct identification). Combining the selected ratio (I425/I350) with routinely obtained physicochemical measurements increased the level of discrimination (91% correct identification). This approach can be easily incorporated into the routine monitoring of maple syrup within the Quality Assurance/Quality Control (QA/QC) process.

A054 Development of hemp nanocellulose-based bioplastics and their application for food packaging Arusha Fleming, arusha.fleming@mail.mcgill.ca, Xiaonan Lu. McGill Univ. Faculty of Agriculture and Environment, Sainte Anne de Bellevue, Quebec, Canada There is a necessity for bioplastics as an alternative to the plastics currently being used. This is particularly important with respect for food-safe packaging use. Hemp is a good source of cellulose and is suitable for a bioplastic due to that fact that it is a reproducible crop. Both the hurd and the bast fiber of the hemp were examined for their cellulose content because of the different physicochemical properties between the fibers. The cellulose extraction from both the hurd and bast fiber consisted of de-waxing, bleaching, and lignin and hemicellulose removal. The hemp bast was found to have a higher cellulose content compared with the hurd, therefore it was chosen to be used to prepare the cellulose nanocrystals. The cellulose nanocrystals where then synthesized and characterized, where hydrolysis times were compared at both 30 minutes and 60 minutes to see which was more suitable to prepare them. It was found that at 30 and 60 minutes there was not a significant difference in the diameter and the length of the nanocrystals, but at 60 minutes there were more surface charges which lead to a degradation in increased sulfate half-ester groups. As a result of this, the preparation time for the cellulose nanocrystals was determined to be 30 minutes using the hemp bast.

A055 Potential of soil enzyme manganese peroxidase to degrade catechin and related polyphenols Meiling Fu, fum6@miamioh.edu, Ann E. Hagerman. Chemistry & Biochemistry, Miami Univ., Oxford, Ohio Environmental stress induces plants to increase their tannin concentration, leading to increased release of tannin into soils from leaching and leaf litter. These changes can in turn alter the soil biology at the level of the microbiome, the invertebrate populations, and the plant systems. Condensed tannin degradation by the soil microbiome, which is critical to the carbon cycle and to soil and plant ecology, is vastly unknown. Here, we are investigating the possible degradation pathway of condensed tannin by the enzyme manganese peroxidase (MnP), which is released into the soil by fungi and microbes that decompose plant matter. MnP catalyzes the oxidation of Mn^{2+} to Mn^{3+}, which is then stabilized by dicarboxylic acids such as oxalate. The metal-oxalate complex is an oxidizing agent for a variety of phenolic substrates related to lignin, leading to identification of MnP as a key enzyme lignin depolymerization. We proposed to explore the possible role of MnP in decomposition of the polymeric polyphenols known as condensed tannins by examining the monomers, (+)-catechin and (-)-epicatechin. We will establish whether the Mn^{3+}-oxalate complex acts on the flavan-3-ols to establish whether MnP could play a role in tannin decomposition. Stereochemical differences between (+)-catechin and (-)-epicatechin will give us insights into how structural features of the tannin polymer could impact its oxidation by MnP. We have monitored the products of hydrogen peroxide-dependent MnP oxidation of the two substrates using HPLC and UV-Visible spectrometry to follow kinetics and product formation. Catechin forms a more complex mixture of products than epicatechin, and the rates constants for the oxidation are different. Our findings highlight the possible importance of MnP in the oxidation of small phenolics related to the more complex condensed tannins, and serve as a first step for identifying key steps in condensed tannin turn over in soil systems.

A056 Analysis and characterization of west Tennessee honeys Ebtisam Ahmed, ebtahme@ut.utm.edu, Bailee Barrett, Abigail H. Shelton. Dept. of Chemistry and Physics, Univ. of Tennessee Martin This study examines properties of honeys from different geographical origins, to include commercially available honeys and direct-sourced honeys, with regard to carbohydrate, metals, and sugar contents, color, pH, ground state absorption, and moisture content. Effects of processing and evidence of tampering will be presented.

A057 Potential for release of toxic alkaloid ricinine and for influence of bacterial functional diversity from castor cake after soil application Kai-Xuan Cheng1, seafood4104039038@gmail.com, Cheng-Hua Liu2, Fo-Ting Shen1, Yu-Min Tzou1, Ya-Hui Chuang1. (1) National Chung Hsing Univ., Taichung, Taiwan (2) Feng Chia Univ., Taichung, Taiwan Castor cake, the primary by-product of castor oil production, has become globally popular organic fertilizer due to its high nitrogen content and rapid mineralization rate, which could fulfill nitrogen sources for organic crop production. However, castor cake also contains alkaloid ricinine, a toxin could stimulate the human central nervous system and cause seizures. Significant amounts of toxic alkaloid ricinine may be released into soils after large scale land application of castor cake, but this potential impact on the soil ecosystem has been overlooked. Better understanding the fate of released toxic alkaloid ricinine in soil and its influence on the functional diversity of bacteria after castor cake application is needed. Therefore, this study used optimized solid-phase extraction (SPE) method coupled with a liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QTOF/MS) to analysis ricinine concentration in soil pore water collected from soil pot experiments with different castor cake application rates. The metabolic potential of bacteria was determined through community level physiological profiling. The release of ricinine was observed in soil pore water with the concentrations decreased with time for all the castor cake application rates. Additionally, the increase in the application rates resulted in the increase of not only the ricinine concentration but also the metabolic potential of fast-growing bacteria. However, the application rate of 20 g castor cake per kilogram soil resulted in the reduce of the functional diversity index of fast-growing bacteria. The utilization of several carbon sources such as β-methyl-D-glucoside, D-galactonic acid γ-lactone, D-galacturonic acid, L-asparagine, D-mannitol, N-acetyl-D-glucosamine, D-cellobiose, and Putrescine was positively related to castor cake application rates. The decrease of ricinine concentration could be the result of bacterial activities, and therefore in-depth studies on determining bacterial community structure is needed to further clarify the relation of released ricinine and bacteria in soils.

A058 Changes of volatile compounds in rice-based distilled spirits, soju aged in different kinds of containers Wan-Keum Kim,

wan9212@hanmail.net, Seungjoo Lee. Culinary and Food Service Management, Sejong Univ., Gwangjin-gu, Seoul, Korea (the Republic of) In this study, changes of volatile compounds in 6, 12 and 18 month-old rice-distilled spirits aged in pottery, oak and stainless steel, respectively were analysed using HS-SPME (Headspace Solid Phase Microextraction) followed by GC-MS. A total of 85 volatile components, including 35 esters, 15 alcohols, 5 ketones, 3 aldehydes, 15 miscellaneous, 14 unknowns, were identified. Esters and alcohols were the largest groups among quantified volatiles. Differences in volatile compounds among the distilled soju samples and possible sample grouping were examined by applying PCA (Principal Component Analysis) to the GC-MS data sets. The first and second principal components explained 51.94% of the total variation across the ten samples. The samples aged in oak showed higher concentrations of ketones, aldehydes, and miscellaneous. In the positive direction of PC1, oak aging samples were positioned. In contrast, pottery or stainless steel aging samples were shown in the far negative side of PC1. The longer aging samples like 18 months were in the positive direction of PC2.

A059 Variability of tannic acid and its role in stabilizing hollow zein nanoparticles Sadeepa Y. Mallikarachchi, malliksy@miamioh.edu, Ann E. Hagerman. Chemistry & Biochemistry, Miami Univ., Oxford, Ohio Tannic acid is a natural plant polyphenol with many biological activities ranging from protein binding to antioxidant activity. Tannic acid is a hydrolysable tannin, comprising a central polyol molecule esterified with one or more galloyl residues. The nominal molecular formula of commercial tannic acid (C76H52O46) suggests the material is decagalloyl glucose, obscuring its complex composition as a mixture of galloyl esters of glucose or other polyols. Owing to its many abundant hydroxyl groups tannic acid forms complexes with proteins based on interactions such as hydrogen bonding and hydrophobic forces. Proteins that are highly amphiphilic and have low water solubility can self-assemble into nanoparticles. Plant proteins are known particularly attractive as potential delivery agents for pharmaceuticals due to their minimum potential to provoke zoonotic disease transmission. However, protein nanoparticles exhibit drawbacks such as low stability under gastrointestinal conditions, so strategies including surface coating or cross linking have been employed to improve delivery potential. In the current study, tannic acid is used as the crosslinking agent to synthesize zein nanoparticles that carry curcumin, a hydrophobic polyphenol extracted from the herb Curcuma longa (turmeric). Although tannic acid has previously been employed to stabilize protein nanoparticles, the role of the chemical and structural variability characteristic of various preparations of tannic acid has not been considered. In this study we characterize different supplies of tannic acid using reverse phase HPLC, and synthesize and characterize zein nanoparticles loaded with curcumin but coated with different tannic acids. We analyze our nanoparticles with DLS to study their particle size, PDI and Zeta potential while imaging is carried out using SEM and TEM. By successful completion of this project, we hope to contribute to the knowledge pool required to synthesize more stable, even and reliable protein nanoparticles for therapeutic and medicinal purposes.

A060 Improving the functional characteristics of sorghum phenolics Jaymi Peterson1, lawrencejay@ksu.edu, Dmitriy Smolensky2, Scott Bean2, Umut Yucel1,3. (1) Food Science Inst., Kansas State Univ., Manhattan (2) GQSRU-ARS, US Dept. of Agriculture, Manhattan, Kansas (3) Animal Sciences and Industry, Kansas State Univ., Manhattan Sorghum is rich in phenolics and can be used for functional food formulation. However, aggregation of phenolics decrease solubility and limit antioxidant activity. Liposomal vesicles (LV) may be used to increase phenolic stability and homogeneously distribute them, improving overall antioxidant activity. The objectives of this study were to characterize sorghum phenolic extracts (SPE), encapsulate extracts with LV to improve antioxidant activity and stability and to evaluate morphology of LV as a function of SPE content. SPEs were obtained by solvent extraction (70% ethanol). LVs were prepared with soy phosphatidylcholine (0.0, 1.0 and 2.0%) and SPE (0.0, 0.1, 0.2, 0.4, 0.8%) at pH 3.8 or 6.5. The samples were prepared using a high-shear (HS) homogenizer (11,000 rpm) or under high-pressure (HP) (500 bar) with aqueous phenolic-buffer dispersions serving as controls. Samples was characterized by their particle size and zeta potential. Encapsulation efficiency was determined by total phenolic content (TPC) and total condensed tannins (TCT) using the Folin-Ciocalteu (FC) and vanillin-HCL methods. Antioxidant activities were determined using the DPPH and ORAC assays. Statistical analysis was performed using general linear model with phenolic-lecithin interactions. Vesicle size for HS samples were greater than 1000 nm and decreased below 50 nm with HP. Addition of phenolics significantly ($p<0.05$) increased particle size (up to 212 nm) for 0.8% SPE concentration with HP and resulted in a monolayer LV. Addition of phenolics increased TPC to 1475 gallic acid equivalents (GAE) at 0.8% SPE. TPC of encapsulated systems were less than SPE dispersions (5% and 10% in HP and HS). The TCT were significantly ($p<0.05$) less in LV than SPE dispersions by 80%. Although measurable TPC and TCT were less in LV than SPE, DPPH capacity improved by 20% and 15% for HP and HS. In addition, ORAC activity saw no significant ($p>0.05$) change between LV and SPE dispersions. LV can improve the homogeneity and stability of SPEs. However, traditional measurement techniques can be misleading when LVs are present and require a combination of different techniques to show change in antioxidant potential.

A061 Influence of the microelements on anticancer metabolites biosynthesis in basidiomycetes Anastasiya Ostrokhishko, ostrokhishko@infochemistry.ru, Anastasiya Pomytkina, Lyubov Levkina, Filipp V. Lavrentev. Infochemistry Scientific Center, Nacional'nyj Issledovatel'skij Univ. ITMO, Sankt-Peterburg, Sankt-Peterburg, Russian Federation Mushrooms and their extracts have long been used in folk medicine and food due to their low calorific value and pleasant taste and are also reported to have beneficial biological activities, thus now found applications in nutraceutical and pharmaceutical products. They are filamentous fungi with fruiting bodies packed with beneficial nutrients such as carbohydrates, fibers, proteins, vitamins, and minerals [1]. Mushrooms with medicinal value are defined as “mushroom nutraceuticals” and are consumed in capsule or tablet form as dietary supplements. Simultaneously, interest in mushrooms as a potential source of bioactive compounds has increased, and much research on the bioactivity of these compounds has been conducted in the last two decades. The secondary metabolites derived from mushrooms have demonstrated diverse biological properties such as anticancer, antidiabetic, immunomodulatory, antimicrobial, anti-inflammatory, antiviral, antiallergic, and antioxidative activities [2]. Basidiomycetes, which were used for the project, were cultivated with the microelements for enrichment. Enrichment basidiomycetes can be used as a dietary supplement in meat products. Microelements that were used are zinc, selenium, and magnesium. For this work anticancer metabolite, ergosterol was chosen to estimate its quantity in dry powder depending on the content of the microelements. The method of the extraction was chosen and optimized based on the number of dry powder samples. Gas chromatography coupled with mass spectrometry of electron beam was chosen as a standard method for the detection of sterols. Correlation between quantitative content of microelements and quantitative content of ergosterol was founded.

A062 Effect and mechanism of Citrus depressa Hayata peel extract against acetaminophen-induced liver injury in mice Zheng-Yuan Su1, zysu@cycu.edu.tw, Po-Yao Tsai1, Guor-Jien Wei2, Xuan-Ru Chen1. (1) Chung Yuan Christian Univ., Taoyuan City, Taiwan (2)

National Yang Ming Chiao Tung Univ. - Yangming Campus, Taipei, Taiwan Acetaminophen (APAP) is a common medication to alleviate pain and reduce fever, but long-term use and overdose of APAP will cause liver injury. In this research, we studied the effect and mechanism of ethanolic extract of Citrus depressa Hayata (CD-EE), Nobelitin (Nob), and Tangeretin (Tan) against APAP-induced liver injury in Balb/c mice. The mice were randomly divided into control, APAP, APAP+N-acetylcysteine (NAC) as a positive control, APAP+CD-EE (250 and 500 mg/kg b.w.), APAP+Nob (50 mg/kg b.w.), and APAP+Tan (50 mg/kg b.w.). The mice were oral administrated with NAC, CD-EE, Nob or Tan once daily for nine weeks, and injected intraperitoneally (ip) with APAP (400 mg/kg) twice a week form the second week. We found that CD-EE, Nob, and Tan significantly decreased APAP-induced serum ALT and AST activities, and decreased the inflammation of liver pathology. As compared with the APAP group, CD-EE, Nob, and Tan can upregulate the mRNA and protein expressions of Nrf2, NAD (P) H: quinone oxidoreductase 1 (NQO1), heme oxygenase-1 (HO-1), and UDP-glucuronosyl transferase 1A (UGT1A), and also restore the activities GPx, GST and catalase, and reduce lipid peroxidation in the liver. These results suggest that CD-EE, Nob, and Tan might reduce APAP-induced hepatotoxicity through regulating Nrf2-mediated defense system in BALB/c mice.

A063 Enhancing the stability of fish oil-in-water emulsions using whey protein- kappa carrageenan complexes Hanna(John) Khouryieh, hanna.khouryieh@wku.edu. Western Kentucky Univ., Bowling Green The aim of this research was to investigate the effect of whey protein isolate (WPI)- kappa (κ-) carrageenan complexes on the oxidative stability of fish oil-in-water (O/W) emulsions. The final O/W emulsions contained 2% WPI and 0, 0.05, 0.1, 0.2, or 0.4% κ-carrageenan. The oxidative stability of the oil droplets was determined by primary lipid oxidation (lipid hydroperoxide values) and secondary oxidation (thiobarbituric reactive substances (TBARS)) for a 2-week period. The physical stability of the emulsions was determined by particle size, zeta potential, creaming index and viscosity tests. The results indicated that pH and concentration of κ-carrageenan had substantially affected the stability of the emulsions. As the κ-carrageenan concentration increased, the emulsion stability increased. Emulsions containing 0.4% of κ-carrageenan were stable when adjusted to a pH of 5 and 6. κ-carrageenan emulsions with 0.2 and 0.4% gum displayed highest viscosities for this gum type at pH 4 and 5, respectively. At pH 3, 4, and 5 zeta potential was near 0 mV indicating minimal electrostatic interactions. The particle size in 0, 0.05, and 0.1% emulsions peaked at pH 4 and 5, indicating increased flocculation due to the low electrostatic interaction. The concentrations of lipid hydroperoxides and TBARs in emulsions significantly decreased with higher concentrations of κ-car. Emulsions with 0.4% of κ-carrageenan had the lowest lipid hydroperoxides at pH 6 and 7, which probably due the high level of electrostatic interaction between the interfacial protein-polysaccharide complex that coated droplets, improving emulsion stability.

A064 Inhibiting ice recrystallization by cellulose nanocrystals: Influences of sucrose concentration and storage time Min Li, mli63@vols.utk.edu, Tao Wu. Food Science, Univ. of Tennessee Knoxville In ice cream products, the presence of ice crystals with sizes over 50 μm leads to an icy texture, affecting mouthfeel and decreasing consumers' acceptance. The increase of ice crystal size mainly results from a thermodynamically favored ice recrystallization (IR) process. To inhibit IR, polysaccharides are commonly used based on a slow-diffusion mechanism. However, their ice recrystallization inhibition (IRI) effects are dependent on measurement conditions, such as concentration and type of sweeteners, and storage temperature and time. This study elucidated the underlying mechanism of how the IRI activity of a newly identified ice recrystallization inhibitor - cellulose nanocrystals (CNCs) is affected by the sucrose concentration and storage time. CNCs demonstrated high IRI activity in low sucrose concentrations (2% ~ 10%), became almost inactive in medium sucrose concentrations (15% ~ 35%), and regained modest activity at high sucrose concentrations (45% ~ 49%). A sufficient storage time was crucial to observe the IRI activity of CNCs in 25% sucrose solution: No IRI activity was observed in a model ice cream system within a short timescale of 0.5-2.0 hours. Over longer timescales, 1.0% CNCs and 0.5% CNCs could completely stop the growth of ice crystals with corresponding final crystal sizes of 25 and 40 μm after 5 and 68 hours, respectively. These results demonstrated that the IRI effect of CNCs is positively related to the surface coverage on ice crystals. These research findings offer a new perspective in understanding the measurement condition-dependent IRI effect of CNCs and outline suitable experimental conditions to evaluate the IRI activity of new materials, which could potentially benefit the ice cream industry in developing new materials and recipes to control ice recrystallization.

A065 Effect of boiling and steaming on the carbohydrates of sweet corns Wenxia Zhang2, Baojie Zhu2, Liangli Yu3, Jing Zhao2, Shaoping Li2, Xianli Wu1, xianli.wu@usda.gov. (1) Methods and Application of Food Composition Laboratory, USDA ARS Beltsville Human Nutrition Research Center, Beltsville, Maryland (2) State Key Laboratory of Quality Research in Chinese Medicine, Inst. of Chinese Medical Sciences, Univ. of Macau, China (3) Dept. of Nutrition and Food Science, Univ. of Maryland, College Park Sweet corn is one of the most consumed vegetables in the US. Fresh sweet corn contains about 20 g/100 g carbohydrates, which makes it an important source of carbohydrates in American diet. Studies have shown that cooking can alter carbohydrate profiles of vegetables. In this study, the effects of two common cooking methods (boiling and steaming) on the carbohydrates of sweet corns were examined. Yellow and bi-color sweet corns were selected as raw materials. The contents of individual simple sugars, oligosaccharides, water-soluble carbohydrates (WSC), starch, total dietary fiber (DF), resistant starch (RS), as well as sugar alcohols were measured in these two varieties before and after cooking. The simple sugars, oligosaccharides and sugar alcohols were quantified by high performance anion exchange chromatography-pulsed amperometric detection (HPAEC-PAD). Other components were measured by AOAC methods with optimization and modification. The results showed that the amounts of carbohydrate components in the two varieties were different. Four simple sugars, sucrose, glucose, fructose and maltose, were identified and sucrose is the predominant one. Boiling and steaming did not change the concentrations of sucrose but resulted in the decreases of the other three sugars. No detectable oligosaccharides were found in these two varieties. Both boiling and steaming did not alter the contents of WSC, starch and DF, but led to huge reduction of RS. RS content decreased by 75.8% and 74.3% after steaming and boiling for bi-color sweet corn, and 84.2% and 83.0% after steaming and boiling for yellow sweet corn, respectively. Sorbitol and mannitol were identified as main sugar alcohols in sweet corn. Sorbitol decreased in cooked samples, while mannitol remained unchanged. In conclusion, boiling and steaming mostly alter RS and simple sugars in sweet corn. The effects of these changes on the digestibility of sweet corn carbohydrates and their biological functions warrant further investigation.

A066 Detection of Campylobacter jejuni in agri-food products using a paper-based microfluidic device based on recombinase polymerase amplification and lateral flow immunoassay Yunxuan Chen1, cassendra.cyx@gmail.com, Yaxi Hu2, Xiaonan Lu3. (1) Food Science, The Univ. of British Columbia, Vancouver, Canada (2) Health Canada, Ottawa, Ontario (3) Food Science and Agricultural

Chemistry, McGill Univ., Montreal, Quebec, Canada Campylobacter jejuni is recognized as the most common species in the genus Campylobacter that causes foodborne diseases globally. Main reservoirs harboring C. jejuni are poultry productions that are associated with the majority of illnesses, making a demand for prompting effective detection methods to understand the transmission route within agri-food systems. The gold standard diagnostic method involves tedious microbiological culture isolation and nucleic acid amplification, specifically polymerase chain reaction (PCR). This analytical workflow is only applicable in laboratory with expensive equipment and experienced technicians, limiting its use in resource-reduced or on-site settings. Therefore, we aimed to integrate paper-based DNA extraction, isothermal amplification and lateral flow detection on a paper-based microfluidic chip that it is portable and easy to use outside laboratory. Recombinase polymerase amplification (RPA) is conducted isothermally and becomes a prevailing alternative to the traditional PCR due to its simplicity in temperature setting and relatively short incubation time (10-20 mins). The endpoint diagnosis is visualized on a lateral flow strip as part of the paper microfluidics. Paper microfluidics was fabricated by wax printing where reaction zones preloaded with amplification reagents were confined within the hydrophilic area. Lysed nucleic acid was extracted by low cost cellulose paper dipstick, and transported onto microfluidic reaction zone without any pipetting. The integrated paper microfluidics enabled performing sample amplification to end-point-detection within 25 mins. Overall, the complete chip demonstrated 100% specificity to C. jejuni including 6 wild strains isolated from our laboratory among 8 other Campylobacter subspecies strains and 11 non-Campylobacter strains. High sensitivity was achieved with the help of lateral flow strip to reduce the detection limit to 100 CFU/mL in Campylobacter culture, 10-fold improvement than visualizing on agarose gel electrophoresis. In addition, the device was capable of detecting C. jejuni spiked at a concentration of 25 CFU/mL on chicken breast meat after enrichment for 12 hrs. Our results suggested the utility of paper-based microfluidic chip on food sample diagnosis with high specificity and sensitivity. It showed the potential as a reliable point-of-care diagnostic platform for in-field conditions owning to its low-cost, portability and simplicity.

A067 Biocatalytic approaches to valorization of food and agriculture waste streams Zhixin Wang, zw485@cornell.edu, Julie M. Goddard. Food Science, Cornell Univ., Ithaca, New York The high lipid, protein and sugar content in agricultural waste streams are ideal for biochemical valorization into value added products. Innovative research on improving the stability and recovery of biocatalysts in extreme environments, typical of waste streams, is essential for their translation in bioprocessing. Here, we explore biocatalytic valorization of lactose in whey permeate to rare sugars. Rare sugars are monosaccharides with near-equivalent sweetness intensity as sucrose, but a fraction of the caloric density and minimal adverse health impacts. Present in very small amounts in nature, an opportunity remains to produce these natural sweeteners from agricultural 'waste' sugars such as lactose. Tagatose and allulose, are of particular interest as they have been granted GRAS status by the USDA. We successfully have bioengineered a recombinant fusion protein, lactase, that can effectively self-immobilize onto cellulose in less than 2 hours and confirmed that the addition of a carbohydrate binding module (CBM) does not alter the optimum reaction conditions of the native enzyme. The protecting effect of sugars on enzymes to improve their catalytic activity was studied. At 50 degrees Celsius, lactase was inactivated within 2 hours, whereas lactase in the same buffer supplemented with 40% (% w/w) trehalose, glucose and sucrose enabled retention of 91 %, 37 % and 79 % of the original enzyme activity, respectively, after 25 hours exposure, an important consideration for higher temperature bioprocessing. To optimize the recombinant enzyme's performance, both rigid and flexible linkers between the enzyme and the CBM will be studied. Improving the stability of enzymes for the valorization of whey permeate waste streams into rare sugars will promote economic and environmental sustainability of global dairy processing. Innovative research to improve or supplement synthetic biology and biocatalyst is crucial in valorizing waste streams into value added products and in reducing the environmental burden of food manufacturing.

A068 Non-fouling and antimicrobial polyurethane coatings to prevent cross-contamination in food processing facilities Autumn Rudlong, amr452@cornell.edu, Julie M. Goddard. Food Science, Cornell Univ., Ithaca, New York Pathogenic and spoilage bacteria can persist as biofilms in Zone 2/3 growth niches (e.g. drains) in food processing facilities which are outside of routine cleaning and sanitization. As both foodborne illnesses and microbial food spoilage continue to be issues, a need remains for new technologies to eliminate favorable growth environments. Here I present my research on the synthesis, characterization and efficacy of non-fouling (NF) and antimicrobial polyurethane (PU) coatings for use in non-food contact environments. Dihydroxy quaternary ammonium bromides, N,N-bis(2-hydroxyethyl)-N-methyl-N-R-1-ammonium bromides (R= -octan {C8QBR}, -decan {C10QBR}, -dodecan {C12QBR}, -hexadecan {C16QBR}, -octadecan {C18QBR}) were synthesized via the reaction of N-methyldiethanolamine and alkyl bromides of varying alkyl chain length. To enhance bactericidal effects of the final PU, minimum inhibitory concentrations (MIC) for each quaternary ammonium bromide were determined against Listeria monocytogenes and Salmonella enterica. C16QBR and C18QBR displayed total inhibitory effects against L. monocytogenes at 2.7ppm. C16QBR showed inhibitory effects against S. enterica at 21.3ppm. Quat sanitizers in the food industry use between 200-400ppm active quaternary. NF PU containing 1-3 wt% perfluoropolyether (PFPE) and NF and antimicrobial PU containing 3% PFPE and derivatized C16QBR were synthesized by step-growth polymerization. Coatings were characterized by ATR-FTIR, GPC, XPS, NMR, and DSC. Dynamic water contact angle demonstrated increasing hydrophobicity with the inclusion of 3% PFPE compared to the control PU (117.2° ± 1.2 versus 87.4° ± 3.8). The PFPE block reduced surface free energy compared to control PU and stainless steel (21.01mN/m, 15.09mN/m, and 0.70mN/m) . Coating performance in preventing microbial adhesion was demonstrated using Psuedomonas poae, a biofilm forming dairy spoilage organism, L. monocytogenes and Salmonella spp.. P. poae biofilms (72 hr) were established using a CDC biofilm reactor, enumerated, and imaged by SEM. Incorporation of the NF block improved the removal of established biofilms. L. monocytogenes and Salmonella spp. were used to determine the bactericidal efficacy of coatings. Antimicrobial coatings showed bactericidal effects against all test organisms. Developing antimicrobial and NF coatings using PU chemistry enhances the translatability, enhancing cleanability and reducing cross-contamination caused illness, product spoilage and waste.

A069 Phenolic metabolites in plasma and urine of children after blueberry consumption Laura Lavefve1, ldlavefv@uark.edu, Rohana Liyanage2, Luke Howard1, Kikumi Ono-Moore3, Renny Lan3,4, Eva C. Diaz3,5,4. (1) Food Science Dept., Univ. of Arkansas Fayetteville (2) Dept. of Chemistry and Biochemistry, Univ. of Arkansas Fayetteville (3) USDA-ARS Arkansas Children's Nutrition Center, Little Rock (4) Dept. of Pediatrics, Univ. of Arkansas for Medical Sciences, Little Rock (5) Arkansas Children's Research Inst., Little Rock Background: Blueberry (BB) native polyphenols undergo extensive conversion through phase II and microbial biotransformation. There is scarcity of data regarding the metabolite profile in biological samples of children after BB consumption. Here, we present preliminary results of BB-derived metabolites measured

in urine and plasma of children (n=6) ages 11 to 12 years participating in a randomized controlled trial at the Arkansas Children's Nutrition Center. Method: Assessors of metabolites were blinded to the intervention assignment. Fasting urine and blood were collected before randomization, and on day 6 of the intervention [BB (15 g bid) vs. placebo]. On day 6, post-prandial blood and urine were collected hourly after the consumption of the study product. Native and conjugated phenolic acid derivatives (n=35) were measured using ultraperformance liquid chromatography-tandem mass spectrometry multiple reaction monitoring (UPLC-MS/MS MRM). Results: A preliminary principal component analysis allowed discrimination between the post-prandial samples from 3 subjects (group A) and the post-prandial samples from the other 3 subjects plus all fasting samples (group B). The most abundant compound was hippuric acid, with an amount up to 10 (urine) and 19 times higher (plasma) in group A compared to group B. In addition, post-prandial plasma and urine concentrations of phloroglucinaldehyde, ferulic, gentisic, sinapic, m-hydroxyhippuric, chlorogenic and 3,4-dihydroxyphenyl acetic acid were higher in children from group A compared to children from group B. Conclusions: Distinct plasma and urine metabolite profiles can be identified in children participating in the ongoing Blueberry Study. Further analyses will be done upon completion of the study to elucidate the changes in metabolite profiles in children following blueberry consumption.

A070 Tailoring protein chemistry for in situ water safety applications: rapid pathogen detection and microplastic degradation Hannah S. Zurier, hsz7@cornell.edu, Sam R. Nugen, Julie M. Goddard. Food Sci. and Tech., Cornell Univ., Ithaca, New York A safe food system depends on maintenance of a safe water system. Both chemical (e.g. microplastics) and biological (e.g. microbial pathogens) hazards present in water can be harmful to agricultural practices and direct consumption. My dissertation research employs principles of protein engineering and synthetic biology in practical solutions to challenges in water safety. I engineered bacteriophage capsid chemistry to enhance rapid bacterial detection in drinking water and manipulated enzyme chemistry to degrade microplastics in agricultural water. To meet regulatory standards, drinking water must have 0 detectable E. coli (a standard indicator of fecal contamination) per sample. Detection systems must therefore reliably indicate 1 colony-forming unit (cfu) of E. coli per standard 100 ml sample, a size difference of 1015 between sample and analyte. Bacteriophages, which specifically bind a tunable range of bacteria, are an ideal biorecognition element in ultrasensitive bacterial detection platforms. I built a T4 bacteriophage-based biosensor using site-specific artificial amino acid incorporation to enable bioorthogonal azide-alkyne "click chemistry" conjugation to magnetic nanoparticles. By combining magnetic separation with the native phage bacterial attachment system, this sensor concentrates the E. coli within the water sample 1000-fold. This signal amplification enables single cfu detection within 7 hours, significantly faster than the 1-2 days required for the standard method. Microplastics (MPs) are plastic particles and fibers <5 mm in their longest dimension. As plastic has become ubiquitous in modern life, MPs have accumulated in a range of environments. MPs can enter agricultural spaces, via treated wastewater (effluent). While the treatment process should render effluent, a common irrigation source, hazard-free, current treatment practices do not adequately address MP contamination. I modified the amino acid composition of a natural plastic-degrading enzyme, PETase, to enable in situ MP biodegradation in wastewater treatment plants. This enzyme degrades a common plastic into soluble monomers readily metabolized by bacteria. Using a combination of computational design, site-directed mutagenesis, and combinatorial engineering, I increased enzymatic activity by over 300%. Overall, my work shows that precise manipulation of amino acid chemistry can transform naturally occurring biologics into potent, practical tools for enhancing water safety.

A071 Evaluation of novel coatings to prevent smoke phenol absorption in Pinot noir grapes Lindsay Garcia, lindsaygarcia.lg@gmail.com, Trung Tran, Darrell C. Cerrato, Michael Penner, Yanyun Zhao, Elizabeth Tomasino. Food Science & Technology, Oregon State Univ., Corvallis Wildfires have been a continuing threat to the wine industry over the years. Smoke exposed grapes result in smoky, ashy, and medicinal sensory characters that are undesirable in wine. To combat this problem, new mitigation techniques are needed to preserve the quality of the grapes. In response to the lack of successful smoke taint reduction techniques, innovative coatings were developed to prevent smoke compounds from entering the grapes. Pinot noir grapes were grown in Woodhall III Vineyards in Oregon and harvested at maturity. After harvest the grapes were coated with four different coating treatments by spraying. Cellulose nanofiber (CNF) was used as a coating forming matrix, and other functional ingredients were incorporated into CNF, including β -cyclodextrin, chitosan, and a mixture of 1:1 β-cyclodextrin/chitosan. Uncoated grapes were used as a control. 13C labeled barley was used as a fuel source to create the smoke in specially designed cages covered in low density polyethylene greenhouse film. The grapes were smoked for 6 hours, achieving a constant smoke density between 20 to 100 mg/m3 for smoke particles >1 μm. After the grapes were smoked, half were washed to determine if the smoke compounds bind or are blocked by the coatings. GCMS and HPLC were used to determine the amount of smoke compounds in the grapes. The results of this study will determine if the novel film coating is a prospective preventative measure to stop wildfire smoke from entering the grapes. Therefore, when a wildfire occurs the wine industry can prevent smoke taint and the potential loss of product.

A072 Electrochemical teardown of a trace pesticide assessment system Vikram Narayanan Dhamu1, vxd171130@utdallas.edu, Chaitra Milan Telang1, Sriram Muthukumar2, Shalini Prasad1. (1) Bioengineering, The Univ. of Texas at Dallas, Richardson (2) EnLiSense LLC, Allen, Texas The large increase in the herbicides tolerant plants has dramatically affected the level of usage of these herbicides recently. There exists an increasing concern about the associated toxicity to the environmental and human health, which instills a need for direct low concentration detection of these herbicides present in various drinking water, food and crop products. In this work, we present the deconstruction of a simple, label-free electrochemical sensor to selectively detect glyphosate. The mapping of the pesticide levels in sample is probed and detected using two electrochemical modalities: Non-Faradaic Electrochemical Impedance Spectroscopy (EIS)-due to its ability to map the subtle chemical interactions occurring at the electrode-electrolyte interfacial double layer and Chronoamperometry (CA)-utilized due to its depiction of transient current representative of the binding effects seen in this affinity biosensing methodology. The study's first focus deals with surveying the effect of the different immobilization steps onto the gold substrate (electrode) by validating the immunochemistry and the binding between the receptor agent and the glyphosate analyte. Next, the temporal factor of incubation and thereby response time is evaluated to optimize the sensor system. Finally, in order to build an overall end-to-end sensing ecosystem: a robust machine learning classification algorithm is integrated to increase the accuracy and precision of the pesticide residue level results. Overall, the sensor has been proven to measure the spiked pesticides doses in real food/water samples with the low limit of detection of 1ppb. The sensing platform therein can be summarized as a micro-volume, high-sensitive, and selective platform which requires no prior sample preparation with the cross-functional ability of machine learning classification. Hence, it can be a potentially

game-changing electrochemical on-field sensing device to measure trace pesticide residues against a threshold limit (as given by various environmental agencies worldwide)-as a precautionary step to alert the common man using the food products as well as farmers working in the agriculture field.

