Division of Agricultural and Food Chemistry of the ACS Spring 2023

CORNUCOPIA

including the AGFD program and abstracts for the

265th American Chemical Society (virtual & live) National Meeting on

March 26 - 30, 2023

in

INDIANAPOLIS

Jonathan Beauchamp, Jason Soares
Program Chairs

Going to Indianapolis?
Join the AGFD Chair's Reception (free refreshments!)
Buca Di Beppo
35 N. Illinois St.
Tuesday, March, 6:00 - 8:00pm

Twelve minute walking directions from Convention Center –
exit the Center onto Maryland Street, turn right, proceed several blocks to N. Illinois Street, cross the street and then turn left. Proceed 1½ blocks. Buca de Beppo is on your right.

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! - https://www.linkedin.com/groups/8154423/

MESSAGE FROM THE CHAIR

I did not expect to be writing this message already. Just over one year ago, at the end of January 2022, I was nominated for the position of Vice-Chair of our technical division – to serve with immediate effect after the incumbent officer for that role unexpectedly stepped down. Words of encouragement and support from Youngmok Kim (past Chair) and Michael Granvogl (Chair-Elect) convinced me to stand, and my appointment was promptly approved by the AGFD Executive Committee. My expectations and intentions were to steadily familiarize myself with my new duties, as is foreseen for incoming officers, by supporting the Chair-Elect before transitioning to that position, then ultimately to Chair; a three-year journey, minus the first couple of months of 2022 due to my late incumbency. Then, only a month later, tragedy struck when Michael Granvogl, my anticipated mentor in the coming years, suddenly passed away; I had expected to learn a great deal from Michael, but that was not to be. My swift progression to Chair-Elect coincided with me inheriting the role of Program Chair for ACS Fall 2022. Michael had put in excellent groundwork in seeding the technical program, yet cultivating it was a daunting challenge due to my lack of prior experience and involvement in such a task. While I acknowledge Michael's fundamental contribution, the great success of the AGFD programming and its implementation for ACS Fall 2022 can be primarily attributed to the steadfast resolve and dedication of LinShu Liu, last year's AGFD Chair. LinShu's unfaltering leadership and support was pivotal in jointly pulling everything together to create a captivating technical program for our members and the wider audience. ACS Fall 2022 featured 20 AGFD symposia on a broad range of topics that comprised 207 oral presentations and 89 posters. The Division can look back with contentment on its success under the circumstances, notably the healthy number of contributions and attendance, which indicate an upturn in conference activity compared to the recent COVID-ridden years.

AGFD has successfully overcome the many challenges faced in the disruptive past three years and we can savor the positive outlook for the year ahead, commencing this month with ACS Spring 2023 in Indianapolis and online. Traditionally, the contributions to the spring meetings are fewer than in the fall, but AGFD can be proud to be coordinating 12 symposia for this meeting, including two interactive panel discussions, with almost 200 abstract submissions. In addition to our regular program events – the General Papers oral and poster sessions (the latter featuring the undergraduate poster competition) – AGFD can boast 14 sessions that cover a diversity of topics, from citrus flavor, the chemistries of alcohol and coffee, functional ingredients, food packaging and preservation, and agri-food sustainability, to food allergens and biomarkers of food and drug intake. We encourage interactive and high attendance in these sessions and hope that this broad range of topics will quell your thirst for hearing the latest developments in the many sub-disciplines of agricultural and food chemistry. Beyond the technical program, the meeting sees the return of the Chair's Reception after the COVID-induced hiatus, which I am delighted to host, especially having the honor of conferring the awards for the best undergraduate poster competition contributions. As with every conference, the success in programming rests on the shoulders of the individual symposium organizers, who have worked tirelessly to create this rich assortment of technical sessions. Accordingly, I would like to thank all symposium organizers for their contributions and achievements: Michael Appel, Lingyun Chen, Nina Cleve (née Buck), Vinka Craver, Kathryn Deibler, William Dixon, Nick Flynn, Brian Guthrie, Zhengze Li, Chris Mattison, Alyson Mitchell , Coralia Osorio Roa, Y Lan Pham, Anne Plotto, Qinchun Rao, Omowunmi Sadik, Majher Sarker, Veronika Somoza, Jane Tseng, Yu Wang, Xian Wu, Tianxi Yang and Liangli Yu. Additional and considerable thanks go to Jason Soares, my Program Co-Chair for this meeting and current Chair-Elect of the Division. Like me, Jason was thrown in at the deep end with a premature call to duty by AGFD, but he has risen to the challenge and provided crucial support in coordinating the programming activities.