A073 Texture and taste flavor characteristics of pecan kernel and the effect of variety Zahra Yusufali1, zyusufali@twu.edu, Xinwang Wang2, Keith Kubenka2, Xiaofen Du1. (1) Nutrition and Food Science, Texas Woman's Univ., Denton (2) USDA-ARS, College Station, Texas Pecan (Carya illinoinensis) is a native North American nut tree that produces pecan kernels which are highly valued worldwide for their sensory, nutritional, and health attributes. Limited work has investigated the pecan kernel flavor among a panel of pecan varieties. This study aimed to analyze the flavor quality (taste and texture) of sixteen native, seven improved, and seven breeding line pecan varieties. The texture was measured with hardness trait and the taste was analyzed by quantifying free amino acids (umami, sweet, bitter), total polyphenols (bitter and astringent), and total soluble solid content (sweet). Texture analysis showed a wide range of hardness (peak force, 12.5-44.2 N) and significant variation among the tested accessions ($p<0.001$). The breeding line 1992-01-0603 and improved cultivar 'Barton' had the highest shearing forces. A total of 20 free amino acids (FAA), quantified with gas chromatography-mass spectrometry (GC-MS) after derivatization and ranged 0.012-44.43 mg/100g of kernel, were identified in pecan kernels. All accessions showed a significant difference in their FAA profiles. Most accessions, especially native and selected breeding lines, showed high amounts of umami contributing FAA (aspartic acid and glutamic acid), ranging 5.35-44.43 mg/100g kernels. Sweetness contributing FAA (alanine, glycine, proline, and glutamine) and the bitterness contributing FAA (arginine) ranged 0.83-17.57 and 7.32-14.93 mg/100g of kernel, respectively, both showed a wide variation among the accessions. Total polyphenols content (TPC) was quantified via the Folin–Ciocalteu reagent assay, which revealed significant difference between accessions, although all samples had high contents with 1.27-6.73 g/100g GAE (Gallic acid equivalent). Total soluble solid content (°Brix) ranged 4.61-7.39% of the whole kernel with significant difference among accessions as well. Knowledge gained in this study could assist in selecting desirable pecan cultivars with better tasting kernels and increasing market values for pecan growers and food industry.

A074 Quantitative variation of taste and texture properties in 165 F2 cucumber progenies Cassidy Duan1, cduan@twu.edu, Yiqun Weng2, Xiaofen Du1. (1) Nutrition and Food Sciences, Texas Woman's Univ., Denton (2) USDA Agricultural Research Service, Madison, Wisconsin Cucumber (Cucumis sativus L.) fruit sensory quality includes textural characteristics, taste (non-volatile compounds), and aroma (volatile), with texture and taste directly linking to consumer acceptance. Limited studies have been conducted to investigate the variation of flavor profiles in F2 cucumber fruit. This study aimed to analyze the variation of texture and taste-related traits of cucumber using an F2 population derived from the cross between two cucumber varieties (9930Q2-1 and W17633) with contrasting flavor attributes. Fruit hardness was evaluated using a texture analyzer among 165 F2 plants which showed a wide variation from 1.34 to 57.26 N and an average hardness of 31.78 N. Fruit pH, TA, and °Brix of 165 F2 plants were measured with a Titrando and a digital refractometer. The F2 progenies had pH ranging 6.02-7.73 (mean value 5.67), TA ranging 0.15%-0.47% (mean=0.26%), and °Brix ranging 1.7-5.7 (mean=2.8). The content of total polyphenols (associated with bitterness and astringency) ranged 6.93-33.58 mg/100 g GAE (Gallic acid equivalent), with an average 19.07 mg/100 g GAE. All the four traits exhibited a largely normal distribution in the F2, suggesting their quantitative nature of inheritance. Two parents and one F1 fruit contained a significant difference of these chemical composition, according to the agglomerative hierarchical clustering analysis. The selection of patents provide potential wide distribution of flavor traits in F2 cucumber populations. This work provides novel insights into the inheritance of attributes contributed to cucumber fruit flavor that may help understanding of their genetic basis and improvement of cucumber fruit quality through molecular breeding.

A075 Black tea polyphenols provide a nutraceutical option for preventing the onset of celiac disease In vitro Paul Mathews, Paul.Mathews@colostate.edu, Charlene Van Buiten. Food Science and Human Nutrition, Colorado State Univ., Fort Collins Celiac disease and related gluten-induced pathologies affect between 1-4% of global population The pathogenesis of celiac disease is a complex cascade involving innate and adaptive immune responses. It has been well established that exposure to gluten amongst genetically susceptible individuals initiates and propagates the disease process, with autoimmunity against intestinal cells and tissue-transglutaminase enzymes manifesting as intra- and extraintestinal symptoms. Currently, the only mitigation of celiac disease is an adherence to a gluten free diet, which can be cost prohibitive, unavailable and socially isolating. Recent advances in synthetic and natural products chemistry may offer therapeutic alternatives to the total abstinence from wheat and related gain products. The objective of our research is to develop a nutraceutical approach to treating celiac disease using dietary polyphenols from tea. Using a variety of spectroscopic techniques, we have shown that black tea polyphenols, which are rich in theaflavins, interact with gluten to form colloidal complexes with gluten in vitro. These complexes cause conformational change in the secondary structure of gliadin, which may reverse its immunostimulatory capabilities. Presently, we are investigating the potential protective effects of theaflavins and other black tea polyphenols against gluten-mediated inflammation and permeability in a Caco-2 cell model of the intestinal brush border. The molecular interactions investigated here offer promise as a nutraceutical, plant-based therapy to acute gluten exposure, offering pre- or post-exposure relief to gluten challenge in susceptible individuals. Because tea polyphenols may impart a prophylactic effect by maintaining intestinal health, they may be a valuable regimen for CD or gluten sensitive individuals to adopt.

A076 Quality characteristics of restructured goat meat jerky as Influenced by natural preservative properties of raisins Beruk B. Lemma, Jung Hoon Lee, leej@fvsu.edu. Agricultural Sciences, Fort Valley State Univ., Fort Valley, Georgia Because of the potential to generate carcinogenic nitrosamines from nitrite-cured meats, there is considerable interest in producing no nitrate/nitrite-added meat products that simulate conventional cured meats. Raisins have been recognized as sensorially compatible with meat products; moreover, their antimicrobial and antioxidant potential appeared in cooked ground meat products. Yet their effect on the quality of goat meat (chevon) has not been studied. Furthermore, homemade jerky products have gained popularity recently in the US and chevon is an excellent raw material for preparation of low fat value-added products. This study, therefore, assessed raisin paste influences on quality parameters of restructured chevon jerky and its stability. Eight batches of restructured chevon jerky were prepared by ground chevon from Spanish goats, mixed with a jerky seasoning either with or without sodium nitrite ($NaNO_2$; 0.015%, w/w), or raisin paste (15%, w/w). Restructured jerky strips were extruded through a stuffing horn, placed in a smokehouse at 93.3 °C for 3.5 h, vacuum packaged, and stored at ambient temperature under fluorescent light for quality analysis at 0, 2, 4, 6, 8, 10 wk. Compared to cured-jerky, jerky prepared with raisin had significantly lower CIE L* (lightness) and

a* (redness) values, moisture contents (33.8 vs 37.9%), water activities (0.79 vs 0.88) pH (5.2 vs 6.2) values, but higher ($P < 0.05$) shear values (2.8 vs 2.6 kg). Furthermore, these quality parameters were also significantly influenced by the storage time whether or not jerky was cured. Inclusion of raisin significantly affected the total microbial counts of jerky. Compared to jerky prepared with or without NaNO2, raisin-jerky had significantly lower aerobic plate counts during storage. Jerky prepared with raisin or NaNO2 significantly decreased TBARS values, which did not change during storage. Cured jerky had higher ($P < 0.05$) sensory color, flavor, texture and overall acceptability scores compared to uncured jerky. However, no significant differences were found in the flavor scores of cured- and raisin-jerky. Jerky prepared with raisin that might be similar to the conventional cured jerky based on its antioxidant and antimicrobial properties. However, unique nitrite-cured sensory properties might not be generated by raisin paste.

A077 Comprehensive analysis of aromatic and metabolic compounds in beer brewed by new wild yeast by GC-MS and special databases Yusuke Tahemori1, takemori@shimadzu.co.jp, Emiko Shimbo1, Yui Higashi1, higashi.yui.jq8@shimadzu.co.jp, Haruna Kawamitsu1, Kazuhiro Kawamura1, Eberhardt R. Kuhn2, Takuma Yamamiya3, Narihiro Suzuki3. (1) Analytical and Measuring Instruments, Shimadzu Corporation, Kyoto, Japan (2) Shimadzu Scientific Instruments, Colunmbia, Maryland (3) Ise Kadoya Brewery, Ise, Japan Various yeasts have been developed to brew characteristic beer. The authors brewed beer using newly collected wild yeast, and comprehensively analyzed the flavor components and hydrophilic metabolites in beers. A wide-scope target analysis was used for the comprehensive analysis of aromatic and metabolic compounds. Acquired data were processed and analyzed by multivariate data analyses to calibrate and visualize beer qualifications. In this study, in order to evaluate new wild yeast, test brewing of beer was carried out by using two kinds of practical beer yeasts and new wild yeast, and these were used as samples. Regarding the analysis of aroma components, a headspace sampler was used, and only the headspace generated from the beer sample was analyzed by GC-MS. The data from the analysis were used to identify aroma components using a special aroma database. On the other hand, the analysis of hydrophilic metabolites was performed using pretreated beer samples. The data from the analysis were used to identify metabolites using a special metabolites database. The data obtained from the analyses of aroma and metabolites were finally processed by Principal Component Analysis (PCA). The score plot of PCA showed clear differences among the three samples. From the loading plot of PCA, it was confirmed that the flavor components of beer brewed by the new wild yeast were relatively rich in terpenes such as Humulene and Isobutyl acetate, and that the hydrophilic metabolites were relatively rich in amino acids such as Glutamine and Glycine. Test brewing of beer was carried out by using two kinds of practical yeasts and new wild yeast, and then three beer samples were analyzed by GC-MS and special databases for comprehensive analysis of aromatic and metabolic compounds. Multivariate analysis of the obtained results confirmed clear differences among the three beer samples and identified the flavor components and metabolites that were relatively abundant in the wild yeast.

A078 Evaluation of non-alcoholic beverages from hop using GC-MS and HPLC Yusuke Takemori1, takemori@shimadzu.co.jp, Mizuki Hayakawa1, Ayako Nomura1, Jun Nagata1, Eberhardt R. Kuhn3, Takuma Yamamiya2, Narihiro Suzuki2. (1) Analytical and Measuring Instruments, Shimadzu Corporation, Kyoto, Japan (2) Ise Kadoya Brewery, Ise, Japan (3) Shimadzu Scientific Instruments, Columbia, Maryland Hops, which give beer its characteristic aroma and bitterness, contain a variety of flavor and functional ingredients. However, it is known that the ingredients originally contained in hops are changed or inactivated during the beer production process or fermentation process. In this study, we analyzed and compared the ingredients of beer and non-alcoholic beverage using the same hop. In this study, a headspace sampler was used to analyze the aroma components of beer and non-alcoholic beverages, and only the headspace generated from the samples was analyzed by GC-MS. The results obtained from the analysis were used to identify aroma components using a special aroma component database. The identified components were subjected to principal component analysis to determine which flavor components were relatively abundant in beer and non-alcoholic beverages. In addition, for the qualitative and quantitative determination of specific functional components, the analysis was done by HPLC, and the comparison between beer and non-alcohol beer was also carried out. PCA (Principal Component Analysis) from the results of GC-MS analysis visually confirmed clear differences in aroma components between beer and non-alcoholic beverages. In particular, methyl isobutyrate, methyl benzoate, 2-acetylthiazole, etc. were detected in non-alcoholic beverages, suggesting that these components decrease or disappear during beer production. On the other hand, 3-Methylbutanal and Ethyl3-methylbutanoate, which are considered to be characteristic aromas of beer, were not detected in non-alcoholic beverages. HPLC analysis confirmed that certain components were detected in non-alcoholic beverages. In conclusion, the aroma components of beer and non-alcoholic beverages were analyzed by GC-MS, and the aroma components could be easily identified using the aroma component database. From the PCA, the clear difference between beer and non-alcoholic beverage was confirmed, and the aroma component which characterized each was able to be specified. HPLC analysis also enabled us to identify the characteristic components of non-alcoholic beverages from hop.

A079 Genotoxicity evaluation of lignin-derivable of six bisguaiacols using in silico, in vitro, and in vivo methods Xinwen Zhang1, wenzhang@udel.edu, Jignesh S. Mahajan2, Thomas H. Epps2, LaShanda Korley2, Changqing Wu1. (1) Animal and Food Sciences, Univ. of Delaware College of Agriculture and Natural Resources, Newark (2) Materials Science & Engineering, Univ. of Delaware College of Engineering, Newark Bisguaiacols, lignin derived bisphenol analogs, are promising and potentially safer bisphenol A (BPA) replacements. Most toxicity studies of BPA or BPA alternatives have focused on the potential estrogenic activity, while limited toxicological data are available on other aspects, such as genotoxicity which is a concern relative to BPA and bisphenol analogs at low exposure levels. In this study, we investigated the genotoxicity of six newly synthesized bisguaiacols (p,p′-BGP, o,p′-BGP, m,p′-BGS, p,p′-BGS, m,p′-BGM, and p,p′-BGM) using a multi-tiered method, consisting in silico simulation, in vitro Ames test, and in vivo comet test. Additionally, we explored the structure-activity relationships (SARs) among bisguaiacols with different methoxy groups and different stereochemistries. The toxicity estimation software tool (TEST) suggested that the majority of the lignin-derived were mutagenic negative. These results were supported by Ames test using five bacterial strains (TA98, TA100, TA102, TA1535, and TA1537) at 0.5 pmol/plate to 5 nmol/plate. Additionally, the potential genotoxicity of bisguaiacols was further evaluated using in vivo comet testing with fetal chicken liver samples. In addition to the standard alkaline comet test, the Fpg enzyme-modified comet assay was applied to investigate oxidative DNA damage in liver samples. Furthermore, the lipid peroxidation level of the fetal liver after three days of treatments was evaluated to understand the mechanism of the genotoxicity of test compounds. Results showed that the signs of mutagenicity (mutagenic index > 1.5) and genotoxicity were not detected for the majority of the lignin-derivable analogues relative to BPA and BPF (bisphenol F).

A080 Identification and quantitation of anthocyanins in berries using liquid chromatography and high resolution tandem mass spectrometry Nebiyu Abshiru1, nebiyu.abshiru@futureceuticals.com, Dawn Randolph1, Boris V. Nemzer1,2. (1) Research and Analytical Center, FutureCeuticals Inc, Momence, Illinois (2) Food Chemistry, Univ. of Illinois at Urbana-Champaign, Urbana Anthocyanins, naturally found pigments in several fruits & vegetables, are widely known for their antioxidant, anti-inflammatory and anti-cancer benefits. In the current study, a comprehensive anthocyanin screening in four freeze-dried berries and VitaCherry® Sport, a commercially available phytonutrients supplement from whole tart cherry, was conducted using high resolution tandem mass spectrometry approach. Quantitation of commonly known anthocyanins was performed by HPLC method. This study identified a total of 26, 30, 27, 20, and 18 anthocyanins in elderberry, aronia, blackberry, acai, and VitaCherry Sport, respectively. The total amount of anthocyanins in decreasing order is elderberry (2.4 mg/g), aronia (2 mg/g), blackberry (0.4 mg/g), VitaCherry Sport (0.2 mg/g), and acai (0.1 mg/g). Moreover, the study showed cyanidin as the most abundant class of anthocyanin in all the berries, ranging in proportion from 63% to 89% of the total anthocyanins.

A081 Phytonutrient composition and potential anti-inflammatory activities of air-dried purslane (Portulaca oleracea) Fadwa Al-Taher1, faltaher1@yahoo.com, Diganta Kalita1, Boris V. Nemzer1,2. (1) VDF FutureCeuticals, Momence, Illinois (2) Univ. of Illinois at Urbana-Champaign, Urbana Purslane (Portulaca oleracea) is a green, leafy plant naturally found in the U.S. It is popular in most regions of Europe, Asia, and the Middle East. There is major potential to produce this herb as a food crop because of its greatly nutritional and antioxidant properties. The purpose of this study was to characterize the nutritional composition of air-dried (AD) purslane. Chemical analysis showed AD purslane contains an excellent source of omega-3 fatty acids (8257 ± 917 mg/100 g), which protects against cardiovascular disease, cancer, and other human conditions. A high content of omega-6 (3158 ± 442 mg/100g) and omega-9 (1120 ± 170 mg/100 g) are also present. Purslane also contains phenolic acids, flavonoids, alkaloids, vitamins, minerals, and amino acids. Aqueous methanolic extract of purslane extract was tested for the inhibition of cyclooxygenase (COX-1 and COX-2) enzyme activities, which is believed to be one of the major targets for the anti-inflammatory activity of nonsteroidal anti-inflammatory drugs and natural products. The aqueous methanolic extract of purslane inhibited the COX2 and COX1 activity in a dose dependent manner with IC50 values of 670 µg/mL and 820 µg/mL respectively. These findings suggest that aqueous extract of purslane possesses potent anti-inflammatory activity. The phytochemical and nutritional composition of purslane makes it important as a raw leafy green, functional food ingredient and for nutraceutical applications.

A082 The evaluation of the fabricated bioactive packaging material using essential oils and natural polymers by electrospray Anto Charles1, Tony Jin2, Richard Mu1, Fur-Chi Chen1, Agnes Kilonzo-Nthenge1, Ying Wu1, ywu@tnstate.edu. (1) Tennessee State Univ., Nashville, (2) USDA Agricultural Research Service, Washington DC In the current study, carvacrol and thymol were used as bioactive antimicrobial compounds in fabrication of bioactive packaging materials by electrospray. Potato starch and water soluble yellow mustard mucilage (WSM) were applied as wall materials. The fabricated nanoparticles were evaluated on their antimicrobial properties and release kinetics. Cherry tomatoes were used to investigate the effect of the fabricated materials on the quality attributes of the product in terms of color, firmness and weight loss. The results indicated that the naoparticles exhibited enhanced antimicrobial effects against Escherichia coli, staphylococcus aureus, salmonella dublin, and pseudomonas fluoroscens by inhibiting them at minimum concentrations compared to their non-encapsulated parallels. The release kinetics followed a controlled release pattern up to 180 h. Investigation over cherry tomatoes showed that the particles positively impacted their color, texture, and weight loss during the 21 day storage period. The active packaged tomatoes significantly maintained the quality attributes and extended the shelf life by 3-4 days. Therefore, the fabricated bioactive packaging materials are recommended explicitly for antimicrobial active packaging. It is a feasible approach to develop active packaging using natural polymers by electrohydrodynamic processing.

A083 Interfacial chemistry of a bioderived active packaging film dictates its performance in complex matrices Ian Kay, ipk7@cornell.edu, Julie M. Goddard, Joshua E. Herskovitz. Food Science, Cornell Univ., Ithaca, New York The convergence of food wasted due to spoilage and disposal of single use, non-compostable plastic packaging represents a significant economic & environmental challenge. The current market trend of reducing additive use in foods is likely to result in an unintended decrease in product shelf life due to increased susceptibility to spoilage reactions such as oxidative degradation. Active packaging technologies which seek to extend ‘clean label’ product shelf life at the post-retail level using bioderived and biodegradable polymers thus represents a unique opportunity in reducing volumes of both wasted food and single-use plastic diverted to municipal solid waste. Real food systems have varying and complex matrices which can impact the performance of active packaging technologies, because the active moieties bound at the interface will perform differently depending on the food matrix itself. Therefore, an understanding of the interfacial behavior is necessary to tailor active materials to meet their end application. Here we present a characterization of the surface pKa for polylactic acid (PLA) films grafted with the antioxidant nitrilotriacetic acid (NTA), PLA-g-NTA. Attenuated total reflectance Fourier transform infrared spectroscopy was used to determine the pKa values of 3.97 and 8.99 for the carboxylic acid groups of NTA and a pH dependent ABTS radical scavenging assay was performed to determine the pKa value of 6.74 for the tertiary amine of NTA. These results indicate that PLA-g-NTA would be useful as an antioxidant material in food systems with pH’s above 6.74, as an electron transfer from the deprotonated tertiary amine was shown to be the largest driver of radical scavenging capacity. Utilizing a biodegradable antioxidant packaging material such as PLA-g-NTA thus gives way to extend shelf of foods while meeting consumer demands for reduced additive use towards the goal of reducing food waste and the environmental impact of petroleum based single-use plastics.

A084 Sorghum DDGS as a renewable source for production of functional packaging films Umut Yucel1, yucel@ksu.edu, Valentina Trinetta1, Scott Bean2. (1) Food Science, Kansas State Univ., Manhattan (2) USDA ARS, Manhattan, Kansas Distiller's dried grains with solubles (DDGS) are byproducts of grain fermentation in ethanol plants, distilleries and breweries. DDGS from sorghum, the third largest grain crop in the US, can be renewed into biodegradable and potentially edible packaging film materials to address environmental and sustainability issues related to food and product packaging. The aim of this study was to produce packaging films from sorghum DDGS with thermal, physical and mechanical properties comparable to traditional plastic films with inherent antioxidant and antimicrobial properties. Sorghum DDGS films were prepared before and after mechanical conditioning via wet milling (Colloid mill) and dry milling (Udy mill) by using a solvent-casting approach. Colloid mill was performed at different pH conditions: acidified water (0.1 M HCl), neutral water, alkaline water (0.1 M NaOH). Films were prepared by using mixtures of organic and aqueous solvents (water:chloroform:ethanol) at various ratios. Final

films were characterized for their thermal properties (DSC), tensile strength (TS), elasticity and elongation (texture analyzer), thickness (micro-caliper), water resistance (gravimetric), oxygen diffusion (oxygen analyzer), and color (hunter LAB colorimeter). The DDGS films prepared without preconditioning were weak, brittle and non-homogenous. Preconditioning significantly improved the structural integrity of films. Colloid milling increased the water resistance of the films more than 80% via solubilization of insoluble fibers and removal of solubles, which also significantly ($p<0.05$) decreased the thickness (145 μm) as compared to Udy (dry) milling (170 μm). Moreover, colloid mill conditioning improved film homogeneity with better mechanical properties: the TS (1:2:1 water:chloroform:ethanol) increased more than an order of magnitude up to 50 MPa as compared to films without preconditioning (3 MPa). The composition of the solvent was a significant ($p<0.05$) factor for film properties. The lack of aqueous fraction resulted in brittle films, while at the optimum conditions (1:2:1 ratio and wet milling) elongation up to 86% was observed exceeding the industrial standards. Furthermore, sorghum DDGS is rich in flavonoids and tannins, which were evaluated for their antimicrobial and antioxidant capabilities, to add value for the use of sorghum DDGS in manufacturing of biodiverse films for functional food packaging applications.

A085 Pre-commercial feasibility evaluation of non-equilibrium pulsed discharge for sanitation of whole and cut fresh Gregory Fridman, gregfridman@gmail.com. AAPlasma LLC, Philadelphia, Pennsylvania We have developed a plasma system to address this issue: plasma jet-like system where an air stream containing small droplets of water is passed through the discharge and onto the surface of produce. The key challenges, addressed in this talk, are the control of temperature of air and water passing through the discharge, and the resulting chemistry generated in the liquid and on the surface of produce. Mixing of plasma-treated water microdroplets with untreated air in the storage chamber is also a major issue with the scale-up and will be addressed in the talk. For our validation experiments, we utilize E.coli, Salmonella, and Listeria with Rifampicin-induced resistance. We coat Petri dishes with Rifampicin and thus are able to repeatably control and observe the rate of initial contamination of each fresh produce sample. As validation samples, packaged or open spinach, kale, lettuce, and strawberries are inoculated with up to 108 cfu (per sample). Samples are then placed into the misting chamber. Treatment times vary from 1 to 30 minutes in an 18” cubic chamber, simulating non-refrigerated storage. Following the treatment, the samples are placed in stomacher bags with 1 ml of PBS, stomached for 120 seconds, and 100 μl of this solution is plated on rifampicin-coated Petri dishes for overnight growth.

A086 Amino acids and their derivatives preventing oxidation of frying oil: Promising natural antioxidants Hong-Sik Hwang, hongsik.hwang@usda.gov. USDA, ARS, NCAUR, Peoria, Illinois Although vegetable oils have many health benefits, these oils are easily oxidized due to the high content of unsaturated fatty acids during frying, resulting in deterioration of oil quality and formation of toxic substances. To reduce the oxidation rate of healthy vegetable oils such as soybean oil during frying, strong antioxidants are needed. Recently, our research group found that amino acids containing a thiol, a thioether, or an extra amine group such as arginine, cysteine, lysine, methionine, and tryptophan had strong antioxidant activity. At 5.5 mM, these amino acids had stronger antioxidant activities than 0.02% (1.1 mM) tert-butylhydroquinone (TBHQ). The synergistic interaction between amino acids and tocopherols seemed to be the most important mechanism for their antioxidant activity in soybean oil. Our research group also examined the derivatives of amino acids, in which the carboxylic acid group was converted to a carboxylate group (-COONa or -COOK). The heating study conducted with 5.5 mM amino acid salts in soybean oil at 180 °C revealed that sodium salts of amino acids including alanine, phenylalanine, and proline and disodium glutamate had significantly stronger antioxidant activity than the corresponding amino acids. Potassium salts had stronger antioxidant activity than sodium salts. One reason for the improved antioxidant activity of amino acid salts was found to be better retention of tocopherols in soybean oil compared to the corresponding amino acids during heating. Amino acid salts also more effective than the corresponding amino acids in preventing oxidation of other vegetable oils including olive, high oleic soybean, canola, avocado, and corn oils. A frying study with potato cubes confirmed the results and showed that phenylalanine potassium salt at 5.5. mM had significantly stronger antioxidant activity than 0.02% TBHQ.

A087 Rapid discovery of novel antimicrobial peptides with machine learning algorithms to improve safety, quality, and shelf-life of clean label food products Changmou Xu1, cxu13@unl.edu, Yuzhen Zhou2, Guangshun Wang3. (1) Dept. of Food Sci. and Tech., Univ. of Nebraska-Lincoln (2) Dept. of Statistics, Univ. of Nebraska-Lincoln (3) Dept. of Pathology and Microbiology, Univ. of Nebraska Medical Center, Omaha With more and more consumers choosing clean label foods with natural and healthy ingredients for better lifestyle, and avoiding foods made with chemical additives to minimize the risk of health and disease, natural food antimicrobials play an increasing critical role in the clean label food market. However, commonly used food antimicrobials present various limitations. Therefore, novel natural antimicrobials are urgently needed by the food industry. The interest in natural antimicrobial peptides and proteins (AMPs) is increasing recently because of their broad range of activity, stability to commonly used food processes, which enable them to represent promising alternatives to traditional antimicrobials. Nevertheless, studies on the discovery and application of AMPs to foods are still quite limited. At present, only few bacterial AMPs, such as nisin, have been approved as a food antimicrobial in multiple countries, leaving thousands of other AMPs in the antimicrobial peptide databased (APD) untapped. It is logical to assume that there are more candidates like nisin in the database, which are suitable for food applications. The search, however, has been hindered as a consequence of limited information, inadequate tools, and ineffective research strategies. This presentation will introduce a novel approach for rapidly discovering potent antimicrobial peptides as natural food antimicrobials to improve safety, quality, and shelf-life of clean label food products. The study integrated a well-recognized Nebraska APD database, deep understanding of antimicrobial peptides, state-of-the-art machine learning algorithms, and solid scientific knowledge of natural food preservatives. How to develop effective applications of natural AMPs in food products also will be discussed. Promisingly, this approach may lead to a breakthrough solution for rapidly discovering novel and natural food antimicrobials of great benefit to the food industry, consumers, and environment.

A088 Antioxidants and antimicrobials to maintain freshness and minimize Listeria contamination of fresh-cut apples Xuetong Fan, xuetong.fan@usda.gov. USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania Fresh-cut apples which offer consumers health benefits and convenience have become popular in recent years. There are two major challenges in the processing of fresh-cut apples: development of cut surface browning and possible contamination with human pathogens such as Listeria monocytogenes. The surface browning that impairs sensory properties and discourages consumer purchase of fresh-cut apples is mainly a result of enzymatic reaction of endogenous phenolics with oxygen catalyzed by polyphenol oxidase (PPO). Many antibrowning agents have been developed and evaluated to inhibit PPO activities

by using reducing agents (antioxidants), chelating agents, acidulants, etc. However, these compounds have no or little antimicrobial activity against human pathogens and spoilage microorganisms. Indeed, there have been numerous Listeria recalls of fresh-cut apples that had been treated with antibrowning agents in recent years. The source of L. monocytogenes could be preharvest and postharvest, which ultimately lead to the contamination of antibrowning solutions and cut apples. Therefore, chemicals that have both antimicrobial and antibrowning properties have been investigated, such as organic acids, sodium chlorite, and sodium acid sulfate. However, individually the compounds have limited effectiveness in inhibiting browning or reducing populations of L. monocytogenes. Combinations of antimicrobial and antibrowning agents have been investigated. Challenges remain to develop formulations that are natural, safe, economical, and consumer-friendly to meet the shelf-life desired by the fresh-cut apple industry.

A089 Grape pomace as a natural antimicrobial and antioxidant and their application in active food packaging Yixiang Xu, sueva2010@gmail.com, Edward Sismour. Agricultural Research Station, Virginia State Univ., Petersburg Grape pomace is the residue of grapes from wine or juice making and consists primarily of the skin, pulp, seeds, and stems. It accounts for approximately 20% of the grapes (by weight) and around 16 million tons of grape pomace were produced in 2018. It is generally treated as a low-valued waste, and the efforts have been made to explore different value-added alternative utilizations for the pomace, including the extraction of bioactive polyphenolic compounds for potential applications as antioxidant and antimicrobial agents in food, pharmaceuticals and cosmetics. Even though Virginia ranks No. 6 in wine grape production in the U.S, the limited information is available concerning pomaces from grape varieties produced in Virginia. The goals of our research are to (1) investigate phenolic compounds, antioxidant and antibacterial properties of pomaces from Virginia-grown grape varieties, (2) incorporate grape pomace extract into starch nanocomposite films to evaluate their antioxidant and antimicrobial effectiveness on ready-to-eat meat. The results indicated that significant differences were found among the different varieties of grape pomaces in relation to the concentrations of total phenolic, total flavonoids, total anthocyanins, tannins, and condensed tannins and to DPPH and ABTS free-radical scavenging assays. All pomace extracts exhibited antibacterial activity against L. monocytogenes ATCC 7644 and S. aureus ATCC 29213, but no activity was observed against E. coli O157:H7 ATCC 3510 or S. typhimurium ATCC 14028. Further, incorporation of grape pomace into starch nanocomposite films improved antioxidant and antimicrobial activities both of the films and following meat application. Nanocomposite films incorporating with grape pomace extract exhibited stronger inhibitory effects against Staphylococcus aureus ATCC 29213 than Listeria monocytogenes ATCC 7644. Application of grape pomace extract enriched-nanocomposite films on the meat surface resulted in progressively lower pH values and increasingly darker coloration throughout the storage periods. The study demonstrated that the starch films incorporating grape pomace extracts have the potential for antimicrobial food packaging application.

A090 Biobased microcarriers for enhanced antimicrobial delivery to improve food safety and quality Kang Huang, kghuang@ucdavis.edu. School of Chemical Sciences, The Univ. of Auckland, New Zealand Despite the rapid development of innovative food products and processes, there are significant microbial food safety and spoilage issues that highlight the limitation of sanitation and washing processes. The conventional antimicrobial approaches are not effective in reducing the load and growth of pathogenic and spoilage microbes on raw or minimally processed foods and minimizing the risk of cross-contamination between foods and food contact surfaces. The current antimicrobial delivery vehicles have limited dispersibility in complex systems, poor stability in harsh environments, and lack of specificity and affinity for target microbes. In our studies, multiple types of novel bio-based antimicrobial delivery systems have been developed to effectively target harmful microbes and deliver antimicrobial molecules to inactivate both bacterial and fungal biofilms. The bio-based microcarriers were developed to encapsulate a broad spectrum of antimicrobial compounds including hydrophilic, lipophilic and even amphiphilic molecules (e.g., chlorine binding polymer, essential oils, curcumin, and metallic nanoparticles). These studies demonstrate the high affinity of bio-based compositions to bind target bacterial and fungal cells and inactivate more than 5 logs of model pathogenic bacteria and fungi in wash water without and with high organic load. In addition, it has been demonstrated that these bio-based compositions can enhance the inactivation efficacy against bacterial and fungal biofilms. The enhanced antimicrobial activity can be attributed to three factors: a) localized high concentration of antimicrobials within bio-based microcarriers; b) high affinity of bio-based microcarriers to bind diverse microbes; c) improved stability of antimicrobials in organic-rich aqueous environment. In summary, these unique attributes of bio-based carriers will significantly enhance the sanitation efficacy of biofilms, reduce persistence and transmission of antimicrobial resistance microbes, limit the use of antimicrobial chemicals, and improve the cost-effectiveness of sanitizers.

A091 Potential new antimicrobials/antioxidants from peptides using high voltage field technology Tony Jin, tony.jin@usda.gov. Eastern Regional Research Center, U.S. Dept. of Agriculture, Wyndmoor, Pennsylvania Natural antimicrobials and antioxidants are greatly demanded by food industry and consumers. In recent years, there has been a growing interest in the use of natural or bio-based antimicrobials or antioxidants for enhancing food safety and food quality. Pulsed electric fields (PEF) technology applies high voltage pulses on food product and has been used for food pasteurization, extraction and dehydration. There is a new research area using high voltage pulses for enhancing peptides' functional properties and health-promoting bioactivities from their precursor proteins. This presentation will focus on the potential of PEF application in the development of new antioxidation and antimicrobial from proteins hydrolysates, using caseinate, soy protein and whey protein as models. Our preliminary study revealed that a significant increase on the DPPH free radical scavenging rate was found in sodium caseinate hydrolysate after PEF treatment; and PEF treated sodium caseinate-typsin, whey protein isolate-trypsin, soy protein isolate-pancreatin hydrolysates had significant greater antimicrobial activities against E. coli and Listeria than those without PEF treatments. This study demonstrates a new approach for producing potential natural antimicrobial and antioxidants using PEF technology.