Returning to my account of the turbulent experiences of last year, I have shared this with you to convey a positive message. The idiom that life can be unexpected holds true, but most challenges can be surmounted with a strong and unwavering support network in place. The AGFD Executive Committee embodies this notion, and I am indebted to many people for their advice and guidance in matters relating to the tasks of Program Chair and incoming Division Chair. Foremost, I sincerely thank Alyson Mitchell, LinShu Liu, Mike Morello, Michael Appell, Michael Tunick, Kathryn Deibler, Brian Guthrie and Jason Soares for their indispensable help that has smoothened my leap from Vice-Chair to Chair within the constricted space of one year. Finally, Carl Frey is gratefully *continues on next page*

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acknowledged for his ever-skillful composition and editing of this eagerly anticipated Cornucopia (and his unrelenting patience in waiting for me to deliver materials with which to fill it.)

As we slowly yet optimistically emerge out of the pandemic, we hope to see physical meeting attendances in greater numbers, accompanied by the much-needed social interactions that all of us sorely missed during times of lockdowns and travel restrictions. Nevertheless, regardless of whether you are attending ACS Spring 2023 in person or virtually, I wish you an enjoyable and insightful meeting; and for those of you heading to Indianapolis, I look forward to meeting you in person, either while perusing the posters, during the coffee breaks of the technical sessions, or enjoying a drink at the Chair's Reception.

Jonathan Beauchamp
AGFD Chair 2023
March 2023
Freising, Germany

CORNUCOPIA EDITORIAL STAFF & CONTACT INFORMATION	
Editor-in-Chief	C. Frey cfreyenterprise@gmail.com
General Manager	P. White
Staff	C. Kent, L. Lane, J. Olsen

Convergent Chemistry Communities (CCC)

Convergent Chemistry Communities (CCCs) are being piloted by ACS as a new platform for enabling Divisions and Members to come together and collaborate on topics of mutual interest that are best explored in a multi-disciplinary fashion. In particular, CCC initiatives center on important new or emerging focus areas and/or highly multidisciplinary topics and facilitate new collaborative interactions involving multiple Divisions. A primary goal of the CCC is to coalesce interest and activities around an exciting science area that demands the focused attention of the ACS. AGFD is actively undertaking to form CCCs in the following areas:

Food Security: Tackling Hunger
Zero Hunger is one of the U.N. Sustainable Development Goals (SDG-2). AGFD is coordinating collaboration with AGRO, ANYL, and ENVR Technical Divisions of ACS to address this goal through the **CCC – Food Security: Tackling Hunger.** The community aims to foster collaboration and disseminate how chemistry is tackling challenges associated with eliminating hunger. Our vision is to 1) foster strong working relationships; 2) coordinate multidisciplinary knowledge sharing through technical programming, webinars, and social media; and 3) cultivate interest in chemists – students to explore or pursue careers that address food security and alleviate hunger. Members, Divisions, committees, and other societies interested in scientific efforts aimed at eliminating hunger are welcome to join us! A LinkedIn group has been established to facilitate connections: https://www.linkedin.com/groups/12750126/. Contact Kenny Xie kyx@usp.org for more information.

ACS Microbiome Research Consortium
AGFD, in collaboration with AGRO, ANYL, BIOT, CARB, COMP, ENVR, MEDI, has proposed to establish the **CCC – ACS Microbiome Research Consortium**. Microbiomes have emerged as critical determinants of many aspects in our life, ranging from the environment, to food production, safety, and human health. This proposal seeks to foster and consolidate ACS-wide microbiome research activities. The proposal contains three main initiatives: 1) Scientific initiative to provide a consolidated interactive platform in microbiome research. 2) Education and diversity initiative to educate students and postdocs and provide sound advice on skillsets to be successful in this research area. 3) Industrial partnership initiative to promote interaction with industrial partners, to highlight ACS members' microbiome research, and as conduits to translate microbiome research toward utility in industry. It is envisioned that the consortium be a broad based, interactive, collaborative cross division community to highlight current research, identify emerging issues and solutions. A kick-off meeting is planned for ACS Fall 2023. Members, Divisions, committees, and other societies interested in the scientific efforts are welcome to join us! Please contact tom.wang@usda.gov, linshu.liu@usda.gov or karley.mahalak@usda.gov for more information.