A092 Discovery of a gut bacterial metabolic pathway that drives α-Synuclein aggregation and neurodegeneration Lizett Ortiz de Ora1, Kylie Uyeda1, Elizabeth Bess1,2, elizabeth.bess@uci.edu. (1) Chemistry, Univ. of California Irvine (2) Molecular Biology & Biochemistry, Univ. of California Irvine A new approach to predict Parkinson's disease (PD) risk and slow its progression may be found in the metabolic reactions performed by the gut microbiota. Pathogenic aggregates of a protein called α-synuclein (α-syn) accumulate in intestinal tissue before spreading to the motor cortex of the brain where they cause neurodegeneration and PD; however, the factors causing α-syn to aggregate in the gut have remained incompletely understood. Although α-syn aggregation has been linked to gut inflammation via oxidative stress, our findings suggest that the oxidizing redox potential created by the gut microbiota—not the host—can modulate α-syn aggregation. More specifically, our

data indicate that nitrite, a potent oxidant produced by gut bacterial nitrate respiration is a critical inducer of α-syn aggregation. Gut bacteria capable of nitrate respiration include members of the bacterial family Enterobacteriaceae, such as Escherichia coli. Respiration of nitrate by E. coli K-12 yielded nitrite, which oxidized Fe2+ to Fe3+ and created an oxidizing redox potential in these bacterial cultures. Fe3+ then caused oxidation of dopamine to a quinone, which induced aggregation of α-syn (Fig. 1). Genetic knockouts of nitrate respiration (ΔmoaA) prevented α-syn aggregation, and only in the presence of nitrite did abiotic incubations of dopamine, iron, and α-syn yield α-syn aggregates. Exposing nitrite, but not nitrate, to enteroendocrine cells, in vitro, induced aggregation of the α-syn that is natively expressed in these cells, which line the intestinal tract. We examined the in vivo relevance of bacterial nitrate respiration to α-syn aggregation using gnotobiotic α-syn-overexpressing (ASO) C. elegans. We discovered that nematodes colonized with nitrate-respiring bacteria displayed significantly elevated levels of α-syn aggregates. Accumulation of α-syn aggregates corresponded with impaired motor function that is characteristic of neurodegeneration, a hallmark of PD. We are expanding our studies to examine the role of nitrate respiration in α-syn aggregation in mice. We are also leveraging the molecular-level insight garnered through this work to discover new ways to prevent intestinal α-syn aggregation.

A093 Discovery and characterization of gut microbial enzymes involved in keto-reductive metabolism Liangyu Qian1, liangyuqian@tamu.edu, Huanrong Ouyang1, Lois Gordils-Valentin2, Joshua Hong3, Arul Jayaraman1, Xuejun Zhu1. (1) Chemical Engineering, Texas A&M Univ., College Station (2) Genetics, Texas A&M Univ., College Station (3) Biology, Texas A&M Univ., College Station Ketone reduction is a central chemical transformation in the gut microbial metabolism of food-derived compounds and small-molecule pharmaceuticals. However, the corresponding bacterial enzyme involved in metabolism remains elusive. Here, we characterized an oxidoreductase from the human gut bacterium Clostridium bolteae capable of reducing the ketone groups residing in two drugs (i.e., nabumetone and hydrocortisone) and two ketone-bearing dietary chemicals (i.e., raspberry ketone and zingerone). In addition, we have also identified additional oxidoreductase homologues that have similar ketone-reducing activities from multiple human gut microbial species. Our results expand the gut bacterial enzymatic inventory for the ketone-reduction of pharmaceuticals and dietary chemicals, but it also serves as the basis for elucidating bacteria-chemical interactions and illuminating strategies for future personalized medicines and dietary plans.

A094 Gut microbial metabolism of aromatic amino acids under dietary and microbiota interventions Chi Chen, chichen@umn.edu, Yuyin Zhou. Food Science and Nutrition, Univ. of Minnesota Twin Cities, Minneapolis The acceptance of gut microbiota as an important metabolic and endocrine organ is mainly based on the energy supply and regulatory functions of their microbial metabolites. Unabsorbed aromatic amino acids (AAAs), undergoing oxidation and reduction as well as lyase-mediated elimination and decarboxylation in microbial metabolism, can form various aryl metabolites with diverse bioactivities, but the contribution of individual metabolic pathways to the formation and distribution of these metabolites as well as their responses to chemical and microbial interventions are not well examined. In this study, deuterated AAAs were used as the sole source of dietary AAAs to trace their metabolic fates in mouse. The results showed that besides dietary AAAs, endogenous AAAs are also the major contributor of microbial metabolites. Tyrosine and phenylalanine undergo both oxidative and elimination reactions, producing phenylacetate (PAA), 4-hydroxyphenylacetate (4HPAA), p-cresol, phenol, and their conjugates as their major microbial metabolites, while tryptophan is mainly degraded by elimination reaction, producing indoxyl sulfate as a major microbial metabolite. Modulation of microbial AAA metabolism by microbiota and chemical interventions were investigated by the treatments of antibiotics, fecal microbiota transplantation (FMT), and green tea polyphenols (GTP). In both humans and mice, the production of p-cresol is highly sensitive to antibiotics and FMT since urinary p-cresol sulfate was depleted by antibiotics and then quickly restored by FMT through drastic changes in the gut microbiota. In contrast, chronic GTP consumption in humans did not significantly alter the microbial composition, but decreased urinary hippuric acid, indoxyl sulfate, and phenylacetylglutamine, potentially through competitive inhibition in the microbial metabolism of GTP and AAAs. Overall, microbial metabolism of AAAs is dominated by oxidative and elimination reactions. Because of its susceptibility to microbiota and chemical interventions, microbial metabolism of AAAs could be a target for dietary and therapeutic modulations of gut microbiota in humans and animals.

A095 Effect of fructooligosaccharide on the adult human gut microbiome in vitro Karley Mahalak1, karley.mahalak@usda.gov, Jenni Firrman1, Lin Liu1, Weiming Hu2, Kyle Bittinger2. (1) USDA Agricultural Research Service, Washington, District of Columbia (2) Division of Gastroenterology, Hepatology, and Nutrition, The Children's Hospital of Philadelphia Research Inst., Philadelphia, Pennsylvania Fructooligosaccharide (FOS) is a well-known carbohydrate that promotes a healthy gut microbiota and has been previously demonstrated to enhance levels of Bifidobacterium and Lactobacillus. In this study, we used a 24 hour in vitro culturing method to compare the effects of FOS on the gut microbiota of 3 different adult age groups that range from young adult to elder adults. The cultured communities were subject to 16s rRNA sequencing to determine the structure and LC-MS/MS analysis to measure short-chain fatty acid (SCFA) levels, which is an indicator of community function. qPCR analysis targeting Bifidobacterium was applied to measure the enhancing effect of FOS on this taxon. The results of this study demonstrate the positive effects of FOS on the gut microbiome, and importantly, how age may play a role in the effectiveness of this prebiotic.

A096 Understanding the gut as a human bioreactor Elaine Holmes, elaine.holmes@imperial.ac.uk. Imperial College London, United Kingdom The research focuses on discovery of metabolic biomarkers of disease. Novel techniques were developed to characterize gut microbiome host metabolic interactions toward the study of gastrointestinal related disease states.

A097 Vitamin derivatives as effective light controlled biocidal agents for food contact surfaces Gang Sun1, gysun@ucdavis.edu, Zheng Zhang1, Peixin Tang1, Nitin Nitin1,2, Luxin Wang2. (1) Biological and Agricultural Engineering, Univ. of California, Davis (2) Food Sci. and Tech., Univ. of California, Davis Recent research and development have revealed that certain vitamin compound and derivatives, including phylloquinone (VK1), menatetrenone (VK2), menadione (VK3) menadiol diacetate (VK4), menadione sodium bisulfite (MSB, soluble VK3 derivative), riboflavin (RF, VB2), and flavin mononucleotide (FMN, VB2 derivative), are photo-active and can produce reactive oxygen species (ROS) under daylight or UVA illuminations. These agents are basically edible and safe for applications for food contact materials without showing any biocidal functions under dark. Their photoactive mechanisms and produced reactive oxygen species, which are the biocides in the systems, are different, thus, their applications may need varied environment to provide the desired light-induced biocidal functions. In addition, the ROS are super reactive and only exist in very short time after

generation. These features make the applications of the agents in various antibacterial surfaces and materials uniquely different and challenging. In this presentation, the photo-induced biocidal mechanisms of representative compounds are discussed with computational modeling and experimental results. Creative applications of the agents in food preservation and reduction of biofilms under varied lighting conditions will be illustrated.

A098 Antioxidant behavior of polypropylene-graft-maleic anhydride Halle Redfearn, hnr22@cornell.edu, Julie M. Goddard. Food Science, Cornell Univ., Ithaca, New York Oxidative degradation in food and beverages is one of the major causes of food spoilage, prompting the need for antioxidant additives to decrease food waste. Development of nonmigratory antioxidant packaging offers an alternative to reliance on direct food additives to control oxidation. Reactive extrusion (an industrially relevant, solvent-free process) has been used to produce polypropylene-graft-maleic anhydride (PP-g-MA), one of the oldest and most common modifications to polypropylene. While the dicarboxylic acid groups should offer the radical scavenging and metal chelating properties demonstrated in other nonmigratory antioxidant packaging chemistries, the antioxidant behavior of PP-g-MA has never been reported. Here, PP-g-MA is compounded with isotactic polypropylene in a twin-screw extruder, leading to partial hydrolysis to form polypropylene-graft-succinic acid (PP-g-SA) that was analyzed for antioxidant behavior. Since radical scavenging and metal chelating capacity of PP-g-MA is dependent carboxylate formation, pH-dependent surface characterization was performed. Partial hydrolysis during extrusion of PP-g-MA films was confirmed using attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR) with absorbances at 1775 cm-1 characteristic of the anhydride group in PP-g-MA and absorbances at 1708 cm-1 representing the carboxylic acid groups in PP-g-SA. ATR-FTIR also confirmed increasing hygroscopicity at pH > 4 by the appearance of a water band at 3000-3600 cm-1, which can be attributed to carboxylate formation. Precise surface pKa's of the PP-g-SA carboxylic acids were calculated using FTIR integration of the carboxylic acid band, and wettability was examined by advancing water contact angle. The extruded films exhibited significant radical scavenging capacity of 2.05 ± 0.43 nmol Trolox(eq)/cm2 and iron chelating capacity of 16.18 ± 0.63 nmol/cm2. Films were further characterized for inhibition of ascorbic acid and lycopene degradation and prevention of lipid peroxidation. This work highlights the potential application of commercial PP-g-MA as a scalable, industrially relevant, and widely available material for non-migratory antioxidant active packaging applications.

A099 Combined effect of biodegradable packaging with natural antimicrobials and physical agents for liquid foods preservation Luis J. Bastarrachea, luis.bastarrachea@usu.edu. Nutrition, Dietetics, and Food Sciences, Utah State Univ., Logan Polylactic acid (PLA) is one of the most functional biodegradable polymers, as it offers similar properties the petroleum-derived plastics offer, such as mechanical strength, machinability, and versatility for chemical modification. Chitosan is a polycation of natural origin with broad antimicrobial spectrum. In the present study, we have modified PLA for it to harbor chitosan and to test its antimicrobial effect during the storage of liquid foods such as fruit juices or milk after they have been exposed to physical agents such as mild heat, ultrasound, or UV light. This antimicrobial biodegradable plastic exhibits high stability and durability against harsh conditions of extreme pH and heat for food processing applications. The modified PLA alone has a microbial inhibitory property, which effectiveness depends on the type of food and on the type of microorganism (Gram positive or Gram negative bacteria). The physical agents (mild heat, ultrasound and UV light) alone or in combination can substantially enhance the antimicrobial effect of the modified antimicrobial PLA due to the injury caused on the microorganisms, which in some cases can be consummated during storage at refrigeration temperatures. This approach may represent a new and sustainable hurdle technology concept for food preservation.

A100 Fungicidal constituents from phytopathogens Kumudini M. Meepagala, kmeepaga@olemiss.edu. USDA-ARS Natural Products Utilization Research Unit, Univ., Mississippi Phytopathogenic fungi use the host plants to survive by absorbing nutrients from the host plant. Some of these phytopathogens produce fungitoxic compounds to compete with other fungi that can infect the host plant. Thus, we speculate that plant pathogenic fungi may be good sources from which to isolate and identify fungicidal compounds that can be used in crop protection. We have isolated and identified fungi that cause disease symptoms on crops and other ornamental plants. These fungi were grown in potato dextrose agar and were identified by molecular techniques. The liquid culture broths of various fungi were extracted with ethyl acetate followed by butanol. We have also observed that the yields of the fungal metabolites were significantly increased when the cultures were grown in the presence of 10% Diaion HP20.These extracts were tested on TLC bioautograpy to detect the presence of antifungal constituents. The fungi belonged to numerous genera such as Diaporthe, Phoma, Didymella and Chaetomium. In this paper extraction, isolation, structure elucidation and bioassay of antifungal constituents from various genera of phytopathogenic fungi will be discussed.

A101 Application of natural antimicrobials for the preservation of fresh produce Xiuxiu Sun1, xiuxiu.sun@usda.gov, Anne Plotto2, Jinhe Bai2. (1) Pacific Basin Agricultural Research Center, USDA Agricultural Research Service, Hilo, Hawaii (2) Horticultural Research Laboratory, USDA Agricultural Research Service, Ft. Pierce, Florida Fresh produce possess high nutritional value with various health benefits, but their shelf life can be relatively short depending on the commodity. Therefore, the extension of fresh produce's shelf life is critical for industry and consumers. Natural additives have been widely applied by the food industry for various purposes. Essential oils are natural compounds extracted from plants, many of which show antimicrobial and antioxidant activities. In our research, an active packaging system containing controlled-release essential oils, in sachet or coating form, was applied to fresh blueberries, strawberries, and papaya. Essential oils containing coatings reduced the populations of bacteria and yeasts/molds on the surface of the blueberries up to 6 logs. The activity of the compounds also resulted in significantly reduced weight loss, better firmness, and better sensory taste of blueberries, strawberries, and papaya. Our research results indicate that natural antimicrobial essential oils could be used for the preservation of fresh produce to extend their shelf life.

A102 New ethyl phenolic branched chain fatty acid arginate products with antimicrobial and surfactant properties Helen Ngo, helen.ngo@usda.gov, Xuetong Fan. USDA Agricultural Research Service, Wyndmoor, Pennsylvania Pathogenic microorganisms are a threat to human health since they can cause severe infectious diseases, and to inactivate these pathogens, numerous antimicrobial agents have been developed. This presentation focuses on a new class of ethyl phenolic branched chain fatty acid arginate products derived from natural reagents such as arginine, phenolic and fatty acid. The products can be prepared in four steps starting with the phenolic branched chain fatty acid material. This multistep synthesis is found to be general and can be applied to any type of fatty acids including iso-oleic acid. All intermediates and desired products can be characterized by attenuated total reflectance fourier transform infrared, mass spectrometry, and nuclear magnetic resonance. From the micro-dilution method, these ethyl phenolic fatty acid arginate products are active against Gram-positive bacteria with the minimum

inhibitory concentration and minimum bactericidal concentration slightly better than commercial ethyl lauroyl arginate. The enhanced bioactive properties come from the hydroxyl functional group on the aromatic ring as it improves the hydrophilicity of the fatty acid. These compounds are also found to have superior ability in lowering the surface tension than the commercial product, which can be developed into antimicrobial surfactants for applications in foods, cleaners, and coatings.

A103 Antimicrobial activity of defence phytochemicals: Prenylated (iso)flavonoids and isothiocyanates Carla Araya Cloutier, carla.arayacloutier@wur.nl, Sylvia Kalli, Silvia Andini, Jean-Paul Vincken. Laboratory of Food Chemistry, Wageningen Univ. & Research, Gelderland, Netherlands Defense phytochemicals are produced de novo in the plant upon stress and have been acknowledged for their antimicrobial activity. Prenylated (iso)flavonoids are the main class of defence phytochemicals in the Fabaceae (e.g. soybean). By simultaneous malting and fungal elicitation of soybeans the amounts of prenylated (iso)flavonoids and consequently their antimicrobial activity can be enhanced. Broad diversity in the (iso)flavonoid skeletons, the number of prenyl groups, and the prenyl configurations can be found in nature. Evidence shows that these variations play a key role in their antimicrobial properties. Diprenylated (iso)flavonoids, bearing two prenyl chains, were among the most active antibacterials against Gram positive bacteria, e.g. L. monocytogenes, with minimum inhibitory concentrations (MIC) of < 10 μg/mL. Furthermore, monoprenylated isoflavonoids showed the best anti-yeast activity, with a MIC of ≤ 15 μg/mL against Z. parabailii. Regarding the mode of action, it was shown that prenylated (iso)flavonoids can rapidly disrupt the integrity of the cytoplasmic membrane. Isothiocyanates (ITCs) are another class of defence phytochemicals released upon degradation of glucosinolates, as a defense response in the Brassicaceae family. Isothiocyanates bear an -N=C=S group, which makes them highly reactive towards nucleophiles. The antimicrobial properties of ITCs, mainly of allyl ITC (AITC), has been reported before, nonetheless, the antimicrobial properties and spectrum of activity of different ITC subclasses, bearing different side chains, have not been investigated before. Isothiocyanates (ITCs) with short chained methylsulfinyl (MS) or methylsulfonyl (MSo) groups showed good antimicrobial activity (MIC 25 μg/mL) against Gram negative bacteria (E. coli). ITCs with a long chained MS/MSo groups showed good antimicrobial activity (MIC ≤ 25 μg/mL) against Gram positive bacteria (B. cereus, L. monocytogenes) and fungi (S. cerevisiae and A. niger spores). The quantitative structure-activity relationships of these natural antimicrobials will be discussed and lead compounds for the development of novel antimicrobial strategies will be highlighted.

A104 Chemical compositions and antioxidant activities of 36 typical pomegranates grown in China Wenhao Zheng2, zhengwenhao@sjtu.edu.cn, Yinghua Luo1, luoyinghua@cau.edu.cn, Boyan Gao2, raphaelgao1985@gmail.com, Liangli Yu3. (1) China Agricultural Univ., Beijing, China (2) Shanghai Jiao Tong Univ., China (3) Univ. of Maryland at College Park, College Park The edible parts of 36 cultivars of pomegranate grown in China were collected to make comparisons of their major chemical compositions and potential bio-activities. The chemical compositions, especially the phenol contents of peels from these pomegranates were also determined using ultra-performance liquid chromatography coupled with quadrupole time-of-flight mass spectrometry (UPLC-Q TOF MS). Besides, the triacylglycerol compositions and fatty acid profiles of oils from pomegranate seeds were identified and semi-quantified. As the results, pomegranates with deeper color of arils contented greater amounts of total phenolic components, total anthycanins, and greater antioxidant activities in general. The peels of all the pomegranate samples contented remarkable phenolic compounds. Individual results showed that pomegranate sample No. 27 has the greatest phenolic content and antioxidant activity, and could be recognized as the major direct edible cultivars of pomegranate. The peel of No. 7 cultivar of pomegranate has the greatest phenolic content, and No. 29 cultivar has the greatest triacylglycerol contents in pomegranate seed. Further development about the byproduct of these pomegranates after industrial processing should be focused on in the future.

A105 Ultrasound improves the antibacterial effect of thyme essential oil nanoemulsions against foodborne pathogens in simulated and real food system Mingming Guo, mingguo@zju.edu.cn, Qiao He, zhehao yang. College of Biosystems Engineering and Food Science, Zhejiang Univ., Hangzhou, China Development of novel and effective antibacterial technologies to ensure the microbiological safety of food items has gained considerable attention, mainly driven by numerous outbreaks. Essential oil nanoemulsions have been proven to have stronger antimicrobial effects compared to the essential oil alone or coarse emulsion. Sonoporation could be the promising candidate to trigger a synergistic effect with thyme essential oil nanoemulsion (TEON) and produce a more effective antibacterial efficacy. Therefore, in our studies, the bactericidal effects of ultrasound (US) in combination with TEON treatments against Escherichia coli (E. coli) O157:H7 and Staphylococcus aureus (S. aureus) were investigated in both liquid simulated system and real food matrix. The optimal ultrasonication and emulsifier concentration conditions for the preparation of three different TEON with enhanced dispersion characteristics and antibacterial activity were obtained by response surface methodology. The results showed that TEON-CPC obtained at 350 W, 14.44 min, and 0.15 mg/mL exhibited excellent antibacterial activity through electrostatic interaction. Afterward, the optimal TEON was selected for the further investigation of antimicrobial effect and mechanism of its combination with US on the microbial inactivation. The combined treatment reduced the E. coli and S. aureus population by 2.16-7.10 and 3.21-4.51 log CFU/mL, respectively, indicating the effects of ultrasonic field on facilitating the antibacterial efficacy of TEON. Moreover, remarkable synergistic effect of the combined treatment was also achieved, which decontaminated the E. coli populations by 4.49–6.72 log CFU/g on the surface of cherry tomatoes. As for the antibacterial mechanism, the combined treatment led to drastically larger extent of membrane disintegration, fluidity reduction, membrane depolarization, and membrane composition modification than the single use of ultrasound and TEON. It could be concluded that US could induce physical damage on cell morphology, facilitating the entry of TEON into the bacteria; reduce the bacterial membrane hydrophobicity that would increase the odds of TEON interacting with the cellular membrane. Overall, US combined with TEON was proved to be a promising and feasible alternative for the reduction of microbiological contaminants in food industry.

A106 Gut microbiome variation influences host responses to diet Federico Rey, ferey@wisc.edu. Dept. of Bacteriology, Univ. of Wisconsin System, Madison We are exploring the relationship between interpersonal differences in gut microbiome and health benefits obtained from the consumption of common vegetables, legumes and whole-grains. These foods represent major sources of fiber among US consumers and have been associated with protective effects against cardiometabolic disease (CMD). However, human studies have revealed a large degree of interpersonal variation in the effects associated with their consumption, with a subset of individuals not exhibiting any benefits. Furthermore, we cannot currently predict who will benefit from their consumption. I will discuss our studies in gnotobiotic mice transplanted with human communities that suggest that protection against CMD associated

with consumption of these high-fiber diets is modulated by the gut microbiome, and the host responses associated with specific microbes and microbial metabolites derived from specific foods.

A107 Mechanistic implications of the synergistic effect of diabetes drug metformin with the lactate dehydrogenase inhibitor sodium oxamate Bishambar Dayal1, dayalb77@gmail.com, Michael A. Lea2. (1) Medicine, RWJ-MS Rutgers Univ., New Brunswick, New Jersey (2) Microbiology, Biochemistry and Molecular Genetics, Rutgers Univ. New Jersey Medical School, Newark Recently we described a critical role of Artificial Intelligence (AI), a screening tool at an early stage for diabetic retinopathy identifying tiny lesions, hemorrhages, discoloration resulting in blindness (ACS April 2021). A description of the biological significance of metabolic inhibitors metformin, phenformin and a mono- guanide (2-aminoguanidine) as anti-diabetic drugs and their comparison with bioactives present in okra seed extract and bitter melon peel as well as their receptor was elucidated. Present studies describe mechanistic implications of the synergistic effect of sodium oxamate with the anti-diabetic drug metformin. Sodium oxamate, is a lactate dehydrogenase (LDH) inhibitor and has been used with phenformin to reduce the side-effect of lactic acidosis. The nucleophilic metabolic inhibitors biguanide, phenformin and a monoguanidie 2-aminoguanidine are associated with more severe lactic acidosis side effects than metformin and were withdrawn in late1970 for the treatment of diabetes. The present studies describe the nature of the chemical compound formed when metformin was treated with sodium oxamate: Briefly, metformin (20 mg) in 2ml ethanol was mixed with sodium oxamate (30 mg), 200 microliters triethylamine and 200 microliters glacial acetic acid and the mixture microwaved for 50 seconds. The reaction mixture was resolved by analytical and preparative TLC and analyzed via Nanodrop Spectrometer and Electrospray Ionization Mass Spectrometry (ES-API, Neg. Scan exhibited m/z 164 (100 %). A tentative reaction mechanism and molecular weight assignment showed a 7 membered ring (m/z 164 (m/z 182-H2O). These observations will be potentially helpful in explaining recent studies advanced by Rajesh Kumar et al. (AACR April 25, 2018) on the efficacy of biguanides metformin and phenformin preventing pancreatic ductal adenocarcinoma (PDAC) where phenformin was demonstrated five times better drug than metformin.

A108 Metabolic interplay between gut microbiome and host FGF21during dietary protein restriction Gertrude Ecklu-Mensah1,2, gecklumensah@health.ucsd.edu, Anthony Martin3, Connie Ha3, Gustaf Hendrick3, Don Layman4, Jack Gilbert1,2, Suzanne Devkota3. (1) Pediatrics, Univ. of California San Diego, La Jolla (2) Univ. of California San Diego Scripps Institution of Oceanography, La Jolla (3) F. Widjaja Foundation Inflammatory Bowel & Immunobiology Research Inst., Cedars-Sinai Medical Center, Los Angeles, California (4) Food Science and Human Nutrition, Univ. of Illinois at Urbana-Champaign, Urbana Alterations in macronutrient intake such as restricting protein intake can induce adaptive changes in host-microbe metabolism and interactions. Fibroblast growth factor 21 (FGF21) is a well-recognized host endocrine molecule necessary to sense, respond and metabolically adapt to dietary protein restriction and macronutrient stress. We were primarily interested in the ability of dietary fibers to attenuate macronutrient stress response on protein restricted (PR) diets. Mice were fed PR diets supplemented with either 5% or 15% of two different fiber types, cellulose, and inulin. We monitored whole-body growth rate, FGF21 protein stress response and gut microbiota alterations. Cellulose supplementation, in the context of protein restriction, attenuated the FGF21 stress response and maintained growth rate in mice. The attenuated FGF21 response accompanying PR cellulose fiber diets involved alterations in the gut microbiota of differentially abundant taxa of several genera including Parabacteroides, Akkermansia, Turicibacter and Oscillopira. In the absence of a gut microbiota, FGF21 could not signal appropriately in the face of protein restriction, suggesting the gut microbiota potentially mediates FGF21 nutrient stress signaling during protein restriction. Overall, our data suggest that cellulose fiber supplementation of PR diets enrich cellulose-specific bacterial species that synthesize bacterial metabolites for host utilization to make up for limited dietary resources. This, in turn, leads to the abrogation of the liver FGF21 stress response to protein restriction, resulting in normalized growth promotion.

A109 Novel combinations of prebiotics and polyphenols and their effects upon gut and cognitive health in active military personnel Briony Sayers, b.sayers@pgr.reading.ac.uk, Glenn R. Gibson, Anisha Wijeyesekera. Dept. of Food and Nutritional Sciences, Univ. of Reading, Berkshire, United Kingdom Active military personnel are often subject to extreme stressors, whether psychological or physical. Such stressors often result in severe gastrointestinal (GI) diseases and cognitive perturbations such as Post Traumatic Stress Disorder (PTSD). Though there are available pharmaceutical treatments, they may not be viable, whether due to poor efficacy, unwanted side effects, or economic detriment. Nutraceutical interventions such as polyphenols and prebiotics may improve psychological and gut health in soldiers and reduce effects of PTSD and related GI issues on health and wellbeing. By exploring nutritional interventions both in vivo and in vitro, it may be possible to establish whether prebiotic and polyphenol combinations are a potential treatment for military personnel. This study's objective is to determine whether increased intake of polyphenols and prebiotics can improve psychological and gut health in soldiers and reduce the effects that PTSD and GI issues have on soldier wellbeing. The hypothesis is that consumption of a novel combination of prebiotics and polyphenols will have a beneficial effect on GI and cognitive health of military personnel. Effects of prebiotics and polyphenols on the gut microbiome have been determined using pH controlled in vitro batch fermentation models. Results will be correlated to neurotransmitter levels using liquid chromatography–mass spectrometry (LCMS) to establish any link between food type consumption and cognitive function. The aim is to identify metabolites present within a cognitive impaired state through comparison to a human study at US Army, Natick (prebiotic effects will be assessed in Reading). Further in vitro work was done by use of fed batch culture with the same LCMS methods as well as DNA sequencing. A further human trial will begin shortly with participants taking a supplement for 2 weeks. Whilst LCMS is ongoing, preliminary results from batch culture work, namely from fluorescent in situ hybridisation flow cytometry, show that a batch culture vessel containing a combination of prebiotics and polyphenols was more effective than inulin alone. Results from GC show that combined batch culture contained increased lactate, which is positive for brain function and mood. Though more analysis is needed, results so far are promising in terms of increased bifidobacteria with combined nutraceuticals. This may improve health in military personnel but needs to be determined in vivo, which is currently underway.

A110 Effects of supplementation with polyphenols and fiber on gut microbiota form and function during parallel batch fermentation Jordan Whitman1, jordan.a.whitman2.civ@army.mil, Laurel A. Doherty1, Ida Pantoja-Feliciano1, J. P. Karl2, Kenneth Racicot1, Syed Hussain1, Jason W. Soares1. (1) Soldier Effectiveness Directorate, DEVCOM Soldier Center, Natick, Massachusetts(2) US Army Research Inst. of Environmental Medicine, Natick, Massachusetts Gut microbial metabolism of recalcitrant food components, particularly polyphenols and insoluble fiber, is associated with numerous beneficial effects to the host. Use of in vitro fermentation to simulate colonic conditions facilitates greater

insight into microbial metabolic processes. Here, we present the results of a parallel batch fermentation study to characterize microbiome response to supplementation with polyphenols and fiber. Fecal inocula were prepared by pooling samples from multiple volunteers to normalize individuals' microbiota. Inocula were added to a nutrient-rich medium supplemented either with a mixture of four purified polyphenols, a blend of three fiber sources, or both in combination at 37oC under controlled anaerobic atmosphere. Aliquots were collected at specific time points during the study and analysis of select bacterial growth and metabolite production was determined using qPCR, GC-FID and benchtop assay analysis. Results from qPCR saw differential growth of observed organisms when supplemented independently with polyphenol or fiber and in combination. Increases in beneficial bacterial genus like Lactobacillus and Bifidobacterium and decreases in antagonistic bacterial species like E. rectale were observed when comparing 0 hour samples to 24 hour samples in vessels containing polyphenols, fiber and their combination. Supplementation independently and in combination of polyphenols and fiber reduced the amount of indole, a product of protein fermentation, generated during the fermentation, compared to vessels without supplementation. Preliminary results suggest an increased production of antioxidants in vessels supplemented with polyphenol, with no additional effect due to fiber supplementation, compared to polyphenol-deficient vessels. The effects of supplementation on short-chain fatty acid and ammonia production will also be presented. Supplementation with polyphenols and fiber independently have beneficial effects on gut microbiome health but the synergistic effects of their combination maximized these benefits. The results of this study will inform an ongoing human nutritional intervention study wherein these components are included in a supplemental food bar. Improved understanding of the interplay between dietary inputs, gut microbial metabolism, and host health furthers our overall goal of improving Soldier resilience to military-relevant stressors through nutritional intervention.

A111 Lactose as a modifier of the gut microbiota Jenni Firrman1, jenni.firrman@ars.usda.gov, Lin Liu1, Karley Mahalak1, johanna lemons1, Peggy Tomasula1, Weiming Hu2, Kyle Bittinger2. (1) USDA Agricultural Research Service, Washington, District of Columbia (2) Division of Gastroenterology, Hepatology, and Nutrition, The Children's Hospital of Philadelphia Research Inst., Pennsylvania Lactose is a disaccharide that consists of the monosaccharides glucose and galactose linked together by a beta-1,4 glycosidic bond and is only found in mammalian milk. The mammalian enzyme lactase produced in the human small intestine hydrolyzes lactose to release glucose and galactose. However, this conversion is not always absolute; one seminal report that measured lactose in ileal aspirations of healthy human adults found that approximately 0-8% of lactose consumed was not broken down and absorbed. Therefore, upon consumption of bovine milk, a small amount of lactose may be available for use by the colon gut microbiota. In particular, lactic acid bacteria and Bifidobacteria, which are ubiquitous members of the gut microbiota, produce the enzyme beta-galactosidase, which is also able to metabolize lactose into glucose and galactose and produce metabolic byproducts such as short chain fatty acids (SCFAs). To fully understand how the dairy component lactose may serve as a mediator of the gut microbiota, we analyzed the effects of lactose on the gut microbiota of donors from healthy adults and elderly adults, through application of the short term, batch incubation culturing platform. Changes to the community function were determined through quantification of short chain fatty acids and gas production. To elucidate the effect of lactose on community structure, 16S rRNA sequencing was performed to provide information on changes to diversity and relative abundance of community members and qPCR analysis was used to specifically analyze the impact of lactose on Bifidobacteria. Together, these results demonstrate the potential for lactose to serve as a mediator of the gut microbiota structure and function for adults and elder adults. These results are important to understanding the contribution of dietary milk to human health through promotion of a healthy gut microbiome.

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A134 Introduction: Chemistry of alcoholic beverages Nick O. Flynn, nflynn@wtamu.edu. Chemistry/Physics, West Texas A&M Univ., Canyon Alcoholic beverages can be classified based on a number of methods which include alcohol content, method of production, fermentables, distillation status and extraction method. This presentation will serve as an introduction to the Chemistry of Alcoholic Beverages and will primarily focus on the alcoholic beverages that are being presented.

A135 Rapid wort color analysis of malts Nick O. Flynn, nflynn@wtamu.edu. Chemistry/Physics, West Texas A&M Univ., Canyon The rapid wort color method is an American Society of Brewing Chemists (ASBC) method used to evaluate the color contribution of malts to beer color measured as the Standard Reference Method (SRM). SRM is important to brewers as it helps them predict the relative color of beer that they manufacture and evaluate how close the final product color is to the style of beer being produced. This method involves the heating of a solution of malt and deionized water followed by filtration and analysis of the resulting solution on a spectrophotometer. Several studies in our laboratory have explored aspects of this method including the effect of pH, initial water temperature, modifications for darker malts and residue contribution to color. This presentation will summarize current findings to date and discuss future directions for improving this method.

A136 Dry-hopping as a general tool to influence the concentrations of key odorants in beer as well as to optimize the overall aroma of alcohol-free beer Michael Granvogl1, michael.granvogl@uni-hohenheim.de, Thomas Hofmann2, Sabrina Brendel2. (1) Food Chemistry, Univ. Hohenheim Fakultat fur Naturwissenschaften, Stuttgart, Baden-Württemberg, Germany (2) Technische Univ. Munchen, Bayern, Germany Both the market for alcohol-free beer and the number of craft-beer breweries increased in the past years. Thus, dry-hopping of beer and also of alcohol-free beer is gaining more and more interest. To better understand the transfer of odorants from hops into alcohol-free beer during dry-hopping, their amounts were analyzed over a period of 7 days. During a lab-scale experiment that simulated the dry-hopping process, major transfer was found within the first 2-3 days. However, the importance of the transferred key aroma-active compounds to the overall aroma can only be evaluated by taking their sensory properties into account. For this purpose, orthonasal odor thresholds and sensorial dose-response relationships were investigated for selected key odorants in an alcohol-free beer matrix. Thereby, sensory tests revealed a nearly linear increase in the odor intensity of several esters, while further typical hop key odorants, e.g., linalool, geraniol, and myrcene, showed a multi-stage increase. The lecture will demonstrate that the technique of dry-hopping can be influenced, for example by the hop dosage and the contact time, to optimize the overall aroma of beer. Thus, brewers will have the opportunity to follow the wishes expected by consumers to obtain a desired specific flavor of the final product.