FUTURE PROGRAMS

SAN FRANCISCO August 13-17 2023 ACS Meeting Theme - Harnessing the Power of Data

ACS Microbiome Consortium Kick-off Symposium Laurel Doherty laurel.a.doherty.civ Masuko Kobori kobori@affrc.go.jp LinShu Liu linshu.liu@usda.gov Karley Mahalak Karley.mahalak@usda.gov Tom Wang tom.wang@usda.gov

Advances in Food Chemical Informatics, Knowledge Bases and Databases Andreas Dunkel a.dunkel.leibniz-lsb@tum.de Brian Guthrie brian_guthrie@cargill.com David Wild djwild@indiana.edu

Artificial Intelligence Applications for Food and Agriculture Michael Appell michael.appell@usda.gov Bosoon Park bosoon.park@usda.gov

Award for the Advancement of Application of Agricultural and Food Chemistry in Honor of Liangli (Lucy) Yu Jonathan Beauchamp jonathan.beauchamp@ivv.fraunhofer.de Michael Morello mjmorello226@gmail.com

Bioproducts from Biomass Helen Ngo helen.ngo@usda.gov Majher Sarker majher.sarker@usda.gov Barjendra Sharma Brajendra.Sharma@usda.gov Madhav Yadav madhav.yadav@usda.gov

Biotechnology and Synthetic Biology for Sustainable Foods, Food Ingredients and Flavor Keith Cadwallader cadwlldr@uiuc.edu Xiaofen Du xdu@twu.edu Yong-Su Jin ysjin@illinois.edu Michael Qian michael.qian@oregonstate.edu YanPing Quin yan.ping.qian@oregonstate.edu

Chemical Intervention Technology to Improve Microbial Stability of Food Xuetong Fan xuetong.fan@usda.gov Tony Jin tony.jin@usda.gov

Chemistry of Wine Elizabeth Chang eabc@vt.edu Gal Kreitman gal.kreitman@ejgallo.com Gavin Sacks gls9@cornell.edu Elizabeth Tomasino elizabeth.tomasino@oregonstate.edu

Food Security: The Role of Alternative Protein Sources in Addressing World Hunger John Finley JFinley@agcenter.lsu.edu Brian Guthrie brian_guthrie@cargill.com Lauren Jackson Lauren.Jackson@fda.hhs.gov Michael Morello mjmorello226@gmail.com Rickey Yada r.yada@ubc.ca

Food Toxicants: Occurance, Detection, Formulation Mechanism and Mitigation Michael Appell michael.appell@ars.usda.gov Xiaohua He xiaohua.he@usad.gov Lauren Jackson Lauren.Jackson@fda.hhs.gov Liangli Yu lyu5@umd.edu

General Papers Jonathan Beauchamp jonathan.beauchamp@ivv.fraunhofer.de Jason W. Soares Jason.w.soares.civ@mail.mil

General Posters Jonathan Beauchamp jonathan.beauchamp@ivv.fraunhofer.de Jason W. Soares Jason.w.soares.civ@mail.mil

JAFC Best Paper Award Thomas Hofmann thomas.hofmann@tum.de Willam King WKing@acs-i.org Jonathan Beauchamp jonathan.beauchamp@ivv.fraunhofer.de

Methods, Data and Their Usage Towards Solving the Food Allergy Problem Yuzhu Zhang yuzhu.zhang@usda.gov

Nutracetical Lipids, Proteins and Biopeptides Fereidoon Shahidi fshahidi@mun.ca Jianping Wu jwu3@ualberta.ca Rickey Yada r.yada@ubc.ca

Oat Bioactives & Their Health Benefits YiFang Chu yifang.chi@pepsico.com Changling Hu chu@ncat.edu Shengmin Sang ssang@ncat.edu

Phthalates and PFOS Environmental Exposure and Toxicology John Finley JFinley@agcenter.lsu.edu

Renewable Polymer Materials: Preparation, Processing, Application and Disposal LinShu Liu linshu.liu@usda.gov Jinwen Zhan jwzhang@esu.edu

Smart Food Safety Xiaonan Lu xiaonan.lu@mcgill.ca Rickey Yada r.yada@ubc.ca

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Sustainable Agriceuticals Hyunsook Kim hyunsuk15@hanyang.ac.kr LinShu Liu linshu.liu@usda.gov Daxi Ren dxren@zju.edu.cn Wally Yokoyama wally.yokoyama@usda.gov Liangli Yu lyu5@umd.edu

Virtual Graduate Student Symposium in Asia-Pacific Region on Agriculturaland Food Chemistry Daxi Ren dxren@zju.edu.cn Chunxiao Zheng czheng@acs-i.org

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

NEW ORLEANS March 17-21 2024 ACS Meeting Theme - The Many Flavors of Chemistry

Chemistry of Alcoholic Beverages Nick Flynn nflynn@wtamu.edu

New Technologies in Flavor Analysis Mike Morello mjmorello226@gmail.com

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

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

Authenticity and Adulteration Analysis Neil Da Costa neil.dacosta@iff.com

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

Mycotoxins Hans-Ulrich Humpf humpf@uni-muenster.de

Microplastics and Nanoplastics in Seafood Changqing Wu changwu@udel.edu Xuetong Fan Xuetong.fan@usda.gov

Agnes Rimando Memorial International Student Symposium Michael Tunick mht39@drexel.edu Roberta Tardugno

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

CCC – Food Security: Tackling Hunger Kenny Xie kyx@usp.org Mike Morello mjmorello226@gmail.com

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

Executive Committee Meeting Minutes

Sunday, August 14,2022 1:00-3:00 pm CDT, via ZOOM
Takes place at each ACS National Meeting

Attendees: LinShu Liu, Jonathan Beauchamp, Alyson Mitchell, Robert McGorrin, Michael Appell, Youngmook Kim, Michael Morello, Michael Qian, Stephen Toth, Michael Tunick, Karley Mahalak, Brian Guthrie, Xiaofen Du, Tony Wang, Carl Frey

AGFD Chair LinShu Liu called the meeting to order at 1:10 p.m. (CDT).

The **minutes** of the spring 2022 Executive Committee meeting were approved with no changes and are published in the spring 2022 Cornucopia.

Michael Morello summarized the **Special Topics Meeting**. The committee discussed how to improve the publication of the special issue papers, based on the symposia of Spring (JAFC) and Fall (J Food Sci. & Tech) Technical Programs. The editoral board of these journals will be contacted to discuss potential ideas (e.g., review article to summarize the meeting, symposia series book, etc.) for these special issues. Michael Morello of the Senior Program Guidance Committee motioned for approval to establishing a new quarterly speaker seminar series with *continues on next page*

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a following social hour to improve PR for the division. This committee will develop recommendations and guidelines to implement this seminar series during the Fall and will send this plan to the Executive Committee for vote and final approval via email. The motion was approved. A need to update Division Bylaws after the upcoming Strategic Planning meeting was also indicated.

The **Awards Committee Report** was given by Mike Morello. All award information can be found on the Division website and is published in the Fall 2022 Cornucopia. Due to on-going COVID-19 issues, the traditional awards banquet will not be held at the Fall meeting. Instead, a Chair's reception will be held at the Fall meeting. All award winners will be recognized at this reception. The call for student and Division awards will be sent out in September via email to Division members. Youngmok Kim will be taking over Michael Granvogl's responsibilities for the Young Scientist Award.

The **Senior Program Guidance Committee (SPGC) Report** was given by Mike Morello. The SPGC was started one year ago. The members of the committee include Mike Morello and Coralia Osario Roa (thru 22), Neil DaCosta and Kanjana Mahattanatawee (thru 23), Lucy Yu and Michael Appell (thru 24). Replacements for this committee need to be identified by the nominations Chair who appoints these positions. Members of this committee cannot be members of the Executive Committee. The committee meets monthly to help advise and steer technical programming. This committee has developed a master list of national meetings from 2001-2022. This committee is working to improve engagement with AGFD subdivisions, and inform subdivision officers an outline of their role and duties as subdivision officers. The committee has also work to improve pre-meeting promotion. For example, a summary of each symposia is compiled for dissemination via social media. Post-meeting promotion is also being focused on (e.g., social media, special journal issues, books, etc.,). New programming opportunities and venues (e.g., webinars and YouTube videos) were identified. Mike Morello indicated that this committee needs volunteers to help accomplish goals and sustain activities (e.g., rotating webinars through the subdivisions).

The **Student Committee Report** was not given as the student graduated and moved on. A new student needs to be identified to carry out these duties. Jonathan Beauchamp asked how our student member numbers are in comparison to previous years. This information was not readily available to the committee. The difficulty of engaging students in AGFD as compared to IFT was brought up by Xiaofen Du as many of the AGFD students research is more related to food science and aligns more with goals of IFT. Additionally, IFT has more student-related events and programs. Michael Qian will contact Alyson Mitchell to discuss forming a committee to address student engagement. This topic will be added to the list of topics to discuss at the Strategic Planning meeting.

The Nomination Reports were given by Youngmok Kim. *Division leadership:* a new Division Chair (Jonathan Beauchamp) and Vice-Chair (Jason Soares) were nominated and approved for incoming Chair and vice-Chair due to the tragic loss of Michael Granvogl. A motion to nominate incumbents officers Steven Toth as Treasurer and Alyson Mitchell as Secretary for 2023 was approved. *Subdivision leadership:* the division has seven subdivisions which include: Flavor (Yu Wang), Functional Foods & Natural Products (Xian Wu), Food Bioengineering (Tianxi Yang), Nutrition (Mathias Sucan), Food Safety (Tony Jin), Diet & Gut Microbiome (Guodong Zhang, Karley Mahalak), Sustainability & Green Technology (Wunmi Sadik) Five of these subdivisions have new secretaries nominated for next year. Youngmok Kim will continue to work with the Flavor and Sustainability & Green Technology subdivisions to identify new officers for next year.