A137 Quantification of capsaicin and dihydrocapsaicin concentration in potentially the hottest beer using HPLC analysis Valerie Ebenki1, valerie.ebenki@gmail.com, Ray Parrish2, Sarah Smith1. (1) Chemistry and Physics, Univ. of Mary Washington, Fredericksburg, Virginia (2) Maltese Brewing Company, Fredericksburg, Virginia Signal One 2.0 Beer from Maltese Brewing Company is a potential candidate for the world's hottest beer infusing approximately 500 carolina reaper chilies during the brewing process. The two capsaicinoids involved in over 90% of the heat in hot peppers are capsaicin and dihydrocapsaicin. The primary objective of this study aims to develop a quantification method that can accurately determine the beer's capsaicin and dihydrocapsaicin concentration using high-performance liquid chromatograpy (HPLC) analysis by a variety of analytical methods including external calibrations and standard additions using HPLC. Results indicate a possibility that capsaicinoid signals are being masked by the complex matrix of the beer. Analyses of the beer sample indicate the hotness in Scoville heat units; possibly supporting the claim of being the hottest beer in the world.

A138 Unveiling the chemistry of sake Eberhardt R. Kuhn, erkuhn@shimadzu.com. Shimadzu Scientific Instruments, Columbia, Maryland Sake is a traditional Japanese alcoholic beverage with a complex aroma profile. Often referred to as "rice wine", it is actually brewed more like beer. In the brewing industry, aroma component analysis is very important due to the pronounced effects on product quality and consistency. Utilizing GCMS and LCMS/MS, we conducted a comprehensive metabolomic analysis of various aspects of sake production and consumption. We identified 86 aroma components, and using Principal Component Analysis (PCA), were able to differentiate different types of sake and measure deterioration characteristics based on storage conditions. The results confirm that performing a complete analysis of metabolites and subsequent multivariate analysis is a useful tool for sake quality evaluation.

A139 Comprehensive aroma characterization of unaged (blanco) tequila Xinhe Huang, xhuang52@illinois.edu, Keith R. Cadwallader. Food Science and Human Nutrition, Univ. of Illinois at Urbana-Champaign, Urbana Tequila ranks fourth in polularity among distilled spirits, and one of the fastest growing alcohol beverages, growing by more than 40% in the past three years. People enjoy this Mexican spirit because of its unique flavor profile, which makes it an essential ingredient of various bar drinks. Despite the importance of this spirit, the understanding of its flavor (aroma) chemistry is limited, and few studies have been undertaken on tequila aroma. None of the previous studies have successfully reconstructed tequila flavor from its component parts, indicating that some of the key odorants of tequila remain unknown. The goal of this research was to comprehensive study various silver or blanco tequilas made from 100% blue agave, to identify odorants that are essential to all unaged tequila. We focused on silver tequila because it contains the essential tequila flavor components, derived from raw materials (agave), fermentation and distillation, but do not possess flavor/aroma constituents derived from aging in oak barrels. This talk will feature a brief overview of previous studies on the flavor of tequila and the progress of the current study. It will include newly discovered essential volatiles that characterize tequila flavor identified using GC-O (Gas Chromatography-Olfactory) and AEDA (Aroma Extract Dilution Analysis) along with methods and techniques based on stable isotope dilution analysis (SIDA) used for quantification of selected volatiles in tequila.

A140 Investigating extraction and reutilization of oak products in model beverage systems Jonathan Belew, jbelew@uttyler.edu, Jordan Beaver. Chemistry and Biochemistry, The Univ. of Texas at Tyler This study seeks to identify key volatiles and polyphenol quality markers and subsequently the rates of extraction in various oak barrels and barrel alternatives in model wine and spirit systems. Considering barrel losses in order to better inform beverage producers/makers who are dependent upon oak products for characteristic key flavors and aromas along with tannins known for mouthfeel properties, and color stabilization; the value of a predictive oak extraction model is apparent. The researcher used model beverage solutions to extract the volatile and polyphenol quality markers, from various oak sources and each trial was monitored for 30, 60, and 90 days. Ninety days is a reasonable endpoint because the wood becomes completely saturated, as seen in other literature. Wood samples and periodic extraction samples were analyzed. Quantification is completed through the liquid-liquid extractions and via Gas Chromatography-Mass Spectrometry(GCMS) for the liquid. Fourier Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy(SEM) on the remaining wood. From these analyses, 7-8 volatiles and tannins both iron reactive and polymerized are quantified, and regression analysis to help build a predictive extraction model for each quality marker over time.

A141 Using Raman spectroscopy for classification of alcohol products Sarah Shidler, sarah.shidler@renishaw.com, Lucy Grainger, Tim Prusnick. Renishaw USA, West Dundee, Illinois The value of alcohol products, especially whiskey, increases with time and rarity, making the market ripe for forgeries. Being able to assess the authenticity of bottles of alcohol, without opening, maintains the value of the product while removing any doubt of forgery. In this talk we will discuss using Raman spectroscopy as a non-contact and non-destructive method for detection of different alcohol products. Raman spectra were collected from different brands of alcohol focusing through the glass of an unopened bottle and then developing a data classification model based on principal component analysis and linear discriminate analysis (PCA-LDA) to predict and classify the products. This method provides fantastic specificity, even where the spectral differences are very subtle.

A142 Elucidating reproducibility of site contributions to composition of Pinot noir wines over multiple vintages: Elemental profile and

organic acids characterization Maisa M. M. Lima1, Desmon Hernandez2, Ron Runnebaum1,2, rcrunnebaum@ucdavis.edu. (1) Viticulture & Enology, Univ. of California Davis (2) Chemical Engineering, Univ. of California Davis Correlations between vineyard site and wine have, historically, been limited due to lack of continuity across multiple vintages, lack of uniformity in scion clone, and lack of controlled pilot-scale winemaking conditions. We have compositional data, including elemental profile and organic acids, characterizing wines across multiple vintages (2017–2019). The experimental design aims to minimize sources of potential variation by using a single scion clone and by using automated 200 L fermentation vessels at the UC Davis Teaching and Research Winery, in which fermentations are highly controlled across vineyard replicates, vineyards, and vintages. Grape clusters were hand-harvested from vineyards which span a distance of more than 1400 km. American Viticultural Areas (AVAs) represented include Santa Rita Hills, Santa Maria Valley, Arroyo Seco, Carneros, Sonoma Coast, Russian River Valley, Anderson Valley and Willamette Valley. Forty-seven elements were profiled in a mass range of 7 to 238 m/z by using inductively coupled plasma–mass spectrometry (ICP-MS) and six organic acids were profiled by using high-performance liquid chromatography coupled with a diode array detector (HPLC-DAD). Wines from specific vineyard sites presented higher lactic acid concentration than possible after malolactic fermentation on the basis of initial malic acid concentration (actual and theorical difference in lactic acid concentrations). Such differences suggest that significant levels of lactic acid were present prior to start of fermentation for these sites. Principal component analysis (PCA) was used to characterize vineyards using only significant elements identified by an analysis of variance (ANOVA) measuring effects of vineyard. Overall, separation and clustering of wines by composition appears consistent across vintages in this experiment. In future work, details to be unraveled aim to further demonstrate consistency of correlations with wine chemistry and sensory.

A143 Determination of histamine, agmatine, and putrescine in wine by ion chromatography single quadrupole mass spectroscopy Terri T. Christison, terri_christison@yahoo.com, Jeffrey Rohrer. Ion Chromatography Products, Thermo Fisher Scientific, Sunnyvale, California Biogenic amines have important biological functions, such as regulating growth, controlling blood pressure, and facilitating neural transmittance. Vintners use malolactic fermentation to create the desired flavors. However, certain strains of the lactic acid bacteria necessary for this fermentation can also produce biogenic amines by decarboxylating amino acids. Putrescine, cadaverine, histamine, and agmatine have been found in red wines, and to a lesser extent, in white wines. In healthy persons, these biogenic amines are rapidly detoxified, in contrast, people with histamine intolerances can experience minor to serious health effects. Cation-exchange chromatography with suppressed conductivity detection (cation ion chromatography (IC)) is a well-established analytical method for determining positively charged ionic species and is frequently used to determine biogenic amines. Mass spectrometry detection provides confirmation of the biogenic amine by the molecular weight of the ion and a different selectivity than suppressed conductivity. In this application note, three biogenic amines (putrescine, histamine, and agmatine) were determined in wine samples using IC with suppressed conductivity and mass spectrometry detections. The biogenic amines were resolved on a high-performance cation-exchange column, detected by suppressed conductivity with the suppressed eluent delivered to electrospray interface of a single quadrupole mass spectrometer designed for ion chromatography and small ion detection. The biogenic amines were detected by MS in selected ion monitoring (SIM) mode. The results from recently opened and 3-day old wine samples were compared. The lowest biogenic amine concentrations were found in the sparkling wine and chardonnay samples and the highest results in the cabernet sauvignon sample. Biogenic amine concentration increased after exposure to air.

A144 Incorporation of 13C as a chemical label for smoke fuel used for smoke affected wine studies Darrell C. Cerrato, cole.cerrato@oregonstate.edu, Lindsay Garcia, Mike Penner, Elizabeth Tomasino. Dept. of Food Sci. and Tech., Oregon State Univ. College of Agricultural Sciences, Corvallis Over the last several decades winemakers in the US have been negatively impacted by the increased intensity of proximal wildfire events. Unlike most food and beverage crops, wine has shown to be particularly sensitive to compounds derived from the ambient smoke at even low densities, often acquiring a medicinal, “ashy” or “burnt rubber” flavors or aromas. The wine industry has long sought more efficient methods of preventing or mitigating the negative sensory characteristics associated with smoke exposure, and unfortunately, some studies have disagreed on the major chemical compounds imparting these sensory characteristics. To develop more targeted approaches to ameliorate the impacts of smoke on wine, this study was developed to inventory the chemicals derived from smoke by chemically labeling a fuel source. Barley, Hordeum vulgare, was exposed to 13C-lablelled CO2 (13CO2) using pulse-labeling techniques in an enclosed environment for 10 days over two weeks. The barley was subsequently dried to constant weight and separated into randomized 5 g bundles. The increased 13C content was evaluated using isotope ratio mass spectrometry (IRMS). This method yielded 13C/12C content as high as 3186.90 ± 737.22‰ relative to VPDB and 4.47 ± 0.75% 13C content compared to 1.10% 13C content of untreated barley. Dried barley bundles were burned and piped “cold” to sealed tents containing Pinot noir or chardonnay grapes from the Woodhall vineyards in Willamette Valley, Oregon. Each replicate of grapes was exposed to a smoke density of 20-100 mg/m3 for smoke particle >1 µm. Standard wine-making methods for the respective styles were employed followed by chemical evaluation using GCMS, HPLC, and 13C-NMR to determine compounds derived from 13C-labelled smoke source.

A145 Simultaneous quantification of 24 aldehydes and ketones in oysters (Crassostrea gigas) with different thermal processing procedures by HPLC-electrospray tandem mass spectrometry Guan-Hua Zhao, zhaoguanhua17@outlook.com. Dalian Polytechnic Univ., Liaoning, China Aldehydes and ketones are secondary oxidation products resulting from lipid oxidation that occurs during food processing. These small molecule compounds not only have an impact on the quality, odor and flavor of food, but also play a role in the pathogenesis of many human diseases. In this study, a HPLC-MS/MS analytical method was developed and validated for the simultaneous determination of 24 aldehydes and ketones. The coefficients of determination (R2) for all aldehydes and ketones were higher than 0.9975 at the range of 0.2-2000 ng/mL. The recoveries were in the range 71.20-108.13% with RSD < 10%. The method was tested by analyzing lipids from oysters with different thermal processing (boiling, frying, roasting and air frying) procedures; the highest concentration for saturated aldehydes and ketones while the highest content of unsaturated aldehydes in boiling treatment. Meanwhile, fatty acid oxidative decomposition was in agreement with aldehydes and ketones formation. Moreover, principal component analysis, orthogonal partial least-squares discriminant analysis and variable importance in projection value showed that lipid oxidation is positively related to the formation of a variety of aldehydes and ketones.

A146 PAM free loop mediated isothermal amplification coupled with CRISPR/FnCas12a cleavage for on-spot detection of three rice pathogens Zaobing Zhu, zbzhu152@sjtu.edu.cn, Litao Yang.

Shanghai Jiao Tong Univ., Shanghai, China The pathogenic diseases are one important factor affecting rice growth, yield and quality, the development and application of rapid diagnostic methods targeting pathogens will contribute to the prevention and control of rice diseases. Herein, we developed one novel PAM-free loop mediated isothermal amplification assisted CRISPR/FnCas12a cleavage (Cas-PfLAMP) assays for the detection of three rice pathogens, such as Xanthomonas oryzae pv. Oryzae (XOO), rice stripe virus (RSV), and rice black-streaked dwarf virus (RBSDV). Furthermore, the Cas-PfLAMP on-spot detection system was also developed by combining solid phase nucleic acids extraction and lateral flow biosensor (LFB). The Cas-PfLAMP assay presented quite high specificity because of the double specific recognition from LAMP primers and FnCas12a/sgRNA, and high sensitivity as low as 10 aM. The results of inoculated rice leaves and practical field rice leaf samples confirmed the high performance of Cas-PfLAMP assay, indicating that the Cas-PfLAMP is one suitable on-spot detection method for rice diseases detection with high specificity, high sensitivity, and easy operation. We believe that the Cas-PfLAMP also could be extended to the other crop diseases detection, and other nucleic acid test fields as well.

A147 Coin operated water vending machines: Bacterial contamination analysis Stephen Bryan Asenjo, brainasenjo8@gmail.com, Rizza Nikka Gerona, izzaikka@gmail.com, Mary Shylle Miñoza, marynalleahreyes@gmail.com, Clisa Mae Flores, clisamae@gmail.com, Ginalyn Sildora, giinafront25@gmail.com. Cebu Normal Univ., Cebu City, Philippines Coin-operated water vending machines (locally known as ATMs) have been an instant and cheap source of drinking water around Cebu City, Philippines. They are mostly located along the sides of roads and streets making them prone to contamination. With the high risk of contamination of these ATMs, this study aimed to determine the bacteriological quality of potable water from coin-operated water vending machines around Cebu Normal Univ.. Bacteriological analysis was done on water samples collected from 5 ATMs around CNU. Various quality parameters were analyzed including total coliform, fecal coliform and heterotrophic plate count (HPC). The results showed that 100% of the samples analyzed has high concentration of total coliform, fecal coliform and heterotrophic bacteria. The level of total and fecal coliforms contamination and heterotrophic plate count have failed to meet the standards of Philippine National Standards for Drinking Water (PNSDW) and Dialysis Water Standard (DWS). By the result of the analysis, it was concluded that ATMs cannot ensure safe water public consumption as bacteriological concentration exceeded the minimum standards set by PNSDW and DWS. It is necessary to maintain cleanliness of the machines, the surrounding environment and help secure reliable water source.

A148 Ovalbumin-specific peptide aptamer selected in the In vitro Selection process using E. coli extract Shin Woong Kim1,2, celllrewp@gmail.com, Akiko Yumoto1, Noriko Minagawa1, Yun Heo1, Kon Son1, Yoshihiro Ito1,2, Takanori Uzawa1. (1) Nano Medical Engineering Laboratory, Rikagaku Kenkyujo, Wako, Saitama, Japan (2) Biological Sciences, Tokyo Toritsu Daigaku, Hachioji, Japan Molecular recognition-based separation and detection systems have attracted much attention in various fields due to their high selectivity for target molecules. Recently, it has become possible to select antibody-like peptides such as antibacterial peptides using molecular evolutionary engineering technology. Selected peptides, called peptide-aptamers, can bind to a variety of target molecules. In vitro selection is the selection of aptamers from random peptide sequences. In this study, we found that E. coli extracts were applicable for peptide aptamer selection when the translation times were very short in ribosome display. Therefore, we hypothesized that utilizing E. coli extract could inhibit RNA degradation by shortening the translation time during the selection process. So, we applied the criteria to select a peptide aptamer for ovalbumin (OVA), a well-known allergen in egg white, by shortening the translation time. It was shown that OVA-binding peptide aptamers selected using E. coli extract could specifically bind OVA even in the presence of various concentrations of serum. Therefore, we conclude that the immediate translation of ribosome display using E. coli extracts has the potential to be useful.

A149 The use of mustard bioherbicide in organic potato production: weed control, soil health, and crop quality Daniel Temmen, John Randall, Inna E. Popova, ipopova@uidaho.edu. Univ. of Idaho, Moscow Organically grown produce accounts for over four percent of total food sales and this number keeps growing to accommodate the consumers' demand for safer and more naturally grown food. According to organic farmers across the US, weed management and soil health represent two major concerns in organic crop systems. To address these concerns, our research program has developed a bioherbicide from yellow mustard (Sinapis alba) seed meal that can be used in organic crop systems to control for more than a dozen problematic weeds including redroot pigweed, Powell amaranth, and green foxtail. While the application of the mustard seed meal extract (MSME) restricts germination and damages weeds, the broader effect of MSME on soil health still needs to be understood. Thus, the objective of this project was to evaluate the overall effect of the mustard based bioherbicide on organic potato production. The use of the MSME can be a viable tool for weed control in organic potatoes systems and it can also positively affect soil health and quality of potatoes through the increased nutrient influx and boosted microbial activity. We have conducted a greenhouse and field study at two organic farms using three different applications to demonstrate this. Weed control efficiency was compared against the commercially available organic herbicide. Soil health was assessed using a combination of soil chemical and biological properties. Crop quality was evaluated using the total phenolics and antinutrient contents. The results obtained provide a critical data for holistic assessment of bioherbicide use in organic systems for short- and long-term sustainability of crop production.

A150 Rapid screening of glycosyltransferases in plants using a linear DNA expression template based cell-free transcription-translation system Xian-Ai Shi, shixa@fzu.edu.cn, Shaobin Guo, Mingdi Wang. College of Biological Science and Engineering, Fuzhou Univ., Fujian, China Plants have an extensively large number of enzymes including glycosyltransferases that are important in the biosynthesis of natural products. However, it is time-consuming and challenging to study these enzymes and only a small percentage of them have been well-characterized. Here, we report a rapid method to screen plant glycosyltransferases using a linear DNA expression template (LET) based cell-free transcription-translation system (TX-TL). As a proof of concept, we amplified and tested glycosyltransferases from Arabidopsis thaliana and showed that the catalytic activity results of these glycosyltransferases from LET-based-TX-TL were consistent with previous studies. We then chose a local medicinal plant Anoectochilus roxburghii, acquired its transcriptome sequences, and applied this method to study its glycosyltransferases. We rapidly expressed all the putative UDP-glucose glycosyltransferases using LET-based-TX-TL and discovered 6 new active glycosyltransferases which can catalyze the glycosylation of quercetin into isoquercitrin. Thus, LET-based-TX-TL was shown to be a powerful tool for researchers to rapidly screen novel plant glycosyltransferases for the first time.

A151 Analytical performance of a portable gluten sensor for celiac disease patients Alena Maric, Katharina Scherf,

katharina.scherf@kit.edu. Karlsruher Institut fur Technologie, Karlsruhe, Baden-Württemberg, Germany Celiac disease (CD) is a lifelong small intestinal inflammation caused by the gluten proteins of wheat, rye and barley. The only treatment is strict dietary avoidance of wheat, rye and barley with a gluten intake of less than 20 mg per day. Eating out and travelling are most difficult to manage and often result in potentially harmful, but conscious gluten intake. To help CD patients overcome these restrictions, a portable gluten sensor was developed. This lateral flow immunoassay-based device allows them to test foods on-site prior to consumption. It carries out sample extraction and analysis within four minutes and shows a smiley (no gluten detected) or a wheat ear (gluten detected). With very limited independent information available on the analytical performance of the sensor, our aim was to test how reliable the sensor really is. We prepared eight high-protein or high-fat and 17 high-starch foods using a gluten-free matrix blended with wheat, rye or barley flours so that the final products contained target values between 0 and 30 mg/kg of gluten. Commercially available products with unknown concentrations of gluten (nine beers, four sauces, three fried potato products, two tofu, three sourdough samples) were also included. All products were tested using the gluten sensor and the gluten content was also determined by R5 Sandwich or competitive ELISA. The sensor found gluten in 95% of samples with ≥20 mg/kg of gluten, which is lower than the 99% claimed by the manufacturer. For the samples with <20 mg/kg of gluten, the sensor showed “gluten detected” in 63% of cases. The results of the sensor agreed with those of the competitive ELISA in 16 out of 21 commercial products. However, it had difficulties in detecting partially hydrolyzed gluten in the five samples that had 20-25 mg/kg of gluten according to the ELISA. There was no evidence for a high-dose hook effect and sample weights between 0,3 g and 0,9 g worked well for different matrices. However, the results of the sensor showed variability between different users, because one user failed to detect gluten in some samples, whereas the other user did detect gluten in the same samples. Overall, the performance of the sensor was acceptable. The systematic variation between different users was concerning and needs to be investigated in more detail outside our well-controlled laboratory setting.

A152 Challenges of detecting an evolving prion disease, chronic wasting disease (CWD) Christopher J. Silva, christopher.silva@usda.gov. USDA Agricultural Research Service, Albany, California Chronic wasting disease (CWD) is a cervid (deer, elk, moose, etc.) prion disease that is readily transmitted among wild and farmed cervids and acquired from CWD-contaminated environments. CWD-infected cervids have been found in 26 states, 3 Canadian provinces (Alberta, Quebec, and Saskatchewan) and CWD was inadvertently exported to South Korea. An independent outbreak of CWD was observed in Scandinavian (Norway, Finland, and Sweden) moose, reindeer, and red deer. The CWD pathology propagates by inducing a natively expressed prion protein (PrPC) to adopt the CWD prion conformation (PrPSc). PrPC and PrPSc differ solely in their respective conformations. Like other prion diseases, CWD is both sporadic and transmissible. The CWD conformation can shift in response to natural selection pressures resulting in new CWD strains with differing phenotypes. CWD alters cervid population genetics, which, in the future, may result in the emergence of novel CWD strains. Millions (11.5) of Americans hunt and annually harvest nearly 6 million deer, indicating that CWD represents an underappreciated potential threat to a significant segment of the American food supply. Should a zoonotic CWD strain emerge, it could negatively impact American hunters and consumers of game meats.

A153 Gas chromatography-based metabolomics to characterize the differences between atypical and dark-cutting beef Ranjith Ramanathan1, ranjith.ramanathan@okstate.edu, Frank Kiyimba1, Joshua Habiger2, Gretchen G. Mafi1. (1) Animal and Food Sciences, Oklahoma State Univ. Division of Agricultural Sciences and Natural Resources, Stillwater (2) Statistics, Oklahoma State Univ. The College of Arts and Sciences, Stillwater Beef color is an important sensory property that influences consumer purchasing decisions. Dark-cutting is a condition in which beef exposed to air does not have a characteristic bright red color. Defective postmortem glycolysis leads to greater than normal muscle pH (> 6.0) in dark-cutting conditions. Dark-cutting beef is characterized by dark red color, and this beef is not sold in retail. Atypical dark-cutting beef represents darker meat at normal-pH, and this beef is not discounted and sold in retail conditions. The darker color of atypical is lower than typical dark-cutting conditions. The objective of the study was to determine the metabolite profiles of normal-pH, atypical dark-cutting, and typical dark-cutting beef. The muscles of all three types were collected from a commercial beef processing facility (n = 6 replications). The surface color was measured using a HunterLab spectrophotometer. The metabolites were extracted in methanol, dried under nitrogen, derivatized, and metabolites were separated by gas chromatography and analyzed by mass spectrometry (GC/MS). Chromatography data were analyzed using Chemstation software, and the spectra were deconvoluted using AMDIS software. The compounds were identified using the Fiehn metabolomics library and the NIST mass spectral library. The data were analyzed using MetaboAnalyst. The average pHs were 5.6 (normal-pH), 5.8 (atypical dark-cutting), and 6.4 (typical dark-cutting). The unsupervised principal component analysis indicated no differences in metabolite profiles between atypical and normal-pH beef, while different clusters were noted between typical dark-cutting and normal-pH beef. In both atypical and typical dark-cutting beef, several metabolites involved in muscle biochemistry such as glucose-6-phosphate, succinic acid, malic acid, aspartate, and citric acid demonstrated a similar trend in abundance. For example, a slight change ($P > 0.05$) was noted between normal-pH and atypical dark-cutting beef. However, the change becomes more significant ($P < 0.05$) between typical dark-cutting and normal-pH beef. The results suggest that darkening may be an outcome of the same etiology, but the muscle darkening and metabolite changes become more prominent with increased pH.

A154 Selective dietary plant extract as inhibitors of cyclooxygenase -1 and cyclooxygenase-2 activities Diganta Kalita1, diganta.kalita@futureceuticals.com, Boris V. Nemzer1,2. (1) Research and Analytical Center, VDF Futureceuticals, Momence, Illinois (2) Univ. of Illinois at Urbana-Champaign, Urbana During last few decades Non-Steroidal Anti-Inflammatory Drugs (NSAIDs) have been widely used for treating numerous inflammatory diseases. One of the pathways that NSAID generates anti-inflammatory activity via inhibiting cyclooxygenase enzyme, that converts arachidonic acid to prostaglandins. Natural products as COX2 inhibitors are promising compared to synthetic ones due to their minimal side effects. In this study we have investigated the potential inhibitory activities of COX1 and COX2 by a dietary supplement S7, a proprietary polyphenol-rich fruit, vegetable and herbs-based material previously reported to reduce reactive oxygen species and to increase level of bioavailable NO in humans. S7 blend includes ingredients: green tea extract (46.5%), green coffee bean extract (46.5%), turmeric extract (5%), whole blueberry powder (0.5%), whole tart cherry powder (0.5%), broccoli powder (0.5) and kale powder (0.5%). The results suggested that S7 blend showed significant inhibition of COX1 and COX2 activities in concentration dependent manner up to 79 and 87 % respectively with the concentration range 1.13-22.27 µg/mL. Among its ingredients green tea extract showed strongest inhibition up to 68 and 97 % respectively in the tested concentrations. Green coffee bean extract

showed moderate inhibition (33%) in the same concentration. Other ingredients did not show significant inhibition against COX1 and COX2 activities in the assay. Selective inhibition of COX2 over COX1 were found to be better by minimizing gastrointestinal effects associated with COX-1. This study of screening of various food product as potential inhibitors against COX1 and CO2 is expected to guide us to develop effective natural dietary plant products that provide anti-inflammatory properties with limited or no side effects.

A155 Sustained release of hydrogen sulfide from poly (lactic acid) micro particles containing a dithiophosphate to enhance plant growth Nimesh Pasan Ranasinghe Ranasinghe Arachchige, nimesh-pasan@uiowa.edu, Eric M. Brown, Ned B. Bowden. Dept. of Chemistry, Univ. of Iowa, Iowa City Hydrogen sulfide (H2S) has emerged as a gasotransmitter capable of exhibiting many beneficial properties in plants including the survival of plants under environment stressors, as well as increase their harvest yields. Although H2S is an exciting new frontier in agriculture, what is needed in this field is a method to add chemicals that slowly release H2S over well-defined time periods, will release biocompatible and safe chemicals in addition to H2S, and will not diffuse away from roots of plants. Here, we report the addition of a dithiophosphate that will release H2S slowly by hydrolysis and its encapsulation into microparticles of poly(lactic acid) [PLA]. The microparticles were prepared by a modified solvent evaporation technique. Tert-butanoldithiophosphate phenethylamine salt was loaded into PLA microparticles. The external morphology and the composition of the tert-butanoldithiophosphate phenethylamine salt loaded particles was examined by scanning electron microscope (SEM), powder X-ray diffraction (PXRD), and energy dispersive X-ray analysis (EDX). It was shown that surface of the microparticles was rough and contained tert-butanoldithiophosphate phenethylamine salt. The release profiles of tert-butanoldithiophosphate phenethylamine salt from the microparticles showed that 61% and 74 % of tert-butanoldithiophosphate phenethylamine salt was released at pH 7.2 and pH 6.0 respectively after 30 days. The H2S release from the microparticles were determined using modified methylene blue method, and it was shown that nearly 20 μM and 12 μM of H2S was released from 20% and 10% loaded microparticles respectively over 4 weeks. To demonstrate the potential applications of micro particles in agriculture, we also describe their effects on the growth of radish 4.5 weeks after exposure to milligram loadings of micro particles.

A156 Investigating protein adsorption on nanoparticle-based sensors and delivery vehicles in plants Elizabeth Voke1, evoke@berkeley.edu, Rebecca L. Pinals2,1, Natalie Goh1, Markita Landry1. (1) Chemical and Biomolecular Engineering, Univ. of California Berkeley (2) Massachusetts Inst. of Technology, Cambridge Climate change and population growth are straining agricultural output. To meet the growing demand for food and energy, monitoring and engineering crops is becoming increasingly important. Nanoparticles have emerged in recent years as tools to advance agricultural practices through plant health sensing and delivery of nutrients or biomolecules for crop genetic engineering. When these nanoparticle-based technologies are applied to plants, they travel through the complex biological matrices, where biomolecules including proteins, metabolites, lipids, and carbohydrates adsorb onto the nanoparticle surfaces, forming a coating known as the “bio-corona”. Understanding the nanoparticle-biomolecule interactions that govern nanoparticle function in plants will be essential to successfully develop and implement nanoparticle-based sensors and delivery of biomolecules into broader agricultural practice. In this work, we characterize the plant protein corona formed on three nanomaterials: polystyrene nanoparticles (a model for the unintentional release of plastics into the environment), DNA-functionalized single-walled carbon nanotubes (ssDNA-SWCNTs; used for sensing plant stress signals and DNA/RNA delivery applications), and gold nanoparticles (similarly used as sensors and delivery vehicles for biomolecules). These nanoparticles, whether or not they internalize into plant cells, interact with extracellular (apoplastic) fluid in plants. Thus, apoplastic fluid was collected from Arabidopsis thaliana, a widely used model plant system with a well-characterized proteome. Nanomaterials incubated with plant apoplastic fluid were analyzed with mass spectroscopy-based proteomics, demonstrating preferential enrichment and depletion of proteins adsorbing to the surface of these nanomaterials. These findings suggest that the plant nanoparticle protein corona cannot be assumed to be compositionally similar to native plant biofluids, with implications for the future development and characterization of agricultural nanobiotechnologies.

A157 Electrostatic interactions of carbon dots with plant model and native cell walls Su-Ji Jeon1, jsuji@ucr.edu, Peiguang Hu1, Kyoungtea Kim2, Christopher Castillo1, Joel A. Pedersen2, Juan Pablo Giraldo1. (1) Univ. of California Riverside (2) Univ. of Wisconsin-Madison The cell wall is a defining plant biosurface that controls the interactions of nanoparticles with plants in the environment. We systematically investigated the influence of nanoparticle zeta potential and charge distribution on the interactions with plant cell walls. For this purpose, we synthesized nanoparticles of environmental and agricultural interest including fluorescent carbon dots (CDs) with positive, neutral, and negative zeta potentials. We also developed novel model plant cell wall biosurfaces built with cellulose or pectin for comparative studies with native cell walls from Arabidopsis plants Coleochaete green algae. We analyzed the interactions between CDs and plant cell walls by confocal fluorescence microscopy, FTIR, XPS, and QCM-D. Our results indicate that positively charged CDs have the strongest affinity to plant cell walls, which is dominated by the ionic bonding between the surface amine groups of CDs and the carboxyl groups of pectin, while CDs with negative or neutral zeta potential exhibited negligible interactions with plant cell walls. This study provides new tools for understanding the interactions of nanomaterials with chemically heterogeneous plant cell walls, insights into nanoparticle design for plant bioengineering and nano-enabled agriculture, and approaches to assess nanoparticle sustainability in the environment.

A158 Eco-friendly targeted pest control using nanomaze lure: Application in agricultural nanotechnology Kamaljit Kaur, kamalvirgo92@gmail.com, Dr.P.S. V. Kumar. Chemical Biology Unit, Inst. of Nano Science and Technology, Mohali, Punjab, India Eco-friendly pest management strategies motivate the search for a platform having the ability to deliver pheromone in a controlled manner. Further, the pest like tomato pinworm Tuta absoluta, which is a leaf minor that dwells inside the host biomass, is hard to control with conventional pesticides. Sustainable agriculture practice uses pheromone trap made out of rubber septa that have a short field life and few other limitations. Hence to overcome this problem a pheromone composite with graphene oxide and amine-conjugated graphene oxide that can extend the diffusion path has been envisaged and developed. The composite with the optimum ratio of matrix and pheromone compound has been found to release the pheromone in the right ratio to kindle the neural network in the antenna and give significant electrophysiological responses. Thus, standardised composite performed well in the field to trap pests, hence it can be beneficial for farmers for longer field efficacy.

A159 Fabrication of electrospun polyacrylonitrile carbon nanofibers with functionalized multi-walled carbon nanotube for electrochemical biosensing applications Ruo-Fan Wang1, Reuben Wang1,2, markmarkmark8g@gmail.com. (1) Inst. of Food Safety and Health, National Taiwan Univ., Taiwan (2) Master of Public Health Program,

National Taiwan Univ., Taipei Several methods for bacterial identification like the enzyme-linked immunosorbent assay (ELISA) or polymerase chain reaction (PCR) are time-consuming, expensive, and laborious in the sample preparation. Here, a novel material was introduced to the electrochemical biosensor, which goals were to enhance the electron transferability and the number of bacteriophages immobilized on the sensor. Specifically, the material was made by the carbonized polyacrylonitrile (PAN) with functionalized multi-walled carbon nanotube (f-MWCNT). With the modification of the screen-printed electrode (SPE), the conductivity and sensitivity of this biosensor could be improved. The fabrication of CNF was performed by electrospinning, stabilization, and high-temperature carbonization. Specifically, 8% (w/v) of PAN solution was prepared by dissolving the PAN powder into the dimethylformamide (DMF) for electrospinning. The electrospun nanofiber was further processed through high-temperature carbonization. The f-MWCNT was obtained by acid oxidation treatment of MWCNT. Briefly, 1g of MWCNT has dispersed in 400mL HNO3/H2SO4(1 : 3) solution and stirred for 12 hours. The acid was then separated by suction filtration and dried in an 80°C oven overnight to obtain the carboxylic acid functionalized MWCNT. For further electrospinning, the PAN/f-MWCNT solution should be sonicated in the ultra-sonication bath for 30 minutes at 80°C. The images of scanning electron microscopy (SEM), which showed the connection between the PAN, f-MWCNT, and the average diameter of nanofiber suggested that 1 wt.% f-MWCNT in 8 wt. % PAN solution resulted in nanofiber with a smooth structure and small diameter (420± 93 nm). For functionalization of MWCNT, it was verified by Fourier-transform infrared spectroscopy (FTIR). No hydroxyl groups and carbonyl groups were found in the FTIR spectra of MWCNT compare to f-MWCNT, which means the functionalization was successfully conducted. Moreover, X-Ray Diffraction (XRD) could be used to analyze the crystal structure in the PAN electrospinning nanofiber, CNF, and MWCNT. Future studies will be focused on calculation the charge transfer resistance (Rct) from the Nyquist plot data through electrochemical impedance spectroscopy (EIS), and try to optimize the methods for bacteriophage immobilization onto the SPE especially through drop-casting accompanied with polyethylenimine (PEI) or chitosan.

A160 Nanoscale biomaterial for developing next-generation agrochemicals Ramesh Raliya1,2,3, rameshraliya@iffco.in. (1) IFFCO Nano Biotechnology Research Center, Gandhinagar, India (2) Smart Aerosol Technologies, Saint Louis, Missouri (3) Center for Rural Development & Technology, Indian Inst. of Technology Delhi, New Delhi, Delhi, India Agrochemicals such as fertilizer, pesticides, herbicides, anti-microbial agents, bio-stimulants, growth factors are being used for enhancing crop production and nutrition, require to feed the global population. However, excessive use of such agrochemicals causes environmental contamination, degradation and also affects the biodiversity of flora and fauna. Further, currently used most agrochemicals having low use efficiency, means they are being used in more amount than optimally required quantity by plants. Unused agrochemicals often transform into another chemical form and release to the environment in form of gaseous emission, leaching, or runoff. For instance, unused nitrogen and phosphatic fertilizer causes eutrophication when ends up in water bodies and affects aquatic life. Similarly, nitrogen fertilizers also get lost in form of ammonia or nitrous oxide, a greenhouse gas, causing global warming. Various attempts were made for enhancing the use efficiency of agrochemicals so that their unintended release into the environment can be minimized or stopped. For instance, coating of hydrophobic lipid (oil) on the surface of urea fertilizer, use of urease inhibitors, however, their success is still not as desired. Therefore, it is essential to develop a platform that enables nutrient to release in a controlled manner, has improved use efficiency and require less by mass volume for obtaining desired crop growth and yield. The present disclosure relates generally to composition based on nanoscale materials synthesized from a raw material originated from biological sources and methods for providing nanotechnology-based agrochemicals to plants as nutrition, growth stimulants, bio-stimulants and crop health protection. More particularly, the present invention relates to a composition including chitosan nanoplatforms and methods for control release of agrochemicals.

A161 Chemically tailored nanomaterials to improve material properties of renewable canola protein-based packaging materials Nandika Bandara1, nandika.bandara@umanitoba.ca, Thilini Dissanayake1, Boon Peng Chang2, Tizazu Mekonnen2, Claudia Narvaez-Bravo1, Senaka Ranadheera3. (1) Food and Human Nutritional Sciences, Univ. of Manitoba, Winnipeg, Canada (2) Chemical Engineering, Univ. of Waterloo, Ontario, Canada (3) School of Agriculture and Food, The Univ. of Melbourne, Victoria, Australia Renewable and biobased polymers have gained enormous attention in the past decade due to the adverse environmental effects and none-renewability of the petrochemical byproduct resin-based synthetic counterparts. Canola protein is a promising biopolymer candidate with versatile, functional properties; however, it suffers from poor mechanical and barrier properties similar to other biopolymers. Nanomaterials could be used to provide solutions to biopolymers' weak functionality, but incorporating nanomaterials into the biopolymer matrix creates major challenges due to poor exfoliation. This study aimed to modify nanocrystalline cellulose's surface using TEMPO (2,2,6,6- Tetramethylpiperidine-1-oxyl) to enhance the exfoliation of nanocrystalline cellulose (NCC) in the canola protein matrix and thereby increase the mechanical, thermal, and barrier properties. Control (0% NCC) and 1%, 3%, and 5% (w/w of protein) modified NCC (TM-NCC) and unmodified NCC (U-NCC) were used to fabricate films. Prepared films were characterized for their mechanical, structural, thermal, and morphological properties to evaluate the addition of chemically modified NCC on film properties. XRD analysis confirmed a successful exfoliation of NCC in polymer matrix up to 3% NCC concentration. The tensile strength of the TM-NCC films was significantly higher than control and U-NCC films. There was no significant difference between TM-NCC and U-NCC films in terms of water vapor permeability and contact angle. However, compared to control, films with 3% and 5% TM-NCC showed significantly higher contact angles. All the films, except 1% U-NCC, showed significantly reduced water vapor permeability. Moreover, the thermogravimetric analysis showed enhanced thermal stability with the addition of NCC. The results demonstrated that the addition of NCC enhanced the thermal, barrier, and mechanical properties of canola films, while TEMPO modification further increased the tensile properties of films.

A162 Tobacco mild green mosaic virus as a multifunctional platform for efficient pesticide delivery Ivonne Gonzalez Gamboa1, igonzalezgamboa@eng.ucsd.edu, Adam Caparco1, Nicole F. Steinmetz1,2,3. (1) NanoEngineering, Univ. of California San Diego, La Jolla (2) BioEngineering, Univ. of California San Diego, La Jolla (3) Radiology, Univ. of California San Diego, La Jolla Plant diseases caused by various pests result in massive crop losses; the Food and Agriculture Organization (FAO) estimates that annually between 20-40% of global crop production are lost due pest manifestation. Pesticides are the basis for defending against these threats. However, the extensive use of pesticides in agriculture causes these toxins to accumulate on crops, in soil, as well as in drinking and groundwater, severely endangering the ecosystem and human health. The first step toward a healthier society is to enhance food security by improving quality and yields (i.e. more effective crop treatment), while protecting the environment and agricultural ecosystems (i.e. preventing the leaching and accumulation of pesticides in the

environment). Toward this goal we deploy biology-derived nanotechnologies as sustainable systems to increase agrochemical efficacy, while protecting the environment. Specifically, we utilize and repurpose the Tobacco mild green mottle virus (TMGMV), a type member of the plant virus tobamovirus group, as a nanotechnology platform for the delivery of active ingredients (a.i.). TMGMV is a 300 x 18 mm rod shaped virus and it is approved by the Environmental Protection Agency as a herbicide. It is comprised of 2,130 identical coat protein subunits, each of which displays three different functionalization sites (NH2, COOH and Tyr side chains). In this work, we focus on the establishment and refinement of chemical bioconjugation methods to load agrochemicals into or onto TMGMV for targeted delivery to plant pests. In one application we are interested to target nematodes and other pests residing in soil, and therefore a.i.-loaded TMGMV nanoparticles were assessed in soil mobility assay. The high aspect ratio shape along with the zwitterionic nature of the protein capsid render TMGMV a suitable platform with favorable soil mobility. These results further extend the understanding of the chemical properties of TMGMV and enable development of novel multifunctional platforms for pesticide delivery and precision farming.

A163 Nutrient compositions of two varieties of tomatoes harvested from single-layer and double- layer high tunnels Augustina Odediran1, Nona Mikiashvili1, Jianmei Yu1, jyu@ncat.edu, Peter L. Coffey2, Sanjun Gu2. (1) Family and Consumer Sciences, North Carolina Agricultural and Technical State Univ., Greensboro (2) Cooperative Extension, North Carolina Agricultural and Technical State Univ., Greensboro Tomatoes are nutritious fruits/vegetables rich in lipid soluble and water soluble antioxidants such as lycopene and vitamin C; they also contain significant amount of sugar and other organic acids which are important to the flavor. The tomatoes grow in warm places/seasons. High tunnel is an inexpensive option to prolong growing season of this high value crop. This study investigated the nutritional quality of two tomato varieties (Brandywine and Rebelski) harvested from single-and double-layer high tunnels with and without plastic mulching by quantifying soluble solid (TSS), titratable acid (TA) and lycopene contents of tomatoes. The TSS, TA and lycopene contents of tomatoes were significantly affected by variety, planting plot, mulching and the plastic layers of high tunnel. Under single-layer high tunnel, tomatoes harvested from plastic covered soil had significantly higher TSS content ($P<0.05$) regardless of variety; with same mulching, Brandywine tomatoes showed higher TSS than Rebelski tomatoes ($P<0.05$). The double-layer plastic high tunnel increased TSS of Rebelski tomatoes regardless of mulching; however, the effects of double-layer high tunnel on TSS of Brandywine tomatoes varied with mulching: increasing the TSS of fruits grown on bare soil, but decreasing the TSS of fruits grown on plastic covered soil ($P<0.05$). The Brandywine tomatoes had significantly higher TA and lycopene contents than Rebelski ($P<0.05$) regardless of growing condition. The TA of tomatoes grown on plastic covered soil was higher than that grown on bare soil ($P<0.05$). Compared to single-layer high tunnel, double-layer high tunnel increased TA of tomatoes grown on bare soil ($P<0.05$), but its impact on TA of tomatoes grown on the plastic covered soil was inconclusive. The impact of double-layer plastic on lycopene content of tomatoes varied with tomato variety and mulching of soil, which was similar to the impact on TSS.

A164 Identification of odorants in American pawpaw fruit, Asimina triloba Sarah Warner, John P. Munafo, jmunafo@utk.edu. Food Science, Univ. of Tennessee, Knoxville The American pawpaw, Asimina triloba, is a small deciduous tree from the custard apple family (Annonaceae). The pawpaw fruit is the largest indigenous fruit in North America. Pawpaw fruits are described as having a sweet, tropical fruit-like aroma that is reminiscent of banana, mango, and pineapple. The fruits have a history of consumption by Native Americans and early American settlers. Despite their long history of use, the fruits have not been successfully commercialized on a large scale due mostly to the fruits having a short post-harvest shelf life. Pawpaw fruits are mostly consumed fresh or are used to flavor various sweet foods including ice cream and baked desserts. Although volatiles present in pawpaw fruit have been reported, the odorants responsible for its distinct aroma profile are unknown. To help fill this knowledge gap, a collection of odorants was identified in tree-ripened pawpaw fruits by employing solvent assisted flavor evaporation (SAFE) and aroma extract dilution analysis (AEDA). Flavor dilution (FD) factors were assigned to each of the identified odorants. Some notable odorants included ethyl butanoate (fruity), ethyl hexanoate (fruity), linalool (floral, citrus), (2E,6Z)-nona-2,6-dienal (cucumber), (E)-B-damascenone (cooked apple), and 4-hydroxy-2,5-dimethyl-3(2H)-furanone (caramel). In addition, coconut-smelling lactones and sulfurous-smelling thiols were identified that appear to contribute the tropical-note observed in the fruits. As a result of this study, a collection of odorants was identified that contribute to the pleasant aroma profile of tree-ripened pawpaw fruits. This study provided a foundation for future quantitative studies on pawpaw fruit aroma which may aid in the development of improved or distinct flavored American pawpaw cultivars.

A165 Identification of odorants in chardonnay marc seeds Sarah Warner, swarne12@vols.utk.edu, John P. Munafo. Food Science, Univ. of Tennessee, Knoxville In the production of Chardonnay wine, the grape juice is first pressed from the skins, seeds, and stems, prior to fermentation. This leftover material is referred to as Chardonnay marc or pomace. This co-product is traditionally discarded, composted or used as animal feed. Chardonnay marc has been reported to contain an abundance of natural molecules that may potentially improve cardiovascular and gut health. Recently, it has been dried, milled and used as a healthy and flavorful food ingredient. Whole Chardonnay marc contains approximately 65% skins, 25% seeds, and 10% stems. The aroma chemistry of Chardonnay marc skins has been previously reported, but the aroma chemistry of the seeds remains unknown. To fill this knowledge gap, first, the seeds, from WellVine Chardonnay marc was manually separated from the skins and the stems. The volatile fraction from the seeds was then isolated using solvent-assisted flavor evaporation (SAFE) and subjected to aroma extract dilution analysis (AEDA) employing gas chromatography-olfactometry (GC-O). A total of 43 odorants were identified including six odorants with flavor dilution (FD) factors ≥ 64. The odorant with the highest flavor dilution factor was (2E, 4E)-deca-2,4-dienal (fatty) with an FD factor of 1024. Five other odorants were identified with an FD factor of 64 including hexanal (green), linalool (floral, citrus), (2E,4E)-nona-2,4-dienal (fatty), 3-methylnonane-2,4-dione (hay-like) and 2-phenylethanol (floral, rose). Based on the results, these odorants may potentially contribute to the overall aroma of the seeds and establishes a foundation for future quantitative studies aimed at determining the contribution of Chardonnay seed-derived odorants to the overall aroma profile of Chardonnay marc powder.

A166 Characterization of odorants from southern mountain mint, Pycnanthemum pycnanthemoides Melissa Dein, m.foley2889@gmail.com, John P. Munafo. Food Science, Univ. of Tennessee, Knoxville Pycnanthemum pycnanthemoides, commonly known as southern mountain mint, is a highly aromatic plant in the mint family, Lamiaceae. This native species grows vigorously in wild populations throughout the southeastern portion of the US and its pleasant mint-like odor suggests it may be a potential source of essential oils or natural ingredients for food, flavor, or cosmetic applications. However, the odorants that contribute to the mountain mint's unique odor have not been previously determined. Therefore,

the objective of this study was to comprehensively characterize the odor of a southern mountain mint through the application of flavor analysis techniques. Twenty-eight odorants were identified in P. pycnanthemoides by coupling solvent assisted flavor evaporation (SAFE) and aroma extract dilution analysis (AEDA). Selected odorants with high flavor dilution factors were quantitated by stable isotope dilution assays (SIDAs) and odor activity values (OAVs) were calculated. The odorants with the highest odor activity values included b-ionone (floral, violet, OAV 100000), linalool (floral, citrus, OAV 15000), myrcene (terpeny, OAV 12000), piperitone (mint, OAV 4200), and piperitenone (mint, OAV 2500). This study offers insight into the odorants that contribute to the complex odor profile of southern mountain mint and provides a foundation for future studies of P. pycnanthemoides and other species of the Pycnanthemum genus.

A167 Synthesis and sensory characterization of novel umami enhancing and kokumi peptide glycoconjugates Jianan Zhang, fez.jianan@mail.scut.edu.cn, Huayang Wang, Guowan Su, Mouming Zhao, Chi-Tang Ho. School of Food Sci. and Eng., South China Univ. of Technology, Guangzhou, Guangdong, China The Maillard reaction products of peptides, especially their Amadori rearrangement products (ARPs), were discovered as good taste-enhancers in many foods. Due to its low concentration (subthreshold concentration) in foods and thermal instability, seldom studies investigated the sensory characteristics of ARPs. Our previous study discovered that some ARPs of peanut peptides might have better umami-enhancing abilities. In this study, five ARPs (EP-ARP, AH-ARP, EE-ARP, β-AH-ARP, RFPHADF-ARP) were synthesized using a food-grade preparation method and their chemical structure was clearly demonstrated by mass spectrometry and 1D/2D NMR. EP, AH, and RFPHADF were peanut peptides with umami or bitter taste. EE and β-AH have similar structures with EP and AH, respectively, as well as good taste. Sensory experiments demonstrated that ARPs had better umami-enhancing abilities than corresponding peptides. ARPs could decrease the umami threshold of MSG and GMP, while only β-AH could enhance the umami intensity of MSG and GMP. RFPHADF had a strong bitter taste without umami and umami-enhancing properties. Its ARP exhibited a slightly bitter taste and excellent umami-enhancing capacity. Within a certain range of expected concentrations, the umami intensity of ARP and MSG solution was promoted when the concentration of ARP was increased. For EP-ARP, it might suppress the umami intensity of MSG when its concentration is higher than 18 mM. Meanwhile, adding EP-ARP could also strengthen the kokumi property of the MSG solution.

A168 Does ultrasound-assisted extraction on berries improve phenolic compounds content in juices? Aude A. Watrelot, watrelot@iastate.edu, Lindsey Bouska. Food Science and Human Nutrition, Iowa State Univ., Ames, Iowa This study aims to investigate high-power sonication to provide a “greener” and quicker process to extract and keep the polyphenol properties of berries. Three solid to solvent ratio and time were applied on chokeberry and Marquette wine grape berries using 50% ethanol or 13% acidified ethanol and compared to a conventional extraction technique. Iron-reactive phenolic compounds, tannins content and color were analyzed during the extractions using UV-Visible spectrophotometry and anthocyanin content was analyzed using HPLC-DAD. At the 1:2 solid to solvent ratio, the color intensity, iron-reactive phenolic compounds and tannins content were improved using the ultrasounds-assisted extraction on Aronia berries. However, the tannin content of Marquette grapes remained the same with both techniques and solvents, suggesting that the plant cell wall structure may have a strong impact on the retention of tannins.

A169 Characterization of an exopolysaccharide (EPS-3A) produced by Streptococcus thermophilus ZJUIDS-2-01 isolated from traditional yak yogurt Feiwei Cao1, caofeiwei@zju.edu.cn, Mingming Liang1, Jianxin Liu1, Phoebe X. Qi2, Daxi Ren1. (1) Zhejiang Univ. Inst. of Dairy Science, Hangzhou, Zhejiang, China (2) USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania Yak yogurt, one of the naturally fermented dairy products prepared by local herdsmen in the Qinghai-Tibet Plateau, contains a diverse array of microorganisms. We isolated and identified a novel Streptococcus thermophilus strain, ZJUIDS-2-01, from the traditional yak yogurt. We further purified and carried out detailed structural, physiochemical, and bioactivity studies of an exopolysaccharide (EPS-3A) produced by S. thermophilus ZJUIDS-2-01. The weight-average molecular weight (Mw) of EPS-3A was estimated to be 1.38×106 Da by High-Performance Gel Permeation Chromatography (HPGPC). The monosaccharide analysis established its composition to be glucose, galactose, N-acetyl-D-galactosamine, and rhamnose in a ratio of 5.2:2.5:6.4:1.0. The molecular structure of EPS-3A was determined by the combination of permethylation analysis, FTIR, and NMR spectroscopic techniques. The ζ-potential measurements indicated that EPS-3A had a pKa value of ~4.40. The DSC yielded a melting point (Tm) of 80.4 °Cand enthalpy change (ΔH) of 578 J/g for EPS-3A, comparable to those of the xanthan gum (XG), a commercial EPS. EPS-3A exhibited better O/W emulsion stability and flocculating capacity than XG. Furthermore, it also demonstrated comparable antioxidant activity to XG and promising in vitro antibacterial properties. This work evidenced that EPS-3A derived from S. thermophilus ZJUIDS-2-01 holds the potential for food and industrial applications.

A170 Determining the distributions of antioxidants from tea extract in oil-in-water emulsions and exploring the effect of chemical structures on the distributions Lu Cheng, lc894@scarletmail.rutgers.edu, Qingrong Huang. Food Science, Rutgers The State Univ. of New Jersey, New Brunswick Efforts to minimize the lipid oxidation in oil-in-water (O/W) emulsions have been made for many years. One of the most effective, economical and convenient employed strategies for food system is addition of antioxidants (AOs). AOs from green tea extract, including (-)-Epigallocatechin-3-gallate (EGCG), (-)-epigallocatechin (EGC), (-)-epicatechin-3-gallate (ECG) and (-)-epicatechin (EC), and from black tea extract, including theaflavin (TF), theaflavin monogallate (TF-1), and theaflavin digallate (TF-2), were reported to effectively inhibit lipid oxidation. For AOs in O/W emulsions, their efficiencies depend not only on their rate constants of scavenging free radicals but also on their distributions. However, determining AOs distributions in intact O/W emulsions is not an easy task because of the physical impossibility of separating the interfacial region from the oil and aqueous regions. In this study, we determined the distribution of the selected AOs in the O/W emulsions, composed of medium chain length triglyceride (MCT), acidic water and Tween 20, via a well-established pseudophase kinetic method. Results indicated that all the individual catechins and theaflavins accumulated in the interfacial region and at the same emulsifier volume fraction, the order of the percentage concentrations in the interfacial regions followed %EGCG< %ECG≈ %EGC< %EC and %TF-2< % TF-1< %TF, indicating that the selected AOs with less galloyl groups or hydroxyl groups were more prone to locate in the interfacial region. An increase in emulsifier concentration promoted the incorporation of AOs into the interfacial region, however, their interfacial concentrations, which were much greater than their stoichiometric concentration, decreased due to the dilution of AOs in the interface region. This research firstly reported the interfacial concentration of AOs from tea extract in the O/W emulsions and explored the effect of chemical structure, especially the number of galloyl groups or hydroxyl groups on the AOs distribution, which is helpful for

developing a guideline to select the optimal antioxidant for food emulsions.

A171 “This fish smells okay, but is it still good?” Using biogenic amines to distinguish seafood species under several stages of decomposition Mayara P. Matos1,2, mpvmatos@umd.edu, Susan Genualdi2. (1) 1. Joint Inst. for Food Safety and Applied Nutrition, Univ. of Maryland at College Park (2) 2. Center for Food Safety and Applied Nutrition, US Food and Drug Administration, College Park, Maryland Biogenic amines (BAs) are low molecular mass compounds formed by the decarboxylation of specific amino acids. These molecules are potential biomarkers of decomposition because they provide indication of spoilage of a product. Currently, the FDA relies on sensory analysis, indole levels and histamine levels to evaluate the degree of seafood decomposition. However, there is a need for other analytical methods to corroborate those analyses. An optimized dispersive liquid-liquid microextraction (DLLME) method was developed for the extraction of putrescine, cadaverine, histamine and tyramine from various decomposition stages of eight types of seafood: sockeye salmon, mahi-mahi, croaker, red snapper, yellowfin tuna, yellowfin canned tuna, vannamei shrimp and scallops. Isotope dilution mass spectrometry and GC/MS were used for quantitative analyses of the BAs, followed by multivariate statistical analysis of the data. The BAs were detectable in at least two decomposition stages of each seafood, depicting very different concentration patterns between the species. These amines were investigated for their ability to distinguish decomposition stages classified by the organoleptic analysis as “borderline pass” (I4) and “borderline fail” (I5) products, which can be indistinguishable by the untrained human nose. One-way ANOVA followed by Tukey-Kramer HSD showed that putrescine was statistically different between I4 and I5 in mahi-mahi, red snapper, yellowfin tuna, canned tuna, scallops, and shrimp samples ($P < 0.05$). Cadaverine and histamine presented the second-best results as biomarkers, being significantly distinct in mahi-mahi, yellowfin tuna, canned tuna, and scallops. Tyramine was significantly different in the borderline increments for red snapper, canned tuna, and scallops. For sockeye salmon, these BAs can be used as biomarkers only if samples are analyzed in grouped increments. None of the BAs could differentiate I4 and I5 in croaker. Principal component analysis demonstrated the visual clustering of the increments within each species. The results suggest that all four analyzed BAs can be potentially used as biomarkers of seafood decomposition, but the choice of biomarker is species dependent. The differentiation between “borderline pass” and “borderline fail” stages of decomposition also demonstrates the suitability of the method to extract compounds that can support the FDA sensory analyses of seafood, ultimately leading to improved consumer protection.

A172 Providing context for chemical effects through compound structure similarity Bethany T. Cook1, bethanycook3@gmail.com, Jaleh Abedini1, Shannon Bell1, John Rooney1, Eric McAfee2, Jason Phillips2, Dave Allen1, Nicole Kleinstreuer3. (1) Integrated Laboratory Systems Inc, Research Triangle Park, North Carolina (2) Sciome LLC, Research Triangle Park, North Carolina (3) National Inst. of Environmental Health Sciences, Research Triangle Park, North Carolina The National Toxicology Program (NTP) Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) recently expanded the Integrated Chemical Environment (ICE, https://ice.ntp.niehs.nih.gov/). ICE now provides structure-based searching capabilities of curated in vivo, in vitro, and in silico data and other computational tools to facilitate the safety assessment of chemicals. One ICE feature, Chemical Quest, allows users to take a structure-based approach to explore ICE’s repository of over 800,000 chemicals, derived from the U.S. Environmental Protection Agency’s (EPA’s) DSSTox database, through a SMILES similarity search utilizing chemical fingerprints. Chemical Quest can be queried through chemical identifiers (CASRN, DTXSID, SMILES or InChiKey) or by drawing a 2D chemical representation. Chemicals identified as structurally similar can be filtered by Tanimoto score or SMART strings and then imported into any ICE tool. Such tools include “Chemical Characterization” which allows for chemical lists to be compared based on physicochemical properties. Results from queries can also be sent to NTP’s Chemical Effects in Biological Systems and the EPA’s Chemical and Products Database, providing further options to examine and compare chemicals based on physicochemical properties, bioactivity, and product use categories. ICE Search provides summary information, curated reference data, and bioactivity details for chemicals and mixtures. Concentration-response relationships from curated high-throughput assays can be examined using the Curve Surfer tool. ICE’s In Vitro to In Vivo Extrapolation tool translates in vitro bioactivity profiles to estimated equivalent in vivo doses for different exposure routes, while the Physiologically Based Pharmacokinetics tool predicts tissue-level concentrations resulting from in vivo doses. This presentation will use case studies to provide an overview of ICE tools and features for chemical analyses and comparisons through structural similarity.

A173 Soy whey protein containing trypsin inhibitors improves the texture of surimi-like gels made with protein recovered from catfish by-products Yan Zhang, yzhang@fsnhp.msstate.edu, Sam K. Chang. Mississippi State Univ., Pascagoula In order to utilize catfish by-products and improve the profitability of catfish farming industry, alkaline protein extraction from catfish by-products has proven economically feasible. However, the gels made from alkaline extracted fish protein was of low elasticity. The study’s objective was to improve the texture quality of the gel made from catfish protein isolate with soybean whey protein, a trypsin inhibitor containing by-product from the production of soy protein isolate. Soybean was defatted and protein isolate was extracted at different pH (7, 7.5, 8, 8.5 and 9) to find the optimal pH to give high protein isolate yield. With the selected extraction pH, whey protein was prepared and subjected to different heating temperatures to find an optimal temperature to eliminate lipoxygenase, but to retain high trypsin inhibitor activity. Under selected conditions, whey protein was prepared and freeze-dried. The whey protein powder was applied at different levels (0, 0.2, 0.4, 0.6, 0.8, 1.0 and 1.2 mg/g) to recovered fish protein to make gel. Texture profile analysis, autolysis and SDS-PAGE were conducted to determine the inhibitory effect of trypsin inhibitors present in whey protein on the proteolysis of fish protein during gelation. Extraction at pH 8.0 achieved 27% soy protein isolate yield and about 45% retention of the TIA in the soybean. Heating at 75 °C for 3 min removed almost 100% lipoxygenase activity and retained 53% TIA in soy whey protein. All texture parameters were improved with the increase of whey protein added, in which springiness increased from 72 to 82% and deformation increased from 6.33 to 8.1 mm. The peptides and amino acids generated during gelation were decreased from 10.19 to 5.89 mmol/g. SDS-PAGE corroborated the protective effect of whey protein on major myofibrillar proteins including myosin, actin and tropomyosin. Disulfide bonds played a vital role in the gel formation. This study solved the textural quality issues of gels made from recovered catfish protein and elucidated the molecular mechanism during gelation.

A174 Data study of the effect of biochar application on greenhouse gas emissions from agricultural soils Celeste Chan, celestechan2000@gmail.com, Simeng Li. Civil Engineering, California State Polytechnic Univ. Pomona A substantial amount of greenhouse gas emissions is from agriculture practices. With the increasing popularity of using biochar as a soil amendment, the question arises as to whether the application of biochar will mitigate greenhouse gas emissions in agricultural fields. This ongoing study aims to synthesize recent research data on biochar’s effects on soil

greenhouse gas (GHG) emissions, particularly CO2, CH4 and N2O. Data were extracted from independent individual studies and then statistically processed for analysis. This synthesis focuses on biochar made from woody and herbaceous feedstocks through fast pyrolysis. Possible impacting factors such as biochar feedstock type, residence time and temperature for biochar pyrolysis, biochar application rate, soil type and soil properties were considered for comparisons. To exclude influences of fertilizer nutrients (e.g., N and P), research that applied fertilizers during the observation periods were not selected. All the emission data collected from different sources were converted into their respective cumulative emissions over 30 days, and the percentage changes in GHG emissions were calculated between the control and experimental values. Our preliminary results indicate that biochar application in most agricultural fields is likely to reduce GHG emissions (particularly N2O emission), but the data from a small group of studies suggest differently. It also has been found that biochar products made from herbaceous feedstock tended to stimulate CO2 and CH4 emission, while those from woody materials exhibited little effects. Understanding biochar's impact on GHG emissions would greatly contribute to building a more resilient agricultural ecosystem against the changing climate.

A175 Automated identification of potential pesticides residues in fruit samples using HRMS data Elisabeth Ortega1, Ismael Zamora1, ismael.zamora@leadmolecular.com, Rosalia Lopez-Ruiz2, Antonia Garrido Frenich2, Roberto Romero-Gonzalez2. (1) Lead Molecular Design, SL, Sant Cugat del Valles, Barcelona, Spain (2) Universidad de Almería, Spain In food safety and related fields, High Resolution Mass Spectrometry techniques applied for multiresidue analysis had become an alternative to the historical routine procedures involving triple quadrupole instruments. This evolution was mainly driven by the possibility to interrogate hundreds or thousands of compounds without a prior individual study of all of them. However, due to the big amount of information that can be generated during the data acquisition, the later data processing and data analysis steps can be quite time demanding. In this presentation we will show how this late step could be automized using Chemical Monitoring workflow included in MassChemSite 3.1. Strawberry, white grape and orange samples providing from Almeria (Spain) greenhouses were acquired in the Univ. of Almería and processed using the Chemical Monitoring data workflow included in MassChemSite 3.1. Data was interrogated against an in-house pesticide database generated by literature search including up to 1500 different pesticides. From the total, up to 10 different pesticides were detected in all the samples in less than five minutes of data processing. The identification step was performed using the MS and MSMS information: MS was used to detect the pesticide in the sample, while fragmentation information was used to finally elucidate the structure of the detected pesticide, by means of a computational fragmentation of the detected pesticide and a later assignation to the MSMS data provided by the instrument. The fitting among computed and experimental fragments is reported as "score" which can be used to discriminate among other structural isobaric compounds associated to the same chromatographic peak. Data analysis and reporting were done in ONIRO server after an automatic uploading of the raw data. Later filtering steps were applied and tracked by the application for further inspection. Additionally, a final report was generated automatically once the experiment was reviewed. Data generated during the acquisition remained on the server for later use or further re-analysis.

A176 Phytochemical characterization of ninety-two Rosinweed (Silphium integrifolium) Genotypes: GC-MS profiles and their chemometric analysis Ayush Chitrakar1, a_chitrakar@coloradocollege.edu, Yiren Zhang1, e_zhang@coloradocollege.edu, Blaze Johnson2, Ebony Murrell2, Edy Chérémond2, Murphy Brasuel1. (1) Dept. of Chemistry & Biochemistry, Colorado College, Colorado Springs (2) The Land Inst., Salina, Kansas Silphium integrifolium, also known as rosinweed, is a common sunflower-like perennial in the Midwest. Because S. integrifolium, like other perennial crops, can be produced without regular soil tillage, it is targeted as an alternative for oilseed production. Vegetable oils, including canola, soy, sunflower, and olive, are used for frying other foods in many traditional cuisines. They improve the availability of lipid-soluble vitamins and provide or enhance food flavor because they provide energy and essential fatty acids not synthesized by humans. S. integrifolium has demonstrated several advantages over other oilseed plants, including a deeper root system leading to drought resistance, excellent pollinator resources, and natural insect herbivore resistance. Terpenoids synthesized by the plant are hypothesized to reduce insect feeding or growth. Natural insect resistance could make this crop well suited to organic or low-input production systems, and silphium breeders want to avoid losing this trait by accident during domestication. In this study, methods for the extraction of biologically active terpenoids from S. integrifolium leaves were explored and optimized. Air-dried leaves from 92 different genotypes were extracted with isopropyl alcohol using a heated ultrasonic-assisted technique. The extracts were then run on a GC-MS to characterize the terpenoids. The genotypes were all from the Midwest but varied in the region they are native to, eastern, central, or western Midwest. The genotypes also varied in their insecticidal activity, which was determined by a fall armyworm-based bioassay. Chemometric characterization of phytochemical data from the GC-MS included the multivariate techniques of cluster and principal component analysis. The analysis determined that each genotype has a unique chemical fingerprint that can be used to establish the likely native region of each S. Integrifolium genotype. Furthermore, an inverse correlation was found between the bioassays and the terpenoid concentrations.

A177 Earthworms increase the potential for enzymatic bioactivation of biochars made from co-pyrolyzing animal manures and plastic wastes Juan Sanchez-Hernandez2, Kyoung Ro1, kyoung.ro@usda.gov, Ariel A. Szogi1, Sechin Chang1, Bosoon Park1. (1) USDA Agricultural Research Service, Athens, Georgia (2) Univ. de Castilla-La Mancha, Teledo, Spain We assessed the enzymatic activation of four different biochars produced from pyrolyzing swine manure and poultry litter, and by co-pyrolyzing these livestock residues with agricultural spent mulch plastic film wastes (plastichars). Enzymatic activation consisted of incubating biochars in soil inoculated with earthworms (Lumbricus terrestris), which acted as biological vectors to facilitate retention of extracellular enzymes onto biochar surface. The activity of carboxylesterase, a pesticide-detoxifying enzyme, was measured in non-bioturbed soils (reference), linings of the burrows created by earthworms, casts (feces) and biochar particles recovered from the soil. Our results revealed that: 1) biochar increased soil carboxylesterase activity respect to biochar-free (control) soils, which was more prominent in the presence of earthworms. 2) The maximum enzyme activity was found in soils amended with plastichars. 3) The plastichars showed higher enzyme binding capacities than that of the biochars produced from animal manure alone, corroborating the pattern of enzyme distribution found in soil. 4) The presence of earthworms in soil significantly increased the potential of the plastichars for enzymatic activation. These findings suggest that the plastichars are suitable for increasing and stabilizing soil enzyme activities with no toxicity on earthworms.

A178 Modeling beer ratings with machine learning Christina N. Vialva1, cv1082971@swccd.edu, Errysteinn Frondarina1, ef1049416@swccd.edu, Gary Fogel2,3, David A. Hecht1,2. (1) Chemistry, Southwestern College, Chula Vista, California (2)

Chemistry and Biochemistry, San Diego State Univ., California (3) Natural Selection Inc, San Diego, California Brewing a good tasting, high-quality beer in a reproducible manner is a very complex and challenging process. A wide range of parameters and factors effect beer quality in nonlinear ways. These include: the composition of the grain bill; the selection of the hops added; the selection of yeast strain(s); the composition of the water used; and optimization of timing and temperature. Here we develop several models that input such features and generate a prediction of beer quality. For this purpose, beer recipes and associated quality rankings (e.g., 1-5 beers, with 5 being the best) were downloaded from www.BeerSmith.com and www.BrewersFriend.com and converted into descriptors. These features were fed into to Molegro Data Modeller and normalized. Feature selection helped reduce the possible input space. We evaluated several nonlinear and/or machine learning modeling methods using features from BrewersFriend for their ability to predict beer quality at BeerSmith. These included: Multiple Linear Regression; Partial Least Squares Regression; Support Vector Machines; Neural Networks; and KNN Classification. The resulting models demonstrated the ability to associate beer recipe features with quality and can be used in the production of novel beers.