LinShu Liu gave the **Program Report**. The 2022 Spring National Hybrid Meeting hosted 12 symposia and 176 abstracts and 77 posters. This is low attendance for our Division and is likely related to the on-going COVID-19 pandemic and technical challenges associated with hosting a hybrid meeting. However, a hybrid meeting offers more flexibility for member engagement and attendance. Student attendance was also low and demonstrates a need to improve engagement with students. The report for the Fall 2022 National Hybrid Meeting was given by Jonathan Beauchamp. The meeting currently has 32 sessions; 14 hybrid, 8 virtual and 10 in-person. The number of papers given will be 207 (215 originally). There will be 45 in-person posters given and 44 virtual posters given. In addition, there will be 32 contributions given at SciMix.

The **Future National Meetings** was summarized by Jonathan Beauchamp. There are 12 symposium and two panel discussions proposed for the 2023 Spring meeting in Indianapolis, in addition to the General Poster Session and Undergraduate Poster Competition and the Graduate Student Symposium. The 2023 Fall San *continues on next page*

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Francisco meeting currently has 16 proposed symposia in addition to JAFC Best Paper Award, Young Scientist Award and Sterling Hendricks Award symposia. A memorial symposium is also proposed in honor of Michael Granvogl. To date there are 4 symposia proposed for the 2024 Spring Meeting in New Orleans.

The **Third International Conference on Flavors** will be held in New Zealand in 2024. The time and date have not been decided. The International Society for Nutraceuticals and Functional Foods will be held in October 2022 in Istanbul, Turkey.

Subdivision Reports were given by subdivision leaders. Xiaofen Du indicated that the Flavor subdivision has not been meeting regularly and needs improvement on re-engaging after a lack of in-person meetings due to COVID-19. Tainxi Yang indicated that Food Bioengineering will hold two symposiua in 2023; Advances in Food Packaging and Preservation and Microplastics in Seafood. Karley Mahalak indicated that Diet & Gut Microbiome will host 3 hybrid sessions at the Fall meeting and that several new people have been recruited into the division. Michael Appell indicated that Sustainability & Green Technology has a virtual and hybrid session that are part of the thematic programming for the Chicago meeting and Indianapolis meetings. This subdivision is meeting regularly.

The **Councilor Report** was given by Michael Tunick. The Council meeting will be held next week at the Chicago meeting. Several petitions are proposed included one related to Divisional activities including a petition to let DAC step in if a Division is having trouble filling all positions.

Council Committee Updates. Michael Tunick gave the DAC update and indicated that there was a strategic planning retreat held last Spring. Several new ideas for improving membership engagement were discussed including encouraging more innovative project grants and strategic planning retreats, among others. The CPRC update was given by Mike Appell who indicated that this committee recently published an article in CE&N titled *Truth Decay*. This committee is also active in doing PR makeovers for divisions. The ComSci update was given by Mike Morello. This committee develops programming such as Frontier Fridays; a webinar series on new and interesting chemistries (e.g., wearable sensors, new battery technology, etc.). This committee also develops policy statements. Finally, this committee helps develop recommendations for non-ACS awards (e.g., National Medal of Science) and is heavily involved in promoting the UN's sustainable development goals (e.g., Zero Hunger). Zero Hunger is a great opportunity to highlight our Division as our programming is in alignment with these goals (e.g., food preservation and sustainable agriculture).

An update on the **Strategic Planning Retreat** was given via email by Lauren Jackson (Chair) who indicated that ACS strategic planning facilitators had not yet contacted her with respect to the October strategic planning retreat and that this may now have to be delayed until the Spring.

Cornucopia editor Carl Frey indicated that the Cornucopia went to the website about 2 weeks ago and 100 copies will be printed for the upcoming Fall meeting. The Cornucopia will look slightly different as the data came from ACS in a different format. For example, the papers are no longer numbered which is not ideal.

Hospitality/Public Relations Report was given by Mike Morello. A Chair's reception is set for the Chicago meeting and will be held at the Marriott on Tuesday from 6:30-8:30 PM. Food will be ordered for 50 people as there are only 10 in-person sessions. Drinks will be limited to beer, wine and soft drinks.

The **Membership Report** was given by Michael Qian who indicated that membership is down. Before the COVID-19 pandemic the Division membership was ~3,200 and we are now down to 1,900. This is not specific to AGFD. Efforts need to focus on re-growing our membership. Mike Appell suggested giving free membership for presenters. The Program Chair has access to all speakers and could reach out to presenters and ask if they want free membership. We may need to work with ACS to get a membership code that could be given to presenters so they could join the Division for free. Michael Qian will consult with Steve Toth and Michael Tunick will consult with DAC to discuss this possibility.