A179 Peanut allergen isolation using ligand bound magnetic nanoparticles Reilly Arena, Gaerielle Nagorite, gjn@email.uscupstate.edu, Anselm I. Omoike. Univ. of South Carolina Upstate, Spartanburg Peanut (Arachis hypogaea) has a balanced and high nutrient composition of fats, proteins, carbohydrates, vitamins and minerals, and it is widely consumed around the globe due to its affordability. The major concern of peanut consumption, however, is the allergenic reactions of some of its protein constituents (Ara h1-17). In the U.S., 2.5% of children and 1.8% of adults have some range of mild to severe peanut allergenicity, which can only be treated through avoidance of consumption or possible immunotherapy. The goal of this study was to develop a cheap, simple, and recyclable extraction technology for allergens removal from peanut extracts. In this study, we functionalized magnetic iron oxide nanoparticles (M) with phytic acid (PA) and evaluated the potential application of the coated particles as an adsorbent for removing allergens from extracts of two varieties of peanuts, the Spanish and the Valencia. The ligand bound magnetic iron oxide nanoparticles (MPA) were characterized using spectroscopic methods. Protein concentrations and protein profiling of the peanut extracts were carried out by bicinchoninic acid (BCA) protein assay and sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE) analysis, respectively. The SDS-PAGE profiles show near complete removal of Ara h1 in the raw and defatted extracts of the two varieties studied after 19 h treatment with MPA (7.9 ± 0.050 mg MPA/mL extract). Ara h1 is the most abundant peanut allergen recognized by the serum IgE in more than 90% of peanut-allergic patients. The MPA are inexpensive, easy to use, easy to retrieve after use, and a prospective adsorbent for highly efficient removal of Ara h1 from raw and defatted peanut extracts. The desorption of adsorbed Ara h1 from MPA for allergy research and therapy processes will be discussed.

A180 Chemical and electrochemical ion intercalation on cobalt hydroxide: Selective phase transformation and application to electrocatalytic reactions Oluwayemi O. Onawumi1, Paul B. Ayoola2, pbayoola@lautech.edu.ng, Olubunmi A. Adewusi3. (1) Dept. of Pure and Applied Chemistry, Ladoke Akintola Univ. of Technology, Ogbomoso, Oyo, Nigeria (2) Dept. of Science Laboratory Technology, Ladoke Akintola Univ. of Technology, Ogbomoso, Oyo, Nigeria (3) Dept. of Chemistry and Biochemistry, Caleb Univ., Lagos, Nigeria Palm wine has been an African drink for ages. It has been used as medicine, juice, drink to appease gods and for many other things. The aim of this study is to evaluate the nutritional benefits and medicinal potential of Raphia palm wine. Fresh and fermented Raphia palm wine were collected from a Raphia palm tree with the assistance of a local palm wine tapper at Yoaco area of Ogbomoso in Oyo state, Nigeria. The following were determined; the pH, which was measured immediately the sampling bottle was opened with a digital pH meter. The brix of the palm wine was determined with a refractometer and the Acid concentration (%TTA) by titrating with a base and expressing it as citric acid equivalent. The fermented and fresh palm wine investigated had pH of 4.26 and 4.35 respectively, Brix values were 2.50 and 4. 00 and % TTA values were 0.83 and 0.94 % respectively. The proximate analysis of the fermented and fresh palm wine revealed the presence of moisture (87.20% and 81.70%), crude protein, (0.01% and 0.03%), crude fat (0.003 and 0.04 %), crude fiber (3.45 and 4.10 %), ash, (6.21% and 7.22 %) respectively while the carbohydrate contents were (6.1 and 9.91 %). The mineral analysis revealed the presence of calcium(Ca) and potassium(K) as the major minerals while sodium(Na) was moderate and magnesium(Mg), iron(Fe), zinc(Zn), manganese (Mn) were in traces and copper (Cu), cadmium (Cd), lead (Pb) and mercury(Hg) were not detected. The result obtained shows that palm wine contain nutrients that are essential as food as well as medicinal due to the presence of some essential elements which are needed for proper functioning of the body system, therefore, possess nutritional and medicinal values.

A181 Improving the extraction and recovery of organic acids from root exudates by WAX-SPE Noryn P. Rosario1, noryn.p.ros@gmail.com, Paul Larsen2, Gregory Barding1. (1) Chemistry, California State Polytechnic Univ. Pomona (2) Biochemistry, Univ. of California Riverside Aluminum toxicity can occur in acidic soils (pH < 5.5) and affects an estimated 35% of arable land in North America and up to 50% of arable land worldwide. These soils are largely unusable for a variety of crops, limiting food access and stability. There are two primary mechanisms plants can use to grow in Al toxic soils. One mechanism is Al tolerance, where Al is internalized but sequestered in a manner that limits the damaging effects of Al to the plant. A second mechanism is Al exclusion, where Al is excluded from the roots by release of chelators. Al exclusion is seemingly the preferred mechanism since prevention of uptake would eliminate the likelihood of any damage related to internalization. Organic acids, such as those containing di- and tri- carboxylic acids, are examples of chelators that can be released into the soil to prevent the uptake of Al by the roots. However, measuring these organic acids are in soil are not trivial; in addition to Al, there are also other common metals present that can be chelated and act as interferants. This work explores the use of weak-anion exchange solid-phase extraction to isolate and Nuclear Magnetic Resonance and Gas-Chromatography coupled with Mass Spectrometry to quantify the production of organic acids exuded from the roots for an Al-protective mechanism. A variety of methods are being evaluated, including the recovery of organic acids in the presence of calcium as a potential interferent and the use of EDTA to limit the interference of calcium or other metals may have on the recovery of organic acids by WAX-SPE. Preliminary work suggests that chelation of calcium by the organic acids can have a significant effect on the recovery of organic acids by SPE and use of a buffer and EDTA can limit the interferents and increase recovery for some organic acids, but not all. We are continuing to evaluate other modifications for SPE to broadly improve the recovery and reproducibility of organic acids exuded by plant roots using WAX-SPE.

A182 WITHDRAWN

A183 Sucrose treatment improves phytochemical levels and bioactivities of mung bean sprouts Junsoo Lee, junsoo@chungbuk.ac.kr, Huijin Heo, Hana Lee. Chungbuk National

Univ., Cheongju, Chungcheongbuk-do, Korea (the Republic of) Sprouting is a simple and inexpensive way to improve the digestibility and nutritional quality of legume. Exogenous treatment with abiotic elicitors can be used to manipulate both metabolite production as well as the qualitative value in leguminous plants. In this study, the effects of sucrose treatment on the growth condition, dietary nutritional quality, and biological activities of mung bean sprouts were investigated. Mung bean seeds were germinated at 25°C in darkness for 4 days and sprayed solutions containing different concentration of sucrose. The results showed that sucrose-treated sprouts have more bioactive compounds including polyphenols, flavonoids, γ-aminobutyric acid, phytosterols, and vitamins than non-treated sprouts. The activities of phenylalanine ammonia-lyase, tyrosine ammonia-lyase, and glutamate dehydrogenase were increased under sucrose treatment. The antioxidant activities were also significantly higher in the sucrose-treated sprouts compared with the non-treated one. The mung bean sprouts treated with 2−3% sucrose markedly improved the insulin resistance and oxidative liver injury in HepG2 cells. Therefore, the present study provides that the sucrose treatment as an abiotic elicitor during mung bean sprouting could be an effective strategy to improve dietary phytochemical compositions as well as the potential health benefits.

A184 Antioxidant and anti-hypertensive effects of sinapic acid via activation of Nrf2/HO-1 pathway in EA.hy926 endothelial cells Hana Lee2, dlgksk0514@naver.com, Hyun-Joo Kim1, Junsoo Lee2. (1) National Inst. of Crop Science Suwon, Gyeonggi-do, Korea (the Republic of) (2) Chungbuk National Univ., Cheongju, Chungcheongbuk-do, Korea (the Republic of) Oxidative stress is a key player in the pathogenesis of hypertension. Increased oxidative stress may impair endothelium-dependent vascular relaxation and constriction. Phenolic acids are widely found in daily foods including fruits, vegetables, and cereals and they are known to have antioxidant and health-promoting properties. Treatment with antioxidants, such as phenolic acids, has been suggested to lower oxidative stress and blood pressure. In this study, to confirm the protective effect of phenolic acids, cell viability, reactive oxygen species generation, nitric oxide production, glutathione depletion, and lipid peroxidation were investigated against H2O2-induced oxidative stress in endothelial cells. Among the 11 phenolic acids, sinapic acid showed the highest protective effect. Therefore, sinapic acid was selected and its anti-hypertensive mechanism was investigated. The phosphorylation of endothelial nitric oxide synthase and protein kinase B was enhanced by sinapic acid in a dose-dependent manner. In addition, the protein expression of phase II enzymes, such as heme oxygenase-1, NADPH: quinone oxidoreductase 1, and gamma-glutamate-cysteine ligase catalytic subunit was dose-dependently increased by sinapic acid treatment. Sinapic acid increased the nuclear factor erythroid 2-related factor 2 protein expression level in the nucleus of EA.hy926 cells. Hence, this study suggests that sinapic acid could be effective in alleviating oxidative stress-induced endothelial dysfunction.

A185 Effects of various pre-treatment and cooking on the levels of biogenic amines in mackerel Hyunwoo Ahn, Yangsu Kim, Kwang G. Lee, kwglee@dongguk.edu. Dongguk Univ., Jung-gu, Seoul, Korea (the Republic of) This study analyses the biogenic amines (BAs) formed in mackerel cooked by various methods and conditions. Five BAs, including tryptamine, β-phenylethylamine, putrescine, histamine and spermidine, were analysed by high-performance liquid chromatography with UV detection. The level of total BAs was higher in the mackerel fillet (108.14 μg/g) than the headed and gutted fish (91.58 μg/g). Roasted, fried and stewed mackerel recorded total BA concentrations of 54.28, 82.25 and 163.05 μg/g, respectively. Stewed mackerel contained about 3-fold more BAs than roasted mackerel. The level of total BAs in mackerel increased significantly up to 190%, 236% and 152% as the roasting temperature increased, upon frying, and as stewing temperature increased, respectively ($p < 0.05$).

A186 Correlation analysis between volatile compounds and α-dicarbonyl compounds in various beans as responses to different roasting conditions Subeen Do, Jooyeon Park, Gaeun Lee, Kwang G. Lee, kwglee@dongguk.edu. Dongguk Univ., Jung-gu, Seoul, Korea (the Republic of) In this study, volatile compounds and α-dicarbonyl compounds (α-DCs; glyoxal, methylglyoxal and diacetyl) content were analyzed with three types of beans (soybean, black soybean, and mung bean) roasted at different time and temperature conditions. Volatile compounds were extracted using a slight modification of distillation under reduced pressure method and analyzed using gas chromatography-mass spectroscopy detector (GC-MSD). Out of 20 volatile compounds identified in bean extracts, 1-octen-3ol, which is relatively abundant in unroasted beans, was reduced by up to 86%, and 1-hexanol was not detected after 25 min roasting. 3-ethyl-2,5-dimethylpyrazine and 2,3,5-methylpyrazine, which were not detected in roasted soybeans, became the main volatile compounds after roasting. Roasting at 180 °C for 25 min had the highest volatile compounds content of all types of conditions. Analysis of α-DCs was performed using chromatography-nitrogen phosphorus detector (GC-NPD). The heat-map showed a relative abundance as blue (negative) to red (positive) scale, and as roasting temperature and time increased, glyoxal changed from red (+2) to blue (-2), and methylglyoxal and diacetyl changed from blue (-2) to red (+2). Roasting at 200 °C for 25 min had the highest α-DCs content of all types of conditions. As the roasting temperature and time increased, the level of α-DCs and volatile substances showed a strong positive correlation (spearman correlation, r = 0.878, 0.867, 0.890 in soybean, black soybean, mung bean, respectively). However, volatile compounds and color values showed a strong negative correlation (spearman correlation, r = -0.917, -0.967, -0.850 in soybean, black soybean, mung bean, respectively). The results of this study suggest 180 °C for 25 min roasting as optimal roasting conditions for beans, in which the generation of flavor components is maximized while the generation of α-DCs is relatively small.

A187 Effect of ultraviolet light exposure and compost tea supplementation on growth and nutrient profile of hydroponically grown mustard greens Robert Castro1, rcastro0271@sdsu.edu, Daniel Pentico2, Stephanie Lu1, Sherry Dinh1, John J. Love3, David Larom5, Ramona Pérez4, Changqi Liu1. (1) School of Exercise and Nutritional Sciences, San Diego State Univ. College of Health and Human Services, California (2) San Diego State Univ., California (3) Dept. of Chemistry and Biochemistry, San Diego State Univ. College of Sciences, California (4) Dept. of Anthropology, San Diego State Univ. College of Arts and Letters, California (5) Dept. of Geological Sciences, San Diego State Univ. College of Sciences, California Hydroponic food production is efficient in water and land use and may help address food insecurity challenges. When practiced in a controlled environment, hydroponic systems are unaffected by a changing climate and can sustain yearlong food production. However, the lack of exposure to UV light and soil microorganisms predisposes the plants to possible antioxidant inadequacy and disease susceptibility. The objective of this study was to investigate the effects of UV light exposure and microbial inoculation on plant growth in hydroponic systems. Garnet Giant mustard greens were hydroponically grown in both indoor and outdoor settings, with and without UV light blocking. One-week-old seedlings were inoculated via foliage with an aerated compost tea consisting of molasses, worm castings, kelp extract, alfalfa meal, mycorrhiza, and azomite to boost beneficial microorganisms. The mustard greens were grown for an additional 14 days. Plant growth and growing conditions were monitored. Moisture, nitrogen, and ash contents, leaf pigmentation,

antioxidant activities, and microbiome of the mustard greens were analyzed. Mustard greens grown in the greenhouses produced 7.3-9.0 times more dry mass than those grown indoor ($P<0.01$). Compost tea supplementation boosted nitrogen and mineral accumulations in the absence of UV-blocking ($P<0.01$). Mustard leaves grown in the UV-passing greenhouse were predominantly red in color while those grown with reduced UV exposures lacked the pigmentation. UV exposure improved ABTS free radical scavenging activity, ferrous chelating activity ($P<0.01$), and ferric reducing power ($P<0.05$) of 80% methanolic extract of the mustard greens, while compost tea supplementation reduced the antioxidant activities ($P<0.05$). Compost tea inoculation resulted in approximately two log-fold increases ($P<0.05$) in beneficial bacteria Pseudomonas oryzihabitans and Leptolyngbya laminosa and a 5.8 log-fold decrease in fungal pathogen Alternaria carotiincultae ($P<0.01$). Overall, our results suggested that exposure to UV radiation and beneficial microorganisms improved the performance and nutrient profile of hydroponically grown mustard greens.

A188 Fluorosulfurylation of amino acid-based sweeteners towards novel high intensity artificial sweeteners Samuel Khasnavis, srka2017@mymail.pomona.edu, Nicholas D. Ball. Chemistry, Pomona College Dept. of Chemistry, Claremont, California The excessive consumption of dietary sugar is a major risk factor for obesity and chronic health conditions such as diabetes and cardiovascular disease. High-intensity artificial sweeteners generally offer consumers the perception of sweetness without the caloric content and elevation of blood sugar levels accompanied by sugar consumption. The most widely used high intensity sweetener, aspartame, binds to the venus flytrap (VFT) domain of T1R2, the predominant binding site of the T1R2/T1R3 sweet taste receptor. Previous functionalizations of a terminal amine on aspartame yielded two new FDA-approved high-intensity sweeteners, neotame and Advantame, with respective potencies 50 and 100 fold higher than aspartame. In recent years, the fluorosulfurylation (addition of an SO2F group) to biologically active molecules has gained attention, due to the unique reactivity of the RSO2F moity. The SO2F warhead displays proximity enabled and context-dependent reactivity, undergoing sulfur fluoride exchange (SuFEx) at the sulfur atom to form a covalent bond in the presence of nucleophilic residues. Owing to these properties, the S(VI)F motif has been incorporated into biologically active molecules to create long-lasting covalent probes and inhibitors of high potency for use in medicinal chemistry and chemical biology. Though the development of S(VI)F-based pharmaceuticals has burgeoned, the use of these covalent warheads in food chemistry remains largely unexplored. Herein we discuss the fluorosulfurylation of amino-acid-derived sweeteners such as aspartame and neotame as part of an effort to create novel artificial sweeteners with higher potency, increased water solubility, and longer-lasting sweetness than their predecessors.

A189 Determination of quaternary amine polar pesticides using improved cation-exchange separation technology combined with suppressed conductivity and tandem mass spectrometry detection Terri T. Christison, terri_christison@yahoo.com, John E. Madden, Jeffrey Rohrer. Ion Chromatography Products, Thermo Fisher Scientific Inc, Sunnyvale, California Quaternary amines are challenging to determine due to their strong interaction with cation-exchange columns and chemical similarity. In addition, some quaternary amines are polar pesticides with toxic and environmental concerns. Here we demonstrate direct determinations of four quaternary amine polar pesticides in food products using a high-performance cation-exchange column designed to resolve quaternary amine pesticides and inorganic cations. The polar pesticides are serially detected by suppressed conductivity and Selective Reaction Monitoring (SRM) of the product and reaction product ions. The pesticides were separated using an electrolytically generated methanesulfonic acid gradient from 3 to 25 mM at 0.3 mL/min and 40 °C. After passing through an electrolytic suppressor, which replaces the acid anion with hydroxide to form water, the pesticides were detected by suppressed conductivity and ionized by positive ESI-MS without make-up solvent for detection by MS. The method was applied to ground, acid-methanol extracted, diluted oat cereal samples following a modified Quechers Polar Pesticide (QePPe) method. Chlormequat was extracted with formic acid whereas paraquat and diquat were extracted with hydrochloric acid. The four quaternary amine polar pesticides exhibited good peak shape with peak asymmetries from 1.0 to 1.1 As(EP) and eluted from the column within 20 min with baseline resolution. The two types of oat cereal samples did not contain paraquat, diquat, mepiquat, or chlormequat. Recoveries of spiked in reagents were ~80%. Sensitivities, as judged by the limits of detection, were single digit µg/L.

A190 Effect of infrared drying method on chemical and microbial stability of cold-hardy grape pomaces Zeinab Shad, zeinabm@iastate.edu, Chandrasekar Venkitasamy, Emily Kuelbs, Aude A. Watrelot. Food Science and Human Nutrition, Iowa State Univ., Ames This study aims to valorize pomace from the cold-hardy grapes grown in the Midwest by drying using hot air and infrared (IR) heating and separating the rice husk with sieving. A catalytic IR heating using natural gas was used to optimize a sustainable drying method for grape pomace. Grape pomace flours were stored under three conditions for 6 months to establish the most appropriate conditions for long term use. The IR drying reduced the initial moisture content (MC) of grape pomace ranged from 50-70% (wet basis) to an MC <10% (w.b.) in 30 min, whereas hot air (HA) drying took about three hours. The quality of IR dried grape pomace samples before and after 6 months of storage, including color and antioxidant content, was determined, and compared with HA dried samples. IR heating at the lowest gap distance (14 cm, distance between an IR emitter and product surface) had the highest drying rate. The color parameters (L*, a*, and b*) and phenolic compounds of IR dried grape pomaces were not significantly different from those of the HA dried pomace before storage. Substantially higher tannin and phenolic contents were found for dried cold-hardy grape pomaces than fresh, raw pomace. The antioxidant activity of dried grape pomace was not different between IR and HA drying methods. The IR drying and sieve separation can be used to produce microbiologically safe and antioxidant-rich grape pomace powder for food and feed application.

A191 Use of 1H NMR spectroscopy to identify fraud in commercial honey samples Vanna Kizirian, vannakizirian@yahoo.com, Rosalee Hellberg. Chapman Univ., Orange, California The objective of this research is to test clover and wildflower honeys sold on the commercial markets for the presence of sugar adulterants. Honey is a common target of fraud, in which cheaper sugar syrups, such as corn syrup, beet syrup, and rice syrup, are added to replace authentic honey. In addition, honey is sometimes diluted with water, which can lessen the concentration of the natural components associated with the benefits of honey. A total of 30 honey samples were obtained from commercial markets in Orange County, CA. The degrees Brix of the honey was measured by a digital refractometer and converted to moisture percentage to validate it was under 18.6% moisture (the maximum level of moisture that should be present in commercial honey samples according to USDA Standards). All honey samples were measured to be under 18.6% moisture. The samples were tested for the presence of adulterants using 1H NMR (Nuclear Magnetic Resonance) Spectroscopy. A standard was made for the common sugar adulterants in honey, including glucose, fructose, sucrose, and 5-hydroxymethylfurfural to obtain the exact chemical shifts in the NMR spectra to compare with the honey samples. Other sugar syrups

such as corn syrup, beet syrup, and rice syrup were obtained for comparison as well. The number signals in the chemical shifts are proportional to the concentration of the particular compound, which can provide insight on the concentration of possible sugar adulterants and other natural components. Overall, the results of this study will improve our understanding of the extent of honey fraud on the commercial market.

A192 Development of novel antioxidant, antibiofilm and hydrophobic cinnamic acid and cinnamic acid derivatives based cellulose nanofibrils (CNF) films for food packaging applications SuriyaPrakaash LakshmiBalasubramaniam1, suriyaprakash.lakshmibalasubrmaniam@maine.edu, Denise Skonberg1, Mehdi Tajvidi2, Cailtin Howell3. (1) School of food and agriculture, Univ. of Maine System, Bangor (2) School of Forest Resources., Univ. of Maine System, Bangor (3) Dept. of Chemical and Biomedical Engineering., Univ. of Maine System, Bangor Cellulose nanofibrils (CNF) are nanoscale fibers commonly obtained from wood pulp through mechanical disintegration. Due to their size and the large number of surface hydroxyl groups, they have the capacity to form strong hydrogen bonds with each other. This hydrogen bonding is the primary reason CNF can form strong flexible films. However, CNF can also hydrogen bond with water molecules making its films susceptible to water. Modification using phenolic acids can improve the hydrophobicity of CNF films making them less susceptible to water and moisture. In this study CNF films were esterified using cinnamic acid and its derivatives (ferulic, coumaric and caffeic acid) using Steglich esterification and tosyl chloride mediated esterification. The modified films were investigated for evidence of esterification, changes in hydrophobicity, mechanical properties, crystallinity, antioxidant activity and antibiofilm activity. It was evident from the results that both esterification techniques resulted in modification of CNF films. After esterification, films acquired antioxidant activity producing a maximum DPPH radical scavenging activity of 79±8% and a TBARS value of 4.58±0.5 mg MDA/kg for films submerged in canola oil at 50 °C for 55 days. An increase in hydrophobicity with a water contact angle value of 101.02 ± 6.41° and water vapor permeability of 0.0075±0.0005 ng cm -1 s -1 pa -1 were also noted. Similarly, modification resulted in a 1 log CFU/mL reduction in viable Bacillus subtills cells on film surface when compared to CNF control. Therefore, modification of CNF films with phenolic acids significantly reduced their susceptibility to water while also providing additional functionality.

A193 Oxygen functionalized MWCNTs decorated with silica-coated spinel ferrite–A nanocomposite for potentially rapid and efficient decolorization of the aquatic environment Zeid A. Al Othman, zeid99@yahoo.com, saikh wabaidur. Chemistry, King Saud Univ., Riyadh, Riyadh Province, Saudi Arabia A silica-coated copper ferrite was decorated on oxidized multi-walled carbon nanotubes for the preparation of nanocomposite. The synthesis was carried out through co-precipitation and hydrothermal reactions. The material was used for the adsorptive removal of cationic dyes from water. Nitrogen adsorption/desorption isotherm confirmed mesoporous nanocomposite surface with 182 m2/g specifics-face area. Spectral bands observed during IR analysis confirmed the successful formation of the nanocomposite. The VSManalysis revealed its ferromagnetic behavior with 0.004 emu/g saturation magnetization. Binding energy peaks observed during XPS analysis further supported nanocomposite synthesis and dyes adsorption over its surface. Dyes adsorption was affected by pH and temperature with equilibrium and kinetic results respectively fitting the Langmuir isotherm and the pseudo-second-order models. Maximum monolayer adsorption capacities determined for CB and MB adsorption on nanocomposite were 714 mg/g (293 K) and 204 mg/g (323 K), respectively. Regeneration studies revealed maximum CB and MB recovery with acetonitrile and methanol, respectively. Therefore, the novel nanocomposite here synthesized is a suitable adsorbent for rapid and effective decolorization of cationic dyes containing wastewaters.

A194 Anti-bacterial, anti-inflammatory activities of lactic acid bacteria-bioconversioned indica rice (Oryza sativa L.) extract Hyunwoo Ahn, Huckjoo Kwon, Kwang G. Lee, kwglee@dongguk.edu. Dongguk Univ., Jung-gu, Seoul, Korea (the Republic of) In this study, indica rice (Oryza sativa L.) was bioconversioned by Lactobacillus plantarum ATCC14917 (LP) and Lactobacillus rhamnosus GG KCTC5033 (LR). Rice extract fermented by LP (LP-RE) and RE fermented by LR (LR-RE) inhibited growth of pathogenic bacteria except E. coli O157:H7 ($P < 0.05$) than RE (control). In biofilm formation assay, the effect of inhibiting biofilm produced by S. aureus exhibited the most by LR-RE (10.81 ± 1.98%). In addition, through real-time PCR, we verified that LP- RE inhibited S. aureus-induced IL-8 expression in Caco-2 cells by 60%. The LC/MS-MS was used to verify for any changes in compound of RE during bioconversion.

A195 Improvement of Robusta coffee aroma with L-leucine powder Hyunbeen Park, Ara Cho, Kwang G. Lee, kwglee@dongguk.edu. Dongguk Univ., Jung-gu, Seoul, Korea (the Republic of) L-leucine powder (LP) were added to improve the aroma of Robusta coffee beans. Treatment was a short soaking (M1) or spraying procedure (M2), then LP was added at varying levels up to 3% (w/w). All samples were roasted (240 °C/15 min) and extracted using an espresso machine. Volatile compounds were analysed by solid-phase microextraction-gas chromatography-mass selective detection. Thirty volatile compounds (6 pyrroles, 8 pyrazines, 3 phenols, 9 furans, 2 ketones, 2 aldehydes) were analysed. In 15 coffee samples, the levels of total volatile compounds (based on peak area ratios) ranged from 8.9 (M1-1) to 15.5 (non-treated Robusta: NTR). Robusta coffee has lower levels of bitter aroma compounds when pre-treated with LP. The sum of bitter volatiles (phenols, pyrroles, pyrazines) was lowest in M1-5 (3% LP), M2-1 (1% LP; both dried at 50 °C/15 min) and M2-7 (3% LP, dried at 70 °C/15 min) compared with NTR ($p < 0.05$).

A196 Reduction of sulfur containing volatiles from antioxidative onion skin extract JiHee Hong1, Mi-Ja Kim2, JaeHwan Lee1, s3hun@skku.edu. (1) Sungkyunkwan Univ. College of Natural Science, Suwon, Korea (the Republic of) (2) Kangwon National Univ., Samchek, Gangwon-do, Korea (the Republic of) Onion (Allium cepa L.) is one of the major sources of dietary flavonoids and has been valued worldwide as medicinal materials, essential seasonings, and spices for processed foods. The aroma and flavor of these Allium species are characterized by a variety of sulfur containing compounds (SCV), which are produced mainly after destruction of cellular structures. Generally, SCV possess an unpleasant odor characteristic, it is necessary to develop methods to control the contents of SCV. The objectives of this study were to screen substances possessing SCV controlling abilities and to evaluate antioxidant activities of onion extract after treatment of deodorization process. The headspace volatiles and antioxidant activities of onion solution were analyzed after treatment by adding 0.5% of α-cyclodextrin (α-CD), β-cyclodextrin (β-CD) and 2-hydroxypropyl-β-cyclodextrin (HP-β-CD), chitosan, and magnesol. The volatiles were analyzed using the solid-phase micro-extraction (SPME) method and identified by GC-MS whereas their antioxidant properties were tested using in vitro assays. The major SCV in the onion solution were methyl propyl disulfide, dimethyl trisulfide, dipropyl disulfide, and dipropyl trisulfide, which accounted for 5.2, 3.5, 15.8, and 60.5% of the total volatiles, respectively. When β-CD

was added to the onion solution, methyl propyl disulfide, dipropyl disulfide, and dipropyl trisulfide were reduced by 64.1, 78.0, and 75.6%, respectively. The content of dimethyl trisulfide was substantially reduced by HP-β-CD compared to the control. These two additives showed the highest deodorizing effects compared to others. Compared to the control, the radical scavenging ability of the sample treated with β-CD decreased by 78.1%, whereas no significant difference was observed when treated with α-CD and HP-β-CD ($p>0.05$). Considering SCV reducing and antioxidant retaining abilities, HP-β-CD is the most suitable substance for reducing the off-flavor of onion while retaining antioxidant properties.

A197 PVA hydrogel film containing lemongrass essential oil emulsion for smart food packaging Hyeongseop Kim1, gudtjq228@naver.com, Umin Park1, Choongjin Ban2, Seokwon Lim1. (1) Dept. of Food Science & Biotechnology, Gachon Univ., Seongnam, Korea (the Republic of) (2) Dept. of Environmental Horticulture, Univ. of Seoul, Dongdaemun-gu, Seoul, Korea (the Republic of) Active packaging is the most promising technology providing antimicrobial barrier for food storage. However, the problem that antimicrobial active package may start to loss its expected function as soon as produced, remains to limit wide ranging industrial applications, because antibacterial functional substances are coated onto packaging, incorporated into packaging layer. Here we demonstrate a controlled release system for antibacterial active food packaging employing a complex of responsive hydrogel and emulsion system with lemongrass essential oil (LGEO), an antibacterial substance. LGEO oil was loaded with O/W emulsion (LGEOE) via ultra-sonication and then incorporated hydrogel. Since relative humidity (RH) is a key feature to bacterial food spoilage, a responsive hydrogel was composed with polyvinylalcohol (PVA), a responsive polymer on RH. Ultimately, LGEOE-PVA hydrogel film were prepared by casting method. The responsive release behavior of LGEOE-PVA film was observed at several RH condition (26, 52, 70, 90% RH) for 72 hours. The content of LGEO oil was 62.04±5.85%, 34.28±18.59%, 15.96±7.76%, and 9.24±10.59%, which decreased as the humidity increased. To confirm the antibacterial activity of LGEOE-PVA film (64 cm2), bacteria were grown in a fixed volume (1840 mL). As a result, the bacteria did not grow within 72 hours, the longest time we observed.

A198 Zn2+ and Ag+ doped oyster shell waste as a natural antimicrobial agent for active packaging Park Kitae, rbdnjs0504@naver.com, Seo Jongchul. Yonsei Univ., Wonju, Korea (the Republic of) Oyster shell wastes have been a significant environmental issue in the southern coast of Korea due to the continues unloading of this food waste into the environment. The oyster shell powder (OSP) poses an antimicrobial potency with a good cytotoxicity profile. However, the application of OSP is limited to the weak antimicrobial activity and low surface interactions. In this study, the OSP was doped with Zn(NO3)2 and AgNO3 in the molar ratio of 1:0.01 M:M using precipitation method. Subsequently, samples were calcined at 750 °C to achieve Zn2+-doped OSP and Ag+-doped OSP. As-prepared materials were thoroughly characterized to identify the chemistry, morphology, and antimicrobial mechanisms. Accordingly, Fourier transform infrared spectroscopy detected peaks corresponding to the Zn2+ and Ag+ on the OSP surface, indicating the surface interaction between OSP and Zn2+ and Ag+. In addition, the morphology and microstructure of samples were identified using transmission electron microscopy and X-Ray diffraction in which doping process rendered the OSP microstructure morphology. Moreover, the antimicrobial activity of as-prepared samples remarkably enhanced against Escherichia coli and Staphylococcus aureus compared to pure calcined OSP, indicating that doping process increased the surface interactions and improved the reactive oxygen species generation as the main biocidal mechanisms. Therefore, the doping process successfully introduced Zn2+ and Ag+ to OSP and enhanced antimicrobial process, which in turn as-prepared materials can be used as natural antimicrobial agents for food, biomedical, and packaging applications.

A199 Quantification of “smoke taint” compounds in grapes and wine by SPME-GCMS Eberhardt R. Kuhn, erkuhn@shimadzu.com, Andy Sandy, Alan Owens, Dominika Gruszecka. Shimadzu Scientific Instruments, Columbia, Maryland “Smoke taint” refers to the aroma that wine takes on when grapes in a vineyard are exposed to smoke from wildfires during ripening, a frequent occurrence in Australia and recently the western US. Wines afflicted with smoke taint are often described as “campfire” or “ash tray”-like and are typically not accepted by consumers. Because of this, a fast and accurate screening method for smoke taint is necessary for winemakers who are faced with remediation, blending, or discarding decisions when grapes are being harvested during or after a wildfire. Guaiacol and 4-methylguaiacol are two compounds typically analyzed as markers of smoke taint, as they are most abundant compared to other smoke-derived odorants like 4-ethylguaiacol, 4-ethylphenol, and eugenol. By combining solid phase microextraction (SPME) sampling prior to analysis by triple quadrupole gas chromatography-mass spectrometry (GCMS), sensitivity of volatiles increases while matrix effects decrease. In SPME, a sorbent fiber is exposed to the headspace of a sample allowing volatiles to ad/absorb to the fiber and then injected into the system where desorption occurs immediately prior to analysis. This technique is ideal for the analysis of ppb-level odorants, such as smoke taint compounds, because of the sensitivity it can achieve while minimizing sample preparation. In this work, a multiple-reaction monitoring (MRM) method with SPME preconcentration was developed for quantification of guaiacol and 4-methylguaiacol in smoke taint-afflicted wines. Method validation was performed on wines containing low-ppb levels of analytes. Sub-ppb detection limits were achieved for both compounds with the use of a deuterated internal standard.

A200 Fermenting beer with maltose negative yeast: The fate of sugars, alcohol, and volatile flavor compounds in nonalcoholic and low alcohol beers Lucille Benedict1,2, lucille.benedict@maine.edu, Samantha J. White1,2, samantha.j.white@maine.edu, Cass J. Riley1,2, Taylor L. Chamberlain1,2, Huy N. Nguyen1,2, Owen McElearney1,2. (1) Chemistry, Univ. of Southern Maine, Portland (2) QC2 Lab, Univ. of Southern Maine, Portland Nonalcoholic and low alcohol beers have been growing in popularity as consumers become increasingly health conscious. While the market share of these beers has grown, they have continually been plagued by sensory issues in comparison with standard beer styles. Yeast strains with genetic mutations that inhibit alcoholic fermentation have been identified that are capable of producing low ABV beers (<2%) and present a needed alternative to physical methods of reducing ethanol concentration. Several maltose negative yeast strains are used in the brewing of low ABV beers due to their reportedly similar flavor profiles to alcohol producing Saccharomyces strains. For this study, four fermentations were performed using different maltose negative yeast all starting from the same low gravity wort. These maltose negative yeast strains are expected to differ from one another in parameters that impact the final product including alcohol content and the composition of organic compounds and sugars in solution. The fate of these parameters were studied through the course of this research. The results from this work will help guide brewers in selecting yeast strains for non alcoholic and low alcoholic beers.