Stephen Toth gave the **Treasurer's Report**. The division has revenues of about $42,000. The Division has not received reimbursement for Councilor travel from the Spring 2022 meeting but has received two $1,000 checks that are not identified for what they are for. The Division spent $22,000 to date this year. Registration and expenses for the Poster session for San Diego was ~$5,000. Total assets for the Division are $942,196, including ~$780,000 in investments and ~$165,000 in the checking and savings accounts. The Division is financially in good shape. The *continues on next page*

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total cost for the Chicago meeting will be in alignment with what was allocated for this meeting. A motion to approve the report as provided was passed.

A **budget** of $25,000 was set and passed for 2023 Spring National Meeting.

The **Communications Report** was given by Michael Appell. The website has been updated to include contact information for the Chair and now links to ACS leadership courses, workshops and jobs as well as other career related resources. The Website now links to over 100 videos on agriculture and food chemistry. Social media resources are also now linked. The website provider also provides a professional letter. Michael indicated that more volunteers are needed to maintain the website.

There is no **New Business.**

The meeting adjourned at 3:15 p.m. *Submitted by Alyson Mitchell, AGFD Secretary*

Meet the new AGFD Vice-Chair Liz Kreger

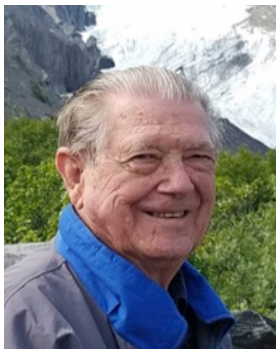
Liz has a Ph.D., [Doctorate & Masters Food Science, U. of Illinois at Urbana-Champaign; B.S Biochemistry, Florida State U.]. Liz leads Innovation and Analytical teams at Sensient Flavors & Extracts NA in research across the spaces of discovery of taste modulators, development of new flavor profiles, delivery systems, and biotechnology. Previous experience includes PepsiCo (performing research to address global flavor issues when reducing sugar), ADM (developing new analytical techniques for flavor molecule discovery) and Nestlé (flavor research to support development of ready-to-drink coffee and cocoa malt products). Liz joined ACS in 2014. She served as Flavor sub-division chair and organized several symposia, most recently in Fall 2022, *Extraction & Biotechnology – A Natural & Sustainable Future for Flavors*

VIRTUAL PROGRAMMING – HOW DOES IT WORK ?

See the ACS website links, below, for the Indianapolis 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/meetings/acs-meetings/spring-2023/attend/faq.html

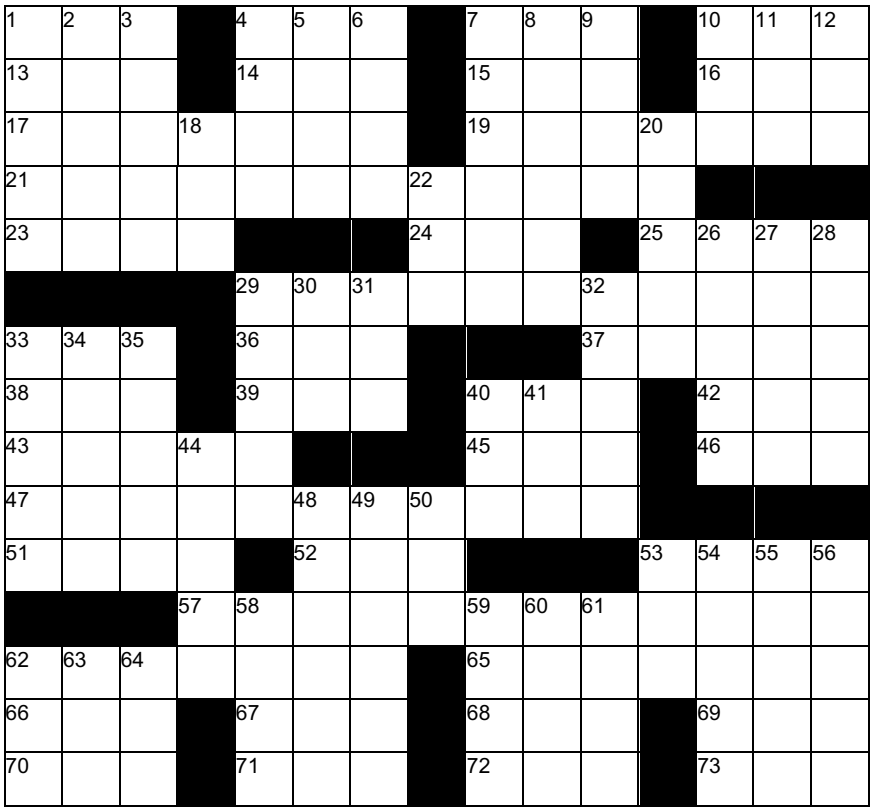
In Memorium
Harold Pattee

6/27/34 – 10/29/22



Harold Edward Pattee was born in Phoenix to Earnest Harold Pattee and Ina Mae Hamblin. On June 8, 1956, he married his high school sweetheart Phyllis Adams at the Latter-Day Saint Temple in Mesa, Arizona. They celebrated almost 59 years together raising one son and six daughters before Phyllis preceded him in death. As an active member of the Church of Jesus Christ of Latter-Day Saints he served on the High Council, as a Temple and Family History Missionary, as Bishop and leaves a legacy of research related to his love of genealogy. He was active in the Boy Scouts of America, receiving the Silver Beaver Award. Harold is survived by his wife, Letha Liddle Pattee; children, Floyd L. Pattee, Phyllis Kofford, Linda Bernard, Deborah Pattee, Sherri Pattee, Sheila Pattee, and Yvonne Lee; 12 grandchildren; 9 great grandchildren; sisters Pat Wilson and Thelma Winters. He earned many prestigious awards over the course of 42 years of USDA research in peanut science at North Carolina State University in Raleigh. Harold presented numerous papers at ACS Meetings. One of his ACS Symposium Series books sold >1000 copies, earning him a Platinum Club Award. He served as AGFD Chair, received the Distinguished Service to AGFD Award and became a AGFD Fellow in 1989. He is remembered as a good friend, mentor and colleague. His many co-workers, collaborators and friends at AGFD miss him and extend condolences to his family

START YOUR PENCILS!



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

ACROSS

1 College student stat
4 Homer's exclamation
7 School in Muncie, IN
10 Animation film unit
13 Tear or shred
14 Gator__
15 FedEx competitor
16 Fish egg
17 Fermentation product
19 Make an echoing noise
21 Purdue's sports teams
23 Some means justify these
24 Cheese go-with
25 Acid + base → ___
29 Waterway slicing Indiana
33 Brain + spinal cord + etc.
36 End of many amino acids
37 Open mouth letter group
38 Cheer for 21 ACROSS
39 Genetic code compound
40 World-wide __
42 S. Afr. anti-apartheid org.
43 Change in face of stress
45 Jackie O's second
46 Maiden name
47 Indy __ race
51 Apple, pear, orange or oak
52 Muscle built with pushups
53 Classic Indian music form
57 *Cat's Cradle* author
62 Allows to decompose
65 What Bert & Ernie are
66 12 months in Tijuana
67 Big ISP
68 Ending for many paraffins
69 180 degrees from NNW
70 Peppy citrus soda: Mtn. __
71 4G phone service acronyn
72 On-line ha-ha
73 JFK & LAX scan pros

DOWN

1 Loon-like bird
2 Climbing hardware
3 A little sucker
4 Niels Bohr, for example
5 Aroma
6 Ship steering apparatus
7 Some full-body covers
8 Oration
9 It fell in 1991
10 It's 'grand' on wine labels
11 A really, really long time
12 Like many new lightbulbs
18 Gore and Einstein
20 Stage & film actor Davis
22 Org. of lots of docs
26 Pertaining to birds
27 W. Africa's Sierra __
28 Agreement to stop fighting
29 Length x __ = area
30 Raggedy __ & Andy
31 'Maude' actress __ Arthur
32 Extreme/fanatical
33 Handiwork ability
34 The lowest low
35 Use for a razor blade
40 Simple full-deck card game
41 Poetic 'before'
44 Looks under the sheets
48 Pull from the ground
49 Weed you might 48 DOWN
50 605 in old Rome
53 Stage of sleep for dreams
54 Age discriminator
55 Surmise without data
56 No longer docked
58 __ Mountains of W. Russia
59 Thesis defense format
60 Taboo
61 Christmas carol
62 Young boy
63 Suffix for an olefin
64 Pull behind

AGFD DIVISION MEMBERSHIP APPLICATION

The Agricultural and Food Chemistry Division (AGFD) of the American Chemical Society (ACS) is a non-profit organization dedicated to the technical advancement of all aspects of agricultural and food chemistry. AGFD encourages technical advancement in the field by -

- organizing symposia/workshops on agricultural/food chemistry at ACS national meetings and other venues
- publishing proceedings of AGFD symposia
- publishing the *Cornucopia* newsletter
- updating members several times a year via e-mail blasts
- hosting social and networking gatherings at ACS national meetings
- providing cash awards and recognition to leading undergraduate and graduate students, young scientists and established scientists in the field of agricultural and food chemistry