A201 Analysis of accelerating the whiskey aging process Shea Walker, sheaw182@gmail.com, Robert Dixon. Chemistry, Southern Illinois Univ. Edwardsville Whiskey aging takes place when ethanol in the barrel interacts with the lignin in the wood. Compounds are

extracted as the ethanol enters and exits the wood over time. This process traditionally takes 3 years or longer to have a completed product. There are generally known methods to accelerate this process, which are heating, sonicating, or increasing the surface area to volume ratio. This experiment utilized ethanol in glass jars with wooden cubes added to mimic barrel conditions. The three methods of accelerating the aging process studied were heating, sonication, and increasing the surface area of wooden cubes present in solution. Samples were taken on a weekly basis. Analysis was carried out using GC/MS with a DB-wax 1301 column. By studying the extraction of aromatic and flavor compounds produced during accelerated aging, businesses may be able to apply these methods to their products and have a profitable product sooner.

A202 Hop (Humulus lupulus) acid and metabolite profiles as a function of growth region by HPLC and GC-MS analysis Celina Paoletta1, celina.paoletta.18@cnu.edu, Christopher Balog1,2, Dmitry V. Liskin1, Andrew Higgs1, Abbie Brehm3, Ronald A. Quinlan1. (1) Molecular Biology and Chemistry, Christopher Newport Univ., Newport News (2) Master of Science in Environmental Science, Christopher Newport Univ., Newport News, Virginia (3) Tradition Brewing, Newport News, Virginia There are many chemical changes that take place during wort boiling, to include the oxidation of polyphenols, production of melanoidins via Maillard reactions, protein precipitation, enzyme inactivation, and isomerization of hop acids. Hops are one of the most important raw materials used in the production of beer as it is responsible for the bitter flavor and aroma of beer. The metabolites from hops also provide beer with other qualities like flavor stability, foam stability, microbial stability, color, and mouthfeel. During the wort boiling, the α-acids are isomerized to iso-α-acids. These products can lead to various ratios of the cis/trans-iso-α-acids, which can affect the kinetics of oxidative degradation as well as the bitter taste development in the final product. Environmental changes to the terroir can lead to alterations in the acid profiles of individual hop cultivars. Here we present our initial findings of acid and metabolite profiles of hops from different growth locations through the brewing process at a local craft brewery using high performance liquid chromatography (HPLC) and gas chromatography – mass spectrometry (GC-MS). The potential for the metabolites to affect the foam stability are also reported.

A203 Characterization of aroma and taste profiles as a function of malt growth region in craft brewing by HPLC and GC-MS Christopher Balog1,2, Celina Paoletta1, Andrew Higgs1, Dmitry V. Liskin1, Abbie Brehm3, Ronald A. Quinlan1, ronald.quinlan@cnu.edu. (1) Molecular Biology and Chemistry, Christopher Newport Univ., Newport News, Virginia (2) Master of Science in Environmental Science, Christopher Newport Univ., Newport News, Virginia (3) Tradition Brewing Company, Newport News, Virginia There are many chemical changes that take place during the wort boiling stage of the brewing process, including oxidation of polyphenols, production of melanoidins via Maillard reactions, protein precipitation, enzyme inactivation, and isomerization of hop acids. Malt is essential part of that process. It is also the sugar source, the starch source, and the primary carbohydrate source for the yeast. Environmental changes and variations to the growth environment can lead to alterations in these starting materials and extraction efficiencies. Here we present our initial findings of the taste and aroma profiles of malts from different growth locations through the brewing process at a local craft brewery using high performance liquid chromatography (HPLC) and gas chromatography-mass spectrometry (GC-MS). These metabolites not only affect flavor and aroma, but color and foam stability as well. We envision that this data will be useful for brewers attempting to maximize a quantitative approach to the selection of malts in the brewing process.

A204 Structures and binding sites of human bitter taste receptors complexed with G protein and agonists Moon Young Yang1, myyang1129@gmail.com, Soo-Kyung Kim1, William A. Goddard1, Brian D. Guthrie2, Stephen B. Liggett3. (1) Materials and Process Simulation Center, California Inst. of Technology, Pasadena (2) Cargill Inc, Minneapolis, Minnesota (3) Dept. of Internal Medicine, USF Health Morsani College of Medicine, Tampa, Florida Bitter taste receptors (TAS2Rs) belong to the G protein-coupled receptor (GPCR) superfamily, which generate signaling through coupling to both the G protein and an agonist. Interestingly, TAS2Rs have been reported recently to be expressed in many extraoral tissues and are known to be involved in health and disease, presenting attractive therapeutic targets. Indeed, TAS2Rs-associated disorders and diseases include cancer, asthma, and cardiovascular diseases. Despite these important roles for TAS2Rs in biological functions and diseases, no X-ray or Cryo-electron microscopy structure is available to provide an understanding of the signal transduction mechanism or to identify the agonist or antagonist binding sites for the 25 TAS2R subtypes. Thus, there is no basis for in silico discovering the endogenous ligands or developing selective ligands with high affinity as new ligands to discover extraoral function or new therapeutic drugs. We report here the three-dimensional structures of the fully activated human TAS2R4 and TAS2R5 predicted using the GEnSeMBLE complete sampling method. We also report the coupling of these GPCRs to cognate G proteins and to several agonists. We discovered that the G protein couples to TAS2Rs through strong salt bridges to each of the three intracellular loops, orienting the Gα5 helix of the Gα subunit to interact extensively with the cytoplasmic region of the GPCR. We show that TAS2Rs exhibit unique motifs compared to typical class A GPCRs, leading to a distinct activation mechanism and a less stable inactive state. We identify several residues in the binding site that play a critical role in ligand binding and activation processes. For TAS2R4, D92 provides a favorable binding energy through polar interactions with an agonist, while triggering rotation of Y239 by changing the hydrogen bond network. For TAS2R5, S89 and Q90 form polar interactions with the 1,10-phenanthroline agonist, which is known to bind specifically to TAS2R5 among the 25 subtypes. Our predicted results explain the subtype selectivity of the agonist and correlate well with experimental results of signaling coefficients against 19 agonists (R2~0.85). These predicted fully activated bitter taste receptor complex structures provide insights into the signal transduction mechanism, a guide to structure-based drug design, and mutation sites for definitive experimental validation of the predicted structures.

A205 Response of metal oxide semiconductor E-nose on aroma compounds and its application in Chinese baijiu Yuzhu Li1, lyz611@foxmail.com, Kangzhuo Yang1, yangkangzhuo@wuliangye.com.cn, Dong Zhao1, 33321523@qq.com, Jia Zheng1, zhengwangi86@163.com, Michael C. Qian2, michael.qian@oregonstate.edu. (1) Flavor Science Innovation Center, Technology Research Center, Wuliangye Yibin Co., Ltd., Yibin, China (2) Dept. of Food Sci. and Tech., Oregon State Univ., Corvallis Electronic nose (E-nose) is usually used to simulates the olfactory organs of animals to recognize complex flavors. Metal oxide semiconductor (MOS) is an ideal material for production of E-nose. In order to explore the feasibility of identifying different types of aroma compounds as well as alcoholic beverage by the MOS based E-nose, the PEN3 E-nose was tested in this study. The results showed that similar characteristic response sensors were detected in different aroma compounds (such as fatty acids, alcohols, esters, ketones, aldehydes, aromatics, pyrazines, and terpenes) as well as ethanol, including W5S, W1S, W1W, W2S, and W2W, while the response intensity varied in different aroma compounds. Classification of different types of aroma compounds could be

achieved according to sensor responses. Lactic acid and β-damascenone had no sensor response in E-nose. The characteristic sensor responses of single aroma compound increased in certain concentration ranges, such as ethanol and ethyl hexanoate. In the binary mixture of ethanol and volatile compound, the addition of aroma compound (e.g., ethyl hexanoate) with content as low as 5‰ could be clearly discriminated by sensor responses and statistical analysis. Based on this, different Chinese baijius were successfully discriminated by E-nose and statistical analysis.

A206 Modified hydroxyapatite nano seed coating for the seedling stage enhancement of Zea Mays Latheesha Abeywardana2, lsa.a@live.com, Madhavi de Silva3, Chanaka Sandaruwan1, Damayanthi Dahanayake1, Gayan Priyadarshana3, Surani Chathurika1, Veranja Karunaratne1, Nilwala Kottegoda3. (2) Sri Lanka Inst. of Nanotechnology Pvt Ltd, Homagama, Western , Sri Lanka (3) Univ. of Sri Jayewardenepura, Nugegoda, Sri Lanka Restraint of crop yields due to the deficiency of plant nutrients calls for an urgent compulsion in developing advanced materials for effective plant nutrient delivery. The hybrid composites incorporating nanoparticles as carriers provide futuristic reinforcement in agronomy. This work communicates the use of zinc doped urea-hydroxyapatite nanohybrids in a novel nano-seed coating on Maize (Zea mays L.) seeds. A one-pot in-situ sol-gel synthetic route was utilized to synthesize the nanohybrids. The advanced seed coating was designed to deliver two macronutrients; nitrogen and phosphorus as well as a micronutrient; zinc during the seedling stage. Successful doping of zinc and incorporation of urea into the hydroxyapatite matrix were reported with a transformation of the lattice environment. The germination study revealed that the Zn doped urea-hydroxyapatite coated seeds exhibited the highest germination percentage (73.3%) with a significant difference ($P < 0.05$) among the treatments at 7 days while resulting in the highest plant height and dry seedling weight after 14 days. Therefore, it can be concluded that the developed nano-seed coating was competent in escalating the growth rate of Maize seeds claiming its applicability as a prospective delivery candidate for nitrogen, phosphorus, and zinc at the seedling stage.

A027 Smart cellulose nanocrystal-based materials for intelligent packaging Zhilong Yu, zhilongyu8901@gmail.com, Xiaonan Lu. Food Science and Agricultural Chemistry, McGill Univ., Montreal, Quebec, Canada Due to predetermined or inaccurate expiration date, not only does food at retail stores go to waste early, but consumers are at higher risk of foodborne illnesses. Intelligent packaging serves as a viable solution to this problem because it can communicate the information on food quality and safety in real time, by detecting direct or indirect indictors for food quality and safety (e.g., humidity, temperature, pH, and freshness). We have fabricated smart biomimetic nanocellulose-based composite films that can respond to humidity and chemicals released during food spoilage. The composite materials are prepared by co-assembling cellulose nanocrystals with biodegradable functional additives, and the material cost is affordable for the industry. The bionanocomposite films show distinct structural colors when exposed to the environments with different humidity levels and volatile amine concentrations. Depending on their advantages in terms of cost, stability, and biodegradability, these smart photonic materials have great potential to be used as indicators installed in intelligent food packaging.

A208 Material degradation inside and out: Contributions to the deterioration of electrospun matrices with encapsulated corn oil Louis Colaruotolo1, Singam S. Singh1, Loong-Tak Lim1, Stacie Dobson1, Azin Sadat1, Iris Joye1, Maria G. Corradini1,2, mariagcorradini@gmail.com. (1) Food Science, Univ. of Guelph, Ontario, Canada (2) Arrell Food Inst., Univ. of Guelph, Ontario, Canada Electrospun nonwovens composed of submicrom fibers are gaining popularity in filtration, coatings, encapsulation and packaging applications. Their production with food-grade biopolymers and the inclusion of bioactive compounds within the fibers ensure their compatibility with food products and increase their functionality and sustainability. However, their potential uses are hindered by their limited stability, particularly when loaded with lipids. The objective of this study was to apply a multi-length scale approach to gain insights into the deteriorative processes that limit the shelflife of these novel materials. A zein solution (20% w/w) prepared in 7:3 propanol:water solution was added with corn oil (3:10 oil:protein ratio). The solution was electrospun through a needle spinneret (0.7 mm diameter orifice) for 10min. Electrospun samples were stored under controlled conditions (dark, 23°C & 33 %RH) for 28 days and tested at selected intervals. Fiber morphology and nonwoven mechanical properties were assessed by scanning electron microscopy (SEM) and tensile tests, respectively. The overall lipid oxidation in the samples was assessed using a TBARS assay. The protein secondary structure was probed using Fourier Transform Infrared Spectroscopy (FTIRS) and the lipid distribution was assessed by microspectroscopic techniques (Raman & luminescence). The photophysical properties of intrinsic (Tyr) and extrinsic (BODIPY C11) lumiphores were also monitored during storage to assess changes in local molecular rigidity and lipid oxidation. SEM revealed ribbon-like fibers whose diameter significantly decreased during storage (700 ± 9 nm vs. 620 ± 10 nm). Extensive breakage of the fibers correlated with increased brittleness of the material, as reported from bulk and local measurements, e.g., decreased extensibility by 30% and increased Tyr emission intensity by 40%. Changes in mechanical properties and matrix rigidity also correlated with a transition in zein secondary structures from unordered (25% vs. 0%) to ordered structures (2% vs. 19%) during storage. Raman micrographs showed oil migration to the ribbon's outer regions during storage, increasing lipid oxidation. The correlation between local rigidity and lipid oxidation suggests the potential interactions between the oxidation products and zein. Understanding the causes of deterioration can aid in developing smart strategies to improve the stability of these novel food-grade materials.

A209 Advances in nanomaterials for food and agricultural applications Iffat Z. Zareen Ahmad, iffat@iul.ac.in. Bioengineering, Integral Univ., Lucknow, Uttar Pradesh, India The advancements in the field of nanotechnology have helped us to synthesize novel nanomaterials for their applications in all spheres of life. The better understanding and the advantages of nanomaterials has made them an alternative to the existing materials which are being used in agriculture and food industries. They have been considered as a potent choice for controlling plant pests and infections. Numerous benefits of nanomaterials have been reported in the prevention of post-harvest loss of fruits and vegetables. They are used in coating and food packaging. The green synthesis of the nanoparticles involving plant extracts poses additional advantages of being easy, suitable, eco-friendly and quick. The nanomaterials synthesized by applying ecological friendly methods might also enhance the agriculture yields by affecting the process of fertilization, germination, synthesis of plant growth regulators, application of herbicides and pesticides, increasing the nutrient absorption in plants. These nanomaterials can also be used for the removal of harmful chemicals that affect the growth of plants. Nanomaterials have gained attention recently because of their unique characteristic properties like large surface area. The popularity of the nano scale materials has increased immensely in the food sector. The devices and materials have become smaller but with good efficacy. They work efficiently in the area of food safety and food packaging. In the area of food packaging, potential results have been obtained as they are reported

to protect food from moisture, rancidity, loss of flavour and unwanted odors. They work effectively to deliver bioactive compounds to the targeted tissues and act as a vehicle. They have been reported as effective anti-microbial agents and prevent food from getting rot. Although several applications of nanomaterials with excellent output is there but still there are many challenges and the scope of improvement in this technology which must be addressed before taking it to commercial level.

A210 Effect of zein and carboxyl-methyl chitosan coated resveratrol nanoparticles on chicken embryonic development as endocrine disruptors Jinglin Zhang1, jinglinzhang@hotmail.com, Xinwen Zhang1, Qin Wang2, Changqing Wu1. (1) Animal and Food Sciences, Univ. of Delaware, Newark (2) Univ. of Maryland at College Park Recently considerable attention has been paid to the potential beneficial effects of resveratrol, a naturally occurring polyphenolic phytoalexin, on human health including antioxidant, anti-inflammatory, anti-carcinogenic activities etc. Because of its poor water solubility, chemical instability and low bioavailability, a variety of nano-resveratrol (nano-Res) formulations have been developed to encapsulate, protect, and deliver resveratrol; however, their safety or nanotoxicity has seldom been reported. In this study, effects of two kinds of nano-Res, i.e., Tween 80 and carboxymethyl chitosan coated zein nanoparticles (Tween-80 and CMCS NPs), on chicken embryonic development and its underlying mechanism were investigated. Different nano-Res formulations with various concentrations (0.01, 0.1, 1 mM resveratrol equivalent) were injected into fertile chicken eggs at Day 6. Toxic effects were observed with embryonic exposure of both nano-Res during 18 days' development as compared to controls. CMCS NPs showed higher death rate (20% at 0.1 mM and 33.3% at 1 mM) than that of Tween-80 NPs (10% at 0.1 mM and 28.6% at 1 mM), with no significant difference on developmental indexes (EWWR: embryo weight to egg weight ratio and LSI: liver somatic index). Results showed that nano-Res significantly elevated the malondialdehyde (MDA) values in chicken embryonic liver ($P<0.05$), implying that inducing oxidative stress might be one mechanism of their toxicity effects. We have also examined the expression of vitellogenin (VTG) and apolipoprotein (apoII) genes, two estrogen-responsive genes, in chicken embryonic liver. The nano-Res promoted the apoII gene expression dramatically, showing their potential toxic effects as endocrine disruptor. Furthermore, the differences in the dissolution and bioavailability of free resveratrol in the embryonic models caused by the different physicochemical properties of NPs were evaluated, to explain the differential toxicity of the two nano-Res in chicken development.

A211 Compressible nanobubbles induced self-assembly of 7S globulins isolated from pea (Pisum Sativum L.) Tianyi Yan, tianyiy4@zju.edu.cn, Donghong Liu. Dept. of Food Science and Nutrition, Zhejiang Univ., Hangzhou, Zhejiang, China Nanobubbles were fabricated in aqueous solutions following a compression-decompression method with a mean hydrodynamic diameter of (332.8 ± 13.7) nm, a zeta potential of – (33.7 ± 1.2) mV, and a concentration of (1.58 ± 0.12) × 1011 particles/mL. The effects of generated nanobubbles on the self-assembly behavior of 7S globulins isolated from pea proteins were systematically investigated. Various factors including pH, protein, and nanobubble concentrations were considered during the formation of self-assembled structures. We found that nanobubbles acted as a soft template to trigger the self-aggregation of 7S globulins adjacent to its isoelectric point (pI~5.5). Furthermore, we proved this process was concentration-dependent. An increase in protein concentration or nanobubble concentration resulted in a larger hydrodynamic diameter of formed nanoparticles, as demonstrated by the dynamic light scattering technique. However, in a low pH condition, the elevated nanobubble concentration destabilized the suspensions and thus nanoparticles were unable to generate. Results from transmission electron microscopy revealed that core-shell architectures were formed at both pH 4.0 and pH 6.0 when mixed with nanobubbles, whereas only solid spherical structures were observed without nanobubble treatment. The formed core-shell architectures at pH 6.0 maintained stable during 25-day storage at 4 °C, while the structures prepared at pH 4.0 gradually shrink within 25 days. The percentage of β-sheets and β-turns in 7S globulins increased, while the percentage of α-helix and intrinsic fluorescence intensity of 7S globulins at both pH 4.0 and 6.0 significantly decreased after the formation of nanobubble-induced nanoparticles. Our results provided a simple, novel, and non-thermal route for food protein self-assembly with a bottom-up strategy.

A212 Hierarchical assembly of safe, pragmatic biocatalytic materials Elizabet Moreno Reyes, em827@cornell.edu, Julie M. Goddard. Food Science, Cornell Univ., Ithaca, New York Enzymes can operate with high specificity under mild conditions of temperature and pH compared to traditional chemical catalysts commonly utilized in non-aqueous systems. To improve biocatalytic performance and potentially replace chemical catalysts, enzymes can be immobilized. However, their industrial application depends on costs associated to carrier materials, functionality recovered after immobilization, efficiency of recovery for subsequent reuse, and particularly for food applications, the use of safe food contact materials. To overcome these challenges, calcium phosphate-based materials can be fabricated in such a way that hierarchical structures are obtained to harness the benefits of both nano and macro scale size regimes by providing microenvironments for enzyme stabilization and reducing the time of recovery of biocatalysts. In this work, we have prepared calcium-based porous microparticles by co-precipitation (particle size range of 5-10 μm and up to 2 μm wide apertures as obtained by scanning electron microscopy) varying the concentration of β-galactosidase (25, 50, 100, 200, and 400 ug/mL) and pH (5.0, 6.0, and 7.0) to achieve maximum activity recovery and immobilization yield. Under optimum conditions of immobilization, the activity of immobilized β-galactosidase was comparable to that of free β-galactosidase and the highest immobilization yield obtained was 88%. To improve retention of enzyme during multiple cycles of recovery and reuse, we employ crosslinking. We have oxidized glucose, sucrose, and lactose to function as crosslinkers that are greener and less likely to denature enzymes compared to standard glutaraldehyde, and we have optimized the process of crosslinking by varying the degree of oxidation (total aldehydes/mol carbohydrate) and concentration of crosslinker. With the combined approach of employing hierarchical structures and greener materials suitable for food applications, such as calcium phosphate and carbohydrates, the reusability and stability of enzymes through immobilization can be improved to enable their wide industrial adoption in food processing and food waste valorization applications.

A213 Synthesis, stability and kinetics of hydrogen sulfide release of dithiophosphates Nimesh Pasan Ranasinghe Ranasinghe Arachchige, nimesh-pasan@uiowa.edu, Eric M. Brown, Arjun Paudel, Ned B. Bowden. Dept. of Chemistry, Univ. of Iowa, Iowa City Hydrogen sulfide (H2S) has been recognized as a key gasotransmiter in many plants. It is has been shown that optimal concentrations of H2S have dramatic effects on plants; increasing the overall size and mass, protecting plants from high salt concentrations or heat and drought conditions, alleviating leaves from freezing stress, increasing root growth, and prolonging shelf-life of harvested fruit. However, application of hydrogen sulfide to plants has been a challenge because of its characteristic odor and toxic effects at high concentrations. We synthesized a series of dialkylthiophosphates and disulfidedithiophosphates that slowly degrade to release hydrogen sulfide upon hydrolysis. Kinetics of hydrolysis of these chemicals were obtained at 85°C and room temperature (23 ± 2 °C). The results

revealed that the structure of the alkyl and sulfides groups had a huge impact on the rate of hydrolysis, and the rate constant varied by more than 14,000x. Many important findings were discovered including that the hydrolysis of the dithiophosphates followed pseudo first order reaction rates. Moreover, the disulfidedithiophosphates hydrolyzed faster than the structurally similar dialkylthiophosphates, free energy values were obtained to explain the large variance in degradation. In addition, dialkoxydithiophosphates synthesized with tertiary alcohols hydrolyzed faster than dialkoxydithiophosphates synthesized with primary and secondary alcohols. Hydrogen sulfide released in water was also quantified using a hydrogen sulfide sensitive electrode. Corn was grown on an industrial scale and dosed with dibutyldithiophosphates to demonstrate that these dithiophosphates have a potential application in agriculture. At a loading of 2 kg per acre, a 6.4% increase in harvest yield of corn was observed.

A214 Resistance mechanism of salmonella typhimurium at low water activity against heat treatment and added trans-cinnamaldehyde or eugenol Qiao Ding1, ding66@umd.edu, Chongtao Ge2, Robert C. Baker2, Robert L. Buchanan1,3, Rohan V. Tikekar1. (1) Nutrition and Food Science, Univ. of Maryland at College Park (2) The Mars Global Food Safety Center, Beijing, China (3) Center for Food Safety and Security System, Univ. of Maryland at College Park We hypothesized that essential oils combined with milder heat treatments can accelerate Salmonella Typhimurium inactivation in low water activity (aw) environment. Although both trans-cinnamaldehyde (CA, 1000 ppm) and eugenol (EG, 1000 ppm) accelerated thermal inactivation of Salmonella in water and food matrices (peanut oil, corn starch and whey protein) with 0.93 aw, a similar effect was not observed at lower (0.35-0.45) aw. Both altered bacterial metabolic activity and membrane properties were hypothesized to contribute to higher resistance. Metabolic activity was measured with resazurin assay where fluorescence produced from metabolism of resazurin was monitored. Faster the sample reaches peak fluorescence intensity (lower tpeak), higher the metabolic activity. Regardless of aw (0.4/ 0.9), metabolic activity following 55 °C treatment in oil (tpeak=95±5/44±0 min), starch (tpeak=293±7/539±13 min), or protein (tpeak=156±14/375±24 min) was lower than at 22 °C (oil tpeak=40±3/17±2 min, starch tpeak=257±7/363±8 min, protein tpeak=117±2/316±12 min) ($P < 0.05$). Addition of CA/ EG further reduced metabolic activity ($P < 0.05$) at both aw compared to 55 °C treatment alone in oil and starch, but not in protein. These results explain bacterial response to thermal treatments at two aw values, but not the response in different matrices at low aw. Membrane fluidity was measured with 1,6-diphenyl-1,3,5-hexatriene, a membrane probe whose rotational movement is restricted by membrane lipid interactions. Its fluorescence polarization value (mPf) reflects membrane fluidity, where a larger value indicates lower fluidity. We also analyzed membrane fatty acid profile using gas chromatography. Bacteria at 0.4 aw had lower ($P < 0.05$) membrane fluidity (mPf=116.3±6.5, Ru/f=0.31±0.01) and unsaturated to saturated fatty acids ratio (Ru/f) than at 0.93 aw (mPf=96.2±1.6, Ru/f=0.34±0.01) or in fresh broth (mPf=97.0±0.8, Ru/f=0.37±0.01), suggesting that bacteria at low aw changed their membrane compositions to increase rigidity and reduce permeability. This explains increased resistance against both heat treatment and essential oils.

A215 Analytical and carbohydrate chemistries of contemporary waterpipe tobaccos John H. Lauterbach, john@lauterbachandassociates.net. Lauterbach & Associates LLC, Macon, Georgia Waterpipe tobacco is the name regulatory authorities have given the products are known to the trade as shisha or as hookah tobacco. The terms shisha and hookah tobacco may bring up memories of mixtures of tobacco and molasses with or without flavors. However, contemporary waterpipe tobaccos contain less than 30% tobacco, often less than 15%. The major ingredients are glycols (glycerol, glycerol -- propylene glycol blends) and sugar syrups such as high fructose corn syrup, regular corn syrup, invert syrup, or molasses or mixtures of those syrups. All commercial products obtained to date are flavored, and all exist as two-phase systems with liquid surrounding tobacco particles saturated with the mixture of glycols, sugars, and flavors. Moreover, none of the commonly used CORESTA Recommended Methods and ISO Standards commonly used to determine major and minor analytes in tobacco products have not been validated with waterpipe tobaccos. Furthermore, there are no reference products available, as there are for most other tobacco products. Consequently, we had over thirty commercial products analyzed for glycols, fructose, glucose, sucrose, water, and other analytes at an ISO 17025 accredited laboratory. In addition, we prepared several control samples using tobaccos prepared for shisha manufacture, commercial sugar syrups, and flavors of known composition. These were all analyzed by the same commercial laboratory and by an additional laboratory that used techniques specifically designed for analyzes of commercial shishas. Particle-size determinations were also conducted on commercial and control products using photomicroscopy of hot-water extracted commercial and control products. The results showed much similarity among commercial products, with the main differences being associated with whether the starting tobacco was flue-cured or dark air-cured.

A216 Characterization of hydroxypropyl methylcellulose bio-composite structures with microcrystalline cellulose-containing natural anthocyanin for developing pH sensing indicator Athip Boonsiriwit, athip8266@gmail.com, Youn Suk Lee. Packaging, Yonsei Univ., Wonju, Gangwon, Korea (the Republic of) Use of the natural pigment for the pH sensing indicator has become increasingly more attention due to the safety trace for a fresh product and the severity of the environmental impacts against synthetic chemicals. A pH sensor in the indicator is generally used for the anthocyanin to incorporate a solid biodegradable matrix. Hydroxypropyl methylcellulose (HPMC) is also widely used as a solid forming agent for film preparing or coating due to a non-toxic, low cost, and eco-friendly material. However, it still has poor mechanical strength together with low moisture and gas barrier properties. This study aimed to improve the HPMC-based composite structures with microcrystalline cellulose (MCC) biomaterial containing anthocyanin for preparing a pH sensing indicator. The HPMC biocomposites with MCC (HMB) were prepared according to the different MCC contents at 10, 20, and 30% (dry basis), respectively. The mechanical, optical, thermal, and gas barrier properties of the prepared HMB samples were evaluated. The results showed that MCC structures could significantly improve tensile property, transparency, and thermal stability. They also represented the highest values in the HMB structures containing the 20% MCC content. Values of the tensile strength, gas barrier properties, and transparency were increased by 62%, 81%, and 266% compared to the control, respectively. 15 mg of anthocyanin as a source of butterfly pea (BA) was incorporated with the HMB structures containing the 20% MCC content (20HMB). The prepared indicator (BA-20HMB) was used for monitoring the pH change according to the ammonia sensitivity. The BA-20HMB indicator showed a clear color change by the pH levels in the atmosphere. It could prove useful for applying intelligent packaging.

A217 Scalable functional cationic swabs for improved pathogenic microbes sampling from food contact surfaces Ahmed El-Moghazy, aelmoghazy@ucdavis.edu, Nicharee Wisuthiphaet, Nitin Nitin. Food Sci. and Tech., Univ. of California Davis Swabbing is the most common technique used for monitoring pathogen contamination on surfaces, determining the sufficiency of the cleaning performance and ensuring the safety of the finished food product. Therefore, the

development of swabbing materials is needed to enhance the swab efficiency and ease of use in the food-processing factory. Functionalized cotton swab was developed based on cationic functionalization for improving the sampling of pathogens from surfaces relying on the robust positive charge of the modified swabs to capture the pathogen through electrostatic interaction. The developed swab was fabricated using UV-induced grafting of cationic monomer (2-(methacryloyloxy)ethyl trimethylammonium chloride, METAC) onto the regular cotton swabs. The prepared cationic cotton swabs displayed a persistent positive charge regardless of the pH conditions. Comparing with the regular cotton swab, the cationic swabs demonstrated 150 to 200 % enhancement in the swab performance for both the Gram-positive and Gram-negative bacteria under any sampling conditions, respectively. Furthermore, the cationic cotton swabs showed at least 4-fold increase in the sampling performance of the bacterial biofilm from the stainless-steel surfaces compared to the cotton swabs. These results illustrate the role of modified swabs in enhancing the sampling of bacteria from contact surfaces and their potential impact on improved monitoring of microbial contamination and verification of surface sanitization.

A218 Ecofriendly extraction of polyphenolic compounds from Vaccinium meridionale fruit by-product with natural deep eutectic solvent (NADES) Gloria Astrid A. Garzon, agarzonm@gmail.com, Carlos E. Gonzalez, Deivison Gonzalez, Carlos D. Mendieta, Valentina Monroy. Chemistry, Univ. Nacional de Colombia, Bogota, Colombia Extraction of bioactive compounds using environmentally friendly solvents is at growing significant interest. Vaccinium meridionale pomace is a rich source of bioactive compounds including anthocyanins and other phenolics. The purpose of this study was to use ultrasound-assisted extraction and Natural deep eutectic solvents (NADES) to achieve an eco-friendly extraction of polyphenols form V. meridionale pomace. NADES based on choline chloride as the hydrogen bond acceptor and malic acid as hydrogen bond donor in 1:1, 2:1 and 1:2 molar ratios, respectively, were prepared. Water was added as the third component of the mixture in 30% and 50% w/w proportions to each mixture. Results were compared to those obtained with the control solvent (80% aqueous methanol). The anthocyanin concentration in the 1:1:50% (31.0 ± 0.6 mg cyanidin-3-glucoside/g DW) and the 2:1:50% (30.2 ± 0.4 mg cyanidin-3-glucoside/g DW) mixtures was significantly higher than that one of the control (12.5 ± 2.8 mg cyanidin-3-glucoside/g DW). The highest total phenolics content were obtained with the 1:2:50% (217.7 ± 7.8 mg GAE/g DW, and the 2:1:30% (228.0 ± 21.3 mg GAE/g DW) with superior extraction capacity with respect to 80 % methanol (82.8 ± 2.4 mg GAE/g DW). The highest antioxidant activity as determined by the ABTS method was found in the extracts obtained with the 1:1:50% (172.8 ± 8.9 mmol TE/g DW), 1:1:30% (166.8 ± 9.9 mmol TE/g DW), and the 2:1:30% mixtures (162.1 ± 2.5 mmol TE/g DW). These results demonstrate that NADES based on choline chloride and malic acid represent an environmentally friendly alternative for the isolation of valuable phenolic compounds from V. meridionale pomace.

A219 Identification of polymers, additives, and contaminants in food contact articles using rapid, direct - high resolution mass spectrometry
Kristen L. Reese1, kleighreese@gmail.com, Janis Rusko2, Ingus Perkons2, Luke K. Ackerman1. (1) Center for Food Safety and Applied Nutrition, US FDA, College Park, Maryland (2) Laboratory of Chemistry, Partikas Drosibas Dzivnieku Veselibas un Vides Zinatniskais Instituts, Riga, Latvia Screening methods are required to estimate consumers' exposure to inadvertently added additives/contaminants in Food Contact Articles (FCAs) during food production. Potential migration of additives/contaminants from FCAs into food is reliably estimated if polymer identity, identity and/or concentration of additive/contaminant, and conditions of use are known. Current non-targeted methods lack either rapid or comprehensive analysis of dozens of known FCA base polymers and thousands of additives/contaminants. Therefore, we are developing a rapid, multi-polymer/contaminant/additive Direct Analysis in Real Time (DART)-HRMS screening method capable of identifying FCAs polymers and small molecules. MS1 parameters on a DART-Thermo Q-Exactive were optimized on robust, documentable, and diverse polymer references (n=5) to produce diverse ions with equi-abundance. The optimized method was applied to n=124 reference materials covering >75% of estimated FCA types in positive and negative modes, generating data for precise HRMS ion databases. Retail/commercial FCAs (n=152) collected between the U.S. and E.U. challenged our method and evaluated usefulness of MS1 reference polymer data. DART-HRMS polymer databases were created by common and unique ion identification using custom open-source workflows developed in KNIME with outputs/averages/merges and lists validated against theory, literature, and vendor software. Reference polymer-specific ion features varied dependent on the polymer and additives present. N=124 reference polymer standards (47 structural classes) were analyzed. Unique ions (~4500) were compiled in an MS1 database. Their accuracy and utility in polymer ID was validated. Separately, a MS1 DART-additive/contaminant (n=210) database was developed from ongoing analyses. Ions within both MS1 databases were assessed for commonality and uniqueness. Polymer-specific common but non-unique ions were prioritized for MS2 analysis to assist in identifying different but related polymers. Workflows to automate polymer classification by cosine-vector matching of more unique ions and/or a-priori defined polymer structural ions are under development. Once completed, this method will provide screening data for responding to food packaging inquiries.

A220 Raman imaging of plant metabolite crystals Sarah Shidler1, sarah.shidler@renishaw.com, Lucy Grainger1, Tim Prusnick2, Anna Lewandowska3. (1) Renishaw USA, West Dundee, Illinois (3) Renishaw Plc, Wotton-under-Edge, Gloucestershire, United Kingdom Understanding plant and crop biochemical mechanisms is fundamental to our ability to maintain ecosystems and provide sustainable nutrition. Environmental, nutritional, and mechanical stresses can impact metabolite production which can be used to study plant health and development. Here we present confocal Raman images detailing the spatial distribution of plant metabolites and tissue structure. Raman imaging is an ideal non-destructive and non-invasive technique for studying plant tissue in the presence of water and in vivo. The high specificity of a Raman spectrum allows for the distinction between different cellular components and Raman images can provide spatially resolved chemical and structural information from plant tissues which influences plant health.

A221 Gossypol effects on mammalian cell growth and gene expression Heping Cao, heping.cao@ars.usda.gov, Kandan Sethumadhavan. Southern Regional Research Center, USDA Agricultural Research Service, New Orleans, Louisiana Gossypol is a plant polyphenol in the small intercellular pigment glands in the leaves, stems, roots, and seeds of cotton plants (Gossypium hirsutum L.). Gossypol has been regarded as an anti-nutritional toxic compound because long-time consumption of gossypol-containing cottonseed oil caused male infertility. Cottonseed meal with gossypol limits its use primarily to feed ruminants, which tolerate the toxic compound. Recently, gossypol has been shown to have potential biomedical applications. Gossypol and related compounds have anticancer activities associated with breast cancer, colon cancer, pancreatic cancer and prostate cancer. It also has anti-obesity, anti-inflammatory and antifungal activities. These discoveries have generated interest in biomedical field. Intensive research has been

directed at understanding the medical utilization of gossypol and related compounds. We recently investigated the effects of gossypol on cell viability and expression of genes involved in glucose transport, lipid biosynthesis, and inflammatory responses in mammalian cells by MTT, qPCR and immunoblotting methods. Our results showed that gossypol inhibited mammalian cell survival, increased many gene expression in mouse macrophages but decreased gene expression in human colon cancer cells. We also demonstrated that gossypol-induced cell death was associated with massive induction of anti-inflammatory tristetraprolin family and proinflammatory cytokine gene expression in mouse macrophages.

A222 Changes in cell wall composition of cool-season pasture grasses over the growing season Sophia Newhuis1, sophia.newhuis@uky.edu, Isabelle A. Kagan2, Brittany Harlow2,1, Michael Flythe2,1, Rachel R. Schendel1. (1) Dept. of Animal and Food Sciences, Univ. of Kentucky College of Agriculture Food and Environment, Lexington (2) USDA ARS Forage Animal Production Research, Lexington, Kentucky Background: Grass cell walls are rich in cellulose and arabinoxylan polysaccharides. Ester-linked phenolic acids such as ferulic and coumaric acids have the potential to cross-link the arabinoxylan polymer both to itself and lignin. Changes in cell wall composition thus affect plants' digestibility for livestock, but there is limited information about how the contents of these structural elements of cool-season grasses' cell walls change over the growing season. Goal: The aim of this project was to investigate changes in the cell wall phenolic acid and monosaccharide profiles of five cool-season pasture grasses harvested over a four month period. Approach: Five cool-season grasses (perennial ryegrass, orchardgrass, tall fescue, Kentucky bluegrass, and timothy) were planted in a randomized block design. Vegetative material was harvested in April, June, August, and October of 2020; lyophilized; milled (< 0.5mm); defatted; and destarched to isolate insoluble cell wall material. Phenolic acids were released via alkaline hydrolysis, extracted with diethyl ether following acidification, and separated, detected, and quantified using high-performance liquid chromatography (HPLC). Trans-o-coumaric acid was used as the internal standard. The monosaccharide profile of the cell wall polysaccharides will be determined via Saeman hydrolysis followed by high-performance anion-exchange chromatography with pulsed amperometric detection (HPAEC-PAD). Statistical significance was analyzed via one-way ANOVA, and Tukey-Kramer post-hoc testing was used to reveal significant pairwise differences. Phenolic acid contents were significantly different over time and between species.

A223 Using ingredient standards to protect food integrity and combat economically motivated adulteration Zhuohong Xie, kyx@usp.org. USP, Rockville, Maryland Food supply chains are becoming increasingly complex especially during the pandemic. This complexity creates multiple opportunities to damage the integrity of the food supply, either intentionally or unintentionally. Ensuring the overall integrity of the food supply system depends on the integration of multiple points of control and information. For foods, including food ingredients, protection relies on being able to demonstrate that each substance has the appropriate composition at every step in the supply chain. Useful standards, along with analytical materials are actionable in that they include explicit parameters to determine whether a particular sample meets the standard for that substance (i.e., acceptance criteria) and the methods needed for making that assessment. This presentation will demonstrate the importance of food ingredient standards and analytical materials using the Food Chemicals Codex, FCC Analytical Materials (FAMs), and USP Reference Standards as examples. Among our offerings are skim milk powder related materials, gluten in oats method development materials, and our first FAM - whey protein method development material, which is to be released in early 2022. In summary, FCC provides users with information on test methods, acceptance criteria, and analytical materials to fight against fraudulent activities and to safeguard overall food ingredient quality.

A224 Use of amino acid fingerprinting in authenticity verification of nonfat dry milk and skim milk powders Sneh D. Bhandari1,2, sdbhandari1@gmail.com, Zhuohong Xie3. (1) Independent Consultant, Crete, Illinois (2) Chemistry, Merieux NutriSciences Corporation, Crete, Illinois (3) US Pharmacopeia, Rockville, Maryland The milk powders including nonfat dry milk (NFDM) and skim milk powders (SMP) are commonly used in reconstitution of milk/dairy products and are widely used in food industry for nutritional purposes and also for their intrinsic advantageous functional properties. The Milk powder is one of the most widely traded food commodities and its adulteration for economical gains is a big motivation to fraudsters. There is an urgent need of robust and rapid methods which can authenticate milk powder samples and help in detection of their adulteration. A study was undertaken to determine amino acid composition of SMP and NFDM samples and effect of their spiking with some potential adulterants. The distribution of each amino acid analyzed in all SMP and NFDM samples was found to be within the corresponding limits of their distribution in authentic SMP and NFDM samples proposed in the Food Chemicals Codex (FCC) standard and thus verified their authenticity. Some of the common plant and animal proteins and potential economically motivated adulterants were found to be different in distribution of some of the amino acids compared to NFDM and SMP samples. Spiking of the NFDM/SMP with potential adulterants was found to affect its amino acid fingerprint at certain spiking levels with some of the adulterants based on data collected on 38 authentic NFDM/SMPs and with potential adulterants in a mini-collaborative study between five laboratories. One-way analysis of variance (AONOVA) with Dunett's post-hoc test indicated that distribution of glycine in milk powders was more sensitive and affected by spiking with most of the studied vegetable proteins and also by gelatin at least at one of the applied spiking levels. Similarly spiking with whey protein isolate also affected NFDM/SMP amino acid fingerprint. This study demonstrates utility of amino acid fingerprinting in verifying authenticity of milk powders samples and use as one of the parameters in detection of adulteration of NFDM/SMP samples.

A225 Development of a LC-QTOF-MS based method for the classification of honeys with different quality attributes Lei Tian1, lei.tian@mail.mcgill.ca, Caren Akiki1, Lan Liu1, Shaghig Bilamjian1, Tarun Anumol2, Daniel Cuthbertson2, Stephane Bayen1. (1) McGill Univ. Faculty of Agriculture and Environment, Sainte Anne de Bellevue, Quebec, Canada (2) Agilent Technologies Inc, Santa Clara, California Novel tools are needed to guarantee the quality, safety and authenticity of food such as honey. For example, fraud (including substitution, adulteration or mislabeling – e.g. origin) is a threat for both consumers and honey professionals, and fraudulent practices may evolve quickly. Non-targeted analysis (NTA), using high-resolution MS (HRMS) and advanced data processing tools has the potential to investigate a wider range of quality attributes simultaneously; and the resulting chemical fingerprints are virtually impossible to imitate for fraudsters due to their complexity. In addition, it has the potential to investigate a wide range of quality attributes simultaneously (e.g. contaminants, authenticity or freshness markers). In the present study, a NTA method based on liquid chromatography (LC) coupled to HRMS was optimized to explore the non-saccharide fingerprints of honeys of different floral origin (incl. buckwheat, clover, linden and blueberry) in honey samples collected in Montreal, Canada. Chemical fingerprints were acquired under a range of LC-quadrupole time-of-

flight (QTOF)-MS instrumental conditions (incl. different mobile phases, types of reverse-phase column, gradient times, ionization and data acquisition modes). The resulting data were analyzed to assess the influence of the LC-QTOF-MS conditions on the classification rate for floral origin. Key molecular features were identified and can be served as markers of origin. This work sets further bases to deploy LC-HRMS based fingerprinting for honey quality, safety and authenticity applications.

A226 Protecting the integrity of plant-based sweeteners: Updating the FCC standard for Steviol Glycosides Tongtong Xu, tongtong.xu@USP.org. USP, Rockville, Maryland Because of growing interest in added sugar reduction in food products and consumer's preferences for "clean label" products, the food and beverage industry are pursuing calorie reduction through product reformulation using low- and no-calorie sweeteners from natural sources. Steviol glycosides obtained from the leaves of Stevia rebaudiana Bertoni consist of a mixture of compounds containing a steviol backbone conjugated to sugar moieties. These products have been used globally as sweeteners in recent years, and the availability of various formulations created to suit the needs of a range of food manufacturers and consumer preferences have led to increased usage. New manufacturing technologies have been applied to make steviol glycosides taste more like sugars, therefore, the composition of steviol glycosides has been evolving. As a part of ongoing efforts to assist the food industry and regulators in protecting the integrity of this ingredient, the Food Chemicals Codex (FCC) has modernized the assay method in the Steviol Glycosides monograph by replacing the existing HPLC method with two example LC-MS methods capable of quantifying 13 major steviol glycosides components. Because of the composition of steviol glycosides can vary, the updated FCC standard also instructs users to develop and validate their own methods, which ensures that the method quality meets FCC's requirements. As a source of global food standards, the FCC seeks to increase the role of public standards and guidance methods, including this publication, to ensure authenticity and protect the integrity of food ingredients.

A227 Exploration of nanobody based immunoassays for the tracing of food fraud Dongyang Li1,2, dylli@ucdavis.edu, Christophe Morisseau2, Yibin Ying1, Bruce D. Hammock2. (1) College of Biosystems Engineering and Food Science, Zhejiang Univ., Hangzhou, China (2) Dept. of Entomology and Nematology and UCD Comprehensive Cancer Center, Univ. of California Davis Immunoassays have been extensively used in many fields, including tacking of food fraud, due to their overwhelming overall advantages in high sensitivity, excellent selectivity, simplicity, fast speed, high throughput, low cost, safety, and general applicability. The key of an excellent immunoassay is the availability of antibodies with high affinity, specificity, and batch-to-batch consistency. Single domain antibody, also termed nanobody or VHH, is an antibody with a single variable domain derived from heavy-chain only antibodies in camelids or cartilaginous fish. This recombinant antibody has received increasing interest owing to their small size, monoclonal nature, genetic manipulability, high thermostability, superior solubility, ease of clone storage and expression in diverse expression platforms, and cost effectiveness for both discovery and continuous production. In this section, we will present the work on the development of nanobodies and the nanobody based immunoassays and further explore their potential applications for tracing of food fraud.

A228 Immunoassays for the detection of meat adulterants Qinchun Rao, qrao@fsu.edu, Xingyi Jiang. Florida State Univ., Tallahassee Around 10% of the foods produced in the US were adulterated, and 7% contained fraudulent ingredients. From 1980 to 2013, the leading reported type of fraudulent foods was animal products, including meat and meat products (7%). Between 2016 and 2017, about 35% of the food recalls were due to the presence of misbranding and undeclared food residues, which is the No. 1 cause of food recalls in the US. In order to (1) reduce the risk of intentional or unintentional contamination of foods, (2) better comply with food regulations, and (3) decrease economic loss to the food industry caused by recall, it is necessary to develop reliable and robust methods for the detection of different food adulterants/contaminants. Recently, different monoclonal antibodies (mAb) specific to two target analytes (i.e., mammalian skeletal troponin and porcine hemoglobulin) were developed using the hybridoma technique in our laboratory. Their properties, such as epitopes and species/tissue-selectivity, were characterized using fluorescent and/or chemiluminescent immunoblotting. Three mAb-based enzyme-linked immunosorbent assays (ELISA) were developed and validated for the detection of mammalian meats and porcine blood residues in foods, respectively. Overall, these immunoassays have high species/tissue-selectivity, low limit of detections, high precision and reproducibility with low inter- and intra-coefficient of variances, and a wide working range. Therefore, they have the potential to fight food fraud, comply with food regulations, and decrease food recalls, which may open up new diagnostic methods for the food industry and the food regulatory authorities.

A229 Rapid methods for detecting the presence of nitrite contamination in food and drink Alexandros Nikolaidis, bane@thermolife.com. Research, NKG Pharmaceuticals, Long Beach, California Nitrite is an ubiquitous pollutant that is a growing concern in drinking water and food alike. Contaminated food, especially vegetables, can contain high amounts of nitrite that can be dangerous and even lethal to sensitive populations, like infants and cardiovascular disease patients. Since presence nitrite is not typically tested for in food or drinks, it has recently come to the author's attention that quite a few innocuously looking food products may contain outright dangerous amounts of nitrite. Traditional methods of nitrite analysis like the Griess reaction require access to equipment and reagents as well as experience in analytical chemistry that are far away from the means of the lay public. To protect the consumer from the dangers of accidental nitrite poisoning, the author has developed a new analytical method that can detect nitrite as well as nitrogen dioxide (a toxic gas that can be formed when nitrite stays in an acidic solution, especially in hot temperatures) with equipment easily available through the internet that requires no experience in analytical chemistry.

A230 Detecting adulteration of red rice yeast dietary supplements by distinguishing between lovastatin and monacolin K Kristen Hannon1, Joshua Sabala1, joshua.sabala@fda.hhs.gov, Kevin Kubachka1, Madhavi Mantha1, Lisa Lorenz1, John Roetting1, Matteo Perini2, Silvia Pianezze2. (1) U.S. FDA, Cincinnati, Ohio (2) Centro Trasferimento Tecnologico, Fondazione Edmund Mach, Trentino, Italy Red Yeast Rice (RYR) is known to contain monacolin K and is marketed as a dietary supplement. Monacolin K is a natural statin that is claimed to lower cholesterol. RYR supplements may be adulterated with lovastatin, an active pharmaceutical ingredient proven to lower cholesterol, to boost efficacy. Monacolin K and lovastatin have identical chemical structures and are difficult to differentiate in testing. However, monacolin K is derived from the mold Monascus purpureus grown on rice, a C3 plant, while lovastatin is fermented from the fungus Aspergillus terreus using mostly C4 plant sources. The stable carbon isotope ratios (δ13C) differ between C3 and C4plants and this difference is passed to monacolin K and lovastatin. This study seeks to develop an optimized preparation method to determine the δ13C values and detect adulteration in the complex matrices of RYR dietary supplements. Study samples (n=31) were first screened for

lovastatin/monacolin K using liquid chromatography-mass spectrometry (LC-MS). Samples with detectable lovastatin/monacolin K were quantified using high performance liquid chromatography with ultraviolet detection (HPLC-UV), and were isolated via fraction collection. Solid phase extraction using graphitized black carbon was used to remove residual pigment contamination. Isolates were analyzed for δ13C values using an elemental analyzer with isotope ratio mass spectrometric (EA-IRMS) detection. Of the samples with sufficient concentrations of lovastatin/monacolin K (>0.8 mg/g), the isolates were analyzed by EA-IRMS (n=13); the δ13C values ranged from -16.3‰ to -31.5‰. A previous study suggests natural monacolin K ranges from -28.2‰ to -30.7‰ and synthetically produced lovastatin ranged from -13.9‰ to -21.6‰. Based on these criteria, 8 of the 13 selected RYR dietary supplements (31 totals surveyed samples) were determined to be adulterated with lovastatin. Five RYR powders from a collaborating lab were also analyzed and the resulting δ13C values from both labs were compared, showing minimal differences (<0.8‰). While this method can provide definitive evidence of adulteration, it is relatively complex and time consuming. Previous reports suggested a ≥2:1 ratio of monacolin K to monacolin K acid indicates adulteration in RYR. Additional experiments investigated any correlation between this ratio and the associated δ13C values. This screening process could reduce the number of samples tested via the isotopic analysis method.

A231 Creation of flavor compounds in cheese Michael H. Tunick, mht39@drexel.edu. Dept. of Food & Hospitality Management, Coll. of Nursing & Health Professions, Drexel Univ., Philadelphia, Pennsylvania When cheesemakers add starter cultures and rennet to milk, a myriad of chemical reactions begin. The carbohydrates, proteins, and lipids break down into compounds that result in the characteristic flavors of the cheese variety. The proteolytic degradation of the casein matrix also generates the distinctive texture of the product. This presentation will deal with the enzymatic and chemical breakdown of these major components of cheese during ripening.

A232 Evolution of volatile compounds during cheddar cheese ripening and discovery of the key flavour compounds related to predetermined cheese qualities YangYi Chen1, Charfedine Ayed1, Qian Yang1, Tim Foster1,2, Nicole Yang1, ni.yang@nottingham.ac.uk. (1) Division of Food, Nutrition and Dietetics, Univ. of Nottingham, Nottinghamshire, United Kingdom (2) Campden BRI, Chipping Campden, Gloucestershire, United Kingdom Cheddar cheese can be pre-determined by Gilles and Lawrence's model linking cheese composition (e.g, moisture, fat, pH) with its grade quality for young cheese after 14 days of manufacturing. During cheese ripening, it is known that biochemical changes of fat, protein, and carbohydrates can lead to significant changes in volatile compounds. Some extreme higher or lower amounts of flavour compounds can cause an imbalanced flavour profile during ripening, which then affects the quality of the end products. This study monitored the evolution of volatile compounds from six different predetermined qualities of cheese during ripening by collecting samples at six stages of ripening (56, 90, 180, 270, 360, 450 days). Solid-phase microextraction gas chromatography-mass spectrometry (SPME GC-MS) was used to characterise key aroma compounds among products at different ripening stages, and descriptive sensory analysis with trained panellists was also conducted on the same cheese samples. Premium Cheddar cheese was found with the highest acetoin level at 56 days than other graded ones, and its level generally decreased to < 20% at 180 days for all samples. Correlation with sensory results indicated that acetoin was highly correlated with a buttery flavour and diary odour (Pearson correlation coefficient r= 0.78 and 0.74 respectively). The level of acetic acid generally increased to its maximum at 270 days, and its level was positively correlated with sour and tangy attributes (r = 0.65 and 0.62 respectively). Other organic acids (e.g., propanoic acid, butyric acid, octanoic acid, valeric acid and caproic acid) showed a steady increase during cheese ripening till 450 days, and their levels were highly correlated with the overall flavour intensity (r =0.74 ~0.88). However, the concentration of acetic acid and organic acids showed no significant difference (p> 0.05) between premium and other graded cheese, particularly at the early stage of ripening (56 and 90 days). Therefore, acetoin, which showed a 30-60% higher level in premium cheese than other graded ones at 56 days, could be the best marker compound to predict the quality of Cheddar cheese.

A233 Multivariate methods in dairy spoilage characterization Lotta Kuuliala2, Lotta.Kuuliala@UGent.be, Jonathan Beauchamp1, Bernard DeBaets2, Frank Devlieghere2. (1) Sensory Analytics and Technologies, Fraunhofer Inst. for Process Engineering and Packaging IVV, Fraunhofer-Institut fur Verfahrenstechnik und Verpackung IVV, Freising, Bayern, DE, other/research, Freising, Germany (2) Faculty of Bioscience Engineering, Universiteit Gent, Belgium The spoilage of dairy products often manifests itself via the generation of offensive off-odors and off-flavors. Typically, this is due to microbial metabolism and oxidative reactions that cause the accumulation of volatile organic compounds (VOCs) in the package over storage time. There has thus been great interest towards identifying spoilage-indicating VOCs and their critical concentration levels corresponding with different spoilage statuses. However, this is a complex task that calls for advanced data analysis. Each food product has its own characteristic volatilome that changes over storage time; furthermore, the volatilome typically consists of several compounds that may be present in different concentration magnitudes and have different olfactory impact. Analyzing and interpreting the VOC datasets thus calls for multivariate statistical analysis and modelling. In this presentation, different multivariate methods for characterizing the volatilome of dairy products packed under gaseous atmospheres are discussed. Firstly, an overview is given of the identification criteria that should be taken into account when aiming at identifying volatile spoilage indicators. A comparison of classical and novel multivariate methods is presented, using examples from different dairy products packed under gaseous atmospheres and stored at refrigeration temperatures (4 °C). Special emphasis will be given on Latent Dirichlet Allocation (LDA), a novel method with promising potential in food spoilage analysis.

A234 Real-time monitoring of VOCs associated with kefir versus kefir-like (plant-based) fermentation induced inoculating diverse microbial resources Vittorio Capozzi1, vittorio.capozzi@ispa.cnr.it, Mariagiovanna Fragasso2, Iuliia Khomenko3, Patrick Silcock4, Franco Biasioli3. (1) National Research Council—Inst. of Sciences of Food Production (ISPA), Foggia, Italy (2) Dept. of Agriculture, Food, Natural Resources, and Engineering, Univ. degli Studi di Foggia, Puglia, Italy (3) Research and Innovation Centre, Fondazione Edmund Mach Centro Ricerca e Innovazione, San Michelle All'Adige, Trentino-Alto Adige, Italy (4) Dept. of Food Science, Univ. of Otago, Dunedin, New Zealand In addition to on-going growth in fermented dairy foods, plant-based dairy analogues are also experiencing rapid growth, however, the diversity of plant-based fermented analogues remains low. One reason for this is that while much is known about the compounds that give fermented dairy products their unique flavour, including how they are derived, this knowledge is missing for plant-based dairy analogues. This is because the flavours generated during fermentation are not only a function of the microorganism(s) involved and fermentation conditions but also the composition of the growth substrate. Of interest in this segment is kefir due to its purported health benefits and sensory attributes. In kefir, fermentation is driven by a heterogeneous microbial consortium aggregated in so-called 'kefir

grains', which consist of different bacterial and yeast genera wrapped in a polysaccharide matrix. Kefir flavour is shaped by a class of secondary microbial metabolites that are volatile and present in trace levels. Due to its ability to measure trace levels of volatile organic compounds (VOCs) in real time Proton Transfer Reaction Time-of-Flight Mass Spectrometry (PTR-ToF-MS) is an ideal tool to measure the generation of these VOCs. In the present work, PTR-ToF-MS was used to determine at what stage of kefir fermentation VOCs were formed and their concentrations in bovine milk and three plant-based milk bases (milk, oat, maize and barley flours). Milks were inoculated with commercial kefir starters, which were diverse microbial consortia. To investigate the integration of additional bacteria into complex microbial communities, a Lactiplantibacillus plantarum strain that allows a bio-enrichment of the riboflavin was also inoculated. The findings improve our understanding of the VOC contributing to kefir flavour and provide information on the influence of fermentation substrate on the generation of VOCs in complex starters that will assist the next generation of plant-based fermented products.

A235 Non-targeted high-resolution mass spectrometry study for evaluation of milk freshness Michele Suman1,2, michele.suman@barilla.com, Cecilia Loffi1,3, Daniele Cavanna1, Giuseppe Sammarco1,3, Dante Catellani1, Chiara Dallasta3. (1) Advanced Research Laboratory, Barilla G e R Fratelli, Parma, Emilia-Romagna, Italy (2) Dept. of Sustainable Food Process, Catholic Univ. of the Sacred Heart, Piacenza, Italy (3) Dept. of Food and Drugs, Univ. of Parma, Italy Milk freshness is an important parameter for both consumers' health and quality of milk-based products. Up to now there have been neither analytical methods nor specific parameters to uniquely define milk freshness from a complete and univocal chemical perspective. In this study, eight molecules were selected and identified as responsible for milk aging, using a liquid chromatography–high-resolution mass spectrometry approach followed by chemometric data elaboration. For model setup and marker selection, 30 high-quality pasteurized fresh milk samples were collected directly from the production site and analyzed immediately and after storage at 2 to 8 °C for 7 days. The markers were then validated by challenging the model with a set of other milk samples, not previously analyzed. Our results demonstrated that the markers identified within this study can be successfully used for the correct classification of non-fresh milk samples, complementing and successfully enhancing parallel evaluations obtainable through sensory measures.

A236 Shelf life of packed UHT milk: Storage test and mathematical modelling Matthias Reinelt, matthias.reinelt@ivv.fraunhofer.de. Materials development, Fraunhofer-Inst. for Process Engineering and Packaging IVV, Freising, Germany The long term shelf life of UHT milk in market available carton board/aluminum packages was investigated under room temperature storage conditions. A major limiting factor for the shelf life (under dark storage conditions) is the radicalic autoxidation of unsaturated fatty acids, which can lead to rancid off-flavors. The rate is influenced by the consumption of oxygen in the milk by the oxidation reaction and the re-supply of oxygen via permeation through the packaging material. The oxygen concentration was measured in the head space and solution during the storage test and modelled by a simplified chemical reaction model coupled to mass transport model for the packaging system (coupled ordinary differential equations). The actual shelf life of the milk was determined by a human sensory panel. From that, a correlation could be determined between the oxygen transmission rate of the packaging system and the expected shelf life. This can be used as a guideline for packaging development. Furthermore, FT-IR spectroscopy, measured on the samples during the storage tests, was used to train pattern-recognition algorithms (perceptron type) to quickly obtain additional information about the samples. Correlations between the FT-IR spectrum and the fat content, storage time, milk producer and general sensory evaluation were investigated.

A237 Sensomics-assisted insights into flavor changes of functional food arising by implementing plant-based proteins as fat-replacer Florian Utz1, florian.utz@tum.de, Johanna Kreissl3, Timo D. Stark1, Christian Schmid1, Caren Tanger2, Ulrich Kulozik2, Thomas Hofmann1, Corinna Dawid1. (1) Chair of Food Chemistry and Molecular Sensory Science, Technische Univ. Munchen, Freising, Bayern, Germany (2) Chair for Food and Bioprocess Engineering, Technische Univ. Munchen, Freising, Bayern, Germany (3) Leibniz-Inst. for Food Systems Biology, Technische Univ. Munchen, Freising, Bayern, Germany Our modern society is facing a multitude of different challenges. One is adiposity. The number of overweight people is constantly increasing, correlating with a wide range of different nutrition-associated diseases, such as diabetes and CVD. The development and promotion of functional food, which is reduced in the amount of e.g., fat, sugar, or salt, may be a promising opportunity to prevent or at least minimize these health risks. Unfortunately, recipe changes result in different flavor profiles and hence, functional food often suffers from low sensory acceptance by consumers. To achieve a fit between consumer preferences and nutritional advantages, the essential flavor-active compounds of the original food must be identified first and gained insights used for knowledge-based flavor optimization of functional analogs. Within a current project, the Sensometabolome of a typical milk dessert containing 15 % fat was decoded to serve as blueprint for processing fat-reduced and flavor-optimized analogs based on functionalized plant proteins. With the help of the Sensomics concept, dairy tastants and odorants were quantitated via UHPLC-MS/MS, HS-SPME-GC-MS or qNMR, based on stable isotope dilution analyses, standard addition, or external calibration. The main requirements for each method were: rapid and simple sample preparations to guarantee precise methods with proper recovery rates and high throughput. Sensory reconstitution experiments of the quantitated compounds also highlighted important flavor-active analytes. Based on these findings, flavor changes within the functional food systems could be identified during manufacturing, explained, and thus minimized by further pre-treatments. In summary, a new way of reducing fat by implementing functionalized plant-based proteins could successfully be established on a laboratory scale and led to functional food products with pleasant flavor profiles. By feasible upscaling, the novel approach shows potential for industrial applications.

A238 Influence of volatile compounds on consumer acceptability of infant formula Graham Eyres1, graham.eyres@otago.ac.nz, Patrick Silcock1, Sophie Gallier2, Louise Tolenaars2, Stephanie Then1. (1) Dept. of Food Sci., Univ. of Otago, Dunedin, New Zealand (2) Dairy Goat Co-operative, Hamilton, New Zealand Flavour is typically an important contributor to consumer acceptability, but how the volatile composition influences the odour and flavour of infant formula (IF), and its impact on acceptability for both parents and infants, is not well understood. The objective of this study was to investigate the volatile composition and consumer acceptability of IF samples to understand the sensory attributes and volatile compounds that determine parents' preference for IF. Eleven commercial IF samples were investigated that varied in composition and processing. Volatile organic compounds (VOC) of the IF samples were analysed using gas chromatography mass spectrometry (GC-MS) with headspace solid phase microextraction (SPME). Consumer acceptability was evaluated for flavour, texture and overall liking with 270 parents of young children. IF products could be differentiated according to the variation in their VOC profiles. IF samples varied in the concentration of lipid oxidation products (e.g. E-2-octenal and E,E-dodecadienal), heat derived products (e.g. furfural) and short chain

fatty acids (e.g. butanoic acid, pentanoic acid). Processing of the whey component had the greatest impact on acceptability, with IF produced with hydrolysed whey being least liked. The VOC profile influenced certain consumers' liking, where compounds were responsible for sensory attributes that decreased their liking scores. Comparison of the VOC concentrations, flavour liking data and comments found that lipid oxidation products were associated with reduced consumer ratings due to fatty, wheaty and plastic characters. Results illustrate that the VOC profile and flavour characteristics significantly influence the relative liking of IF products.

A239 Photooxidation of milk Phil J. Bremer1, phil.bremer@otago.ac.nz, Mohammad Asaduzzaman2, Patrick Silcock1, Erika Zardin4,3, Jonathan Beauchamp4. (1) Dept. of Food Science, Univ. of Otago, Dunedin, New Zealand (2) Faculty of Science and Technology, Libera Univ. di Bolzano, Bolzano, Trentino-Alto Adige, Italy (3) Chemical Work Environment group, National Inst. of Occupational Health STAMI, Oslo, Norway (4) Sensory Analytics and Technologies, Fraunhofer-Institut fur Verfahrenstechnik und Verpackung IVV, Freising, Bayern, Germany The susceptibility of milk to photooxidation in the presence of natural or artificial light and the subsequent development of flavour defects has been studied for almost a century. Despite intermittent interest in this phenomenon over the years, a comprehensive understanding of intermediate compounds formed during the early stage of light exposure, and their transient changes and links to flavour development, is still lacking. It is known that the light activated flavour arises within 15 minutes of light exposure through the oxidation of proteins and amino acids and imparts a flavour described as burnt protein, cabbage and/or mushroom-like. This flavour has been postulated to arise owing to sulphur containing amino acid in proteins, especially methionine being oxidatively deaminated and decarboxylated to methional and a cascade of further decomposed volatile organic compounds (VOCs), such as methanethiol, dimethyl disulphide (DMDS), dimethyl sulphide (DMS) and hydrogen sulphide. However, as methional is not always detected in light struck milk, its relative role in the formation of methanethiol and the mechanisms of VOC formation is still a matter debate. This paper presents the results from dynamic, real-time headspace VOC analysis of model solutions or milks exposed to light using proton transfer reaction-mass spectrometry (PTR-MS). A better understanding of photooxidative flavour development in milk will help in the development of strategies to prevent light-activated off-flavour development and ensure the stability and quality of milk products during storage.

A240 Understanding microbially induced flavor quality changes in milk Mohammad Alothman, Patrick Silcock, pat.silcock@otago.ac.nz, Karen Lusk, Phil J. Bremer. Dept. of Food Science, Univ. of Otago, Dunedin, New Zealand Generally, spoilage of pasteurised milk is a quality failure not a food safety issue. As such whether the milk is suitable for consumption, is generally determined immediately prior to consumption by the consumer using visual and/or odour cues. Microbial spoilage of milk in New Zealand and Australia is typically due to gram negative bacteria like Pseudomonads and occurs as a result of post pasteurisation contamination. Our objective was to the understand relationship between microbial numbers and off-odour generation, including the types of microorganisms present; the types and concentration of volatile compounds (odour) microorganism generate; and how this related to consumers' perception of product quality. This was achieved by measuring volatile organic compounds (VOCs) by proton transfer reaction mass spectrometry (PTR-MS) in milk stored at 4°C with and without inoculation of bacteria isolated from spoiled milk. Consumer perception of milk quality was determined using rejection threshold methodology. In milk stored at 4°C a significant increase in VOC was not observed until a threshold number of microorganisms of about 1x107 CFU/mL were present. Consumers determined that the quality of the stored milk was inferior to freshly produced milk when microbial numbers were about 2.7x107 CFU/mL. In addition, it was found two Pseudomonas fluorescensstrains produced different levels of VOCs at the same microbial numbers. Therefore, spoilage microorganisms differ in the concentration and composition of the VOC they produce, with some microorganisms capable to causing the rejection of the food by consumers at lower total bacterial numbers than others. A better understanding of the progression of spoilage and the factors that cause consumers to reject food products and the associated microorganisms responsible for the spoilage will allow food manufacturers to optimise product shelf life.

A241 Exploring volatile spoilage markers and sensory defects of UHT milk in accelerated shelf-life tests Antonia Krempl, Bettina Handwerker, Andrea Strube, Klaus Rieblinger, Jonathan Beauchamp, jonathan.beauchamp@ivv.fraunhofer.de. Fraunhofer Inst. for Process Engineering and Packaging IVV, Fraunhofer-Institut fur Verfahrenstechnik und Verpackung IVV, Freising, Bayern, DE, other/research, Freising, Germany Accelerated shelf-life (ASL) tests offer a means to examine food spoilage and estimate shelf-life on shorter timescales compared to conventional storage regimes. Ultra-high temperature (UHT) processed milk has an extended shelf-life compared to its fresh milk counterpart of typically at least six months at room temperature (ca. 20-24 °C). Kinetic models allow chemical changes in food systems to be predicted according to temperature. The Q10 approach, for example, characterises the reaction rate coefficients at temperatures that differ by 10 °C. For UHT milk, this model predicts a reaction rate increase by a factor of two from 20 °C to 30 °C storage, and equally from 30 °C to 40 °C. Accordingly, the shelf-life of UHT milk stored at 30 °C or 40 °C is expected to be, respectively, half or a quarter of that compared to storage at 20 °C. Assuming a shelf-life at room temperature of 150 days, this equates to a 75 days shelf-life at 30 °C, and a 38 days shelf-life at 40 °C. UHT milk samples with different fat content (0.1 %, 1.5 % and 3.5 %) were subjected to these three storage regimes in order to examine volatile spoilage metabolites and sensory defects according to shelf-life. The former were analysed in the headspace of milk sample replicates at regular intervals up to and beyond the shelf-life by means of proton transfer reaction mass spectrometry (PTR-MS) and gas chromatography-ion mobility spectrometry (GC-IMS), whereas the latter were evaluated by a trained sensory panel according to appearance and odour using the check-all-that-apply (CATA) approach. Empirical data from these studies indicate that ASL tests at 30 °C exhibit volatile spoilage markers of potential utility in predicting shelf-life, whereas the sensory defects in milk samples held at 40 °C were predominantly associated with temperature-induced chemical changes, e.g., Maillard reaction products.

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Schedule of Technical, Business and Social Meetings

Sunday March 13	11 am – noon	Future Programs	via Zoom
Sunday March 13	1 pm – 2 pm	Special Topics and Business	via Zoom
Sunday March 13	3 pm – 6 pm	Executive Committee	via Zoom
Sunday March 20	8 pm – 10 pm	Undergrad Poster Competition	via Zoom
Monday March 21	8 pm – 10 pm	Sci-Mix	Convention Center & Zoom
Tuesday March 22	7 pm - 9 pm	Undergrad Poster Competition and AGFD Social Reception	Convention Center