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

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

	APPLICATION FOR AGFD DIVISION MEMBERSHIP (7623P)
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[ ]	I am an ACS member and wish to join AGFD ($10.00)
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Be cool **J O I N** **A G F D**	Return application, with payment (payable to American Chemical Society), to AGFD Membership Chair: Michael Qian, Professor Department of Food Science and Technology Oregon State University Corvallis OR 97330

ROSTER OF AGFD OFFICERS & COMMITTEE LEADERSHIP

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

AGFD TECHNICAL PROGRAM

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

SUNDAY MORNING & AFTERNOON March 26
Advances in Biomass-Based Biodegradable Polymers Spons POLY, Cospons AGFD, BIOT, CELL, I&EC, PMSE

SUNDAY EVENING 7 – 9 pm Conv. Ctr Hall F-H
AGFD General Poster Session and Undergraduate Poster Competition
J. Beauchamp, K. Deibler, J. W. Soares, *Org.*
(note-first 19 posters listed below also presented at Monday Evening Sci-Mix)

Synopsis: This session showcases the talents of undergraduate students, provides a professional forum for presentation of their research and promotes their continued education in food & agricultural chemistry. Participation is open to all undergraduate students at certified universities actively participating in research projects/programs in the areas of food and agricultural chemistry. Students chosen to participate as finalists in the symposium receive travel expenses ($750 max.) to attend and present their research during the Spring ACS meeting. Undergraduate Research Award winners receive a cash award of $500, $250, and $100 for first, second and third place, respectively. Contact Dr. Kathryn Deibler (kdd3@cornell.edu) for information.

01--Comparison of the amino acid metabolism of genetically different brewing yeasts. **A.R. Cicali**, E.M. Diaz-Aceituno, S.A. Morton, S. Harper, C.A. Hughey
02--Identification and quantification of carcinogen compounds in carotenoid foods through solid-phase microextraction gas-chromatography mass spectrometry . **A. Pons**, M. Tarrance, K. Barnes
03--Hop *(Humulus lupulus)* phytochemical profiles as a function of growth region by HR LCMS and GCMS analysis. **C. Paoletta**, C. Balog, A. Dew, D.V. Liskin, A. Higgs, K. Kingsbury, A. Brehm, R.A. Quinlan
04--Effect of trans vaccenic acid on glucose homeostasis in a mouse model of diet-induced obesity and insulin resistance. **C.M. Prajogo**, Y. Xu, P. Vahmani
05--Evolution of kombucha in an air-permeable bag. **E. Oberholtzer**, L. Black, J. Kegerreis, J.N. Richardson, L. Stains
06--Characterization of total antioxidant capacity in spent coffee ground extracts by roast and brewing method via UV-Vis spectrometry. B.G. Yust, N.Z. Rao, **E. Schwarzmann**
07--Analysis of free, conjugated and insoluble-bound phenolics in buriti fruit shells as a potential source of functional dietary fiber. **G. Guerrero**, E. Esparza, E. Cosio
08--Design of new, and environmentally safe herbicides using AI and molecular modeling. **J.A. Darsey**, M. Shaver
09--Quantification of nitrate in pomegranate extract using ion-pair reverse-phase HPLC. **J.Powell**, R. Tan, P.M. Joyner
10--Beer processomics: Evolution of volatile and nonvolatile hop compounds throughout boiling and fermentation with genetically different yeast. **J.M. Garcia**, E. Nasipova, S.A. Morton, S. Harper, C.A. Hughey
11--Plasticizing capabilities of glycerol: Acetic acid and choline chloride: Urea in potato thermoplastic starch film. **K. Collier**, R. Singh, J. Staker, E. Collier, A. Ansar, A. Tovar, A. Siegel
12--Isolation of monomeric anthocyanins from *Vitis vinifera* utilizing low-cost and high throughput methodologies. **L. Arce-Rosales**
13--Determination and comparison of xanthophyll carotenoid content in age related macular degeneration vitamins versus vegetables through UV-visible spectrometry and high performance liquid chromatography. **M. Tarrance**, A. Pons-Aguade, K.W. Barnes
14--Induction of viable but nonculturable *Campylobacter jejuni* in various stress conditions. **P. Longchamps**, K. Wang, X. Lu
15--Evaluating the efficacy of smoke-water towards ripening of banana *(Musa paradisiaca)*. **R. Khursheed**, S. Baba
16--Phytoremediation of toxic heavy metals from soils using sunflowers *(Helianthus annuus)*, ferns *(Nephrolepis biserrata)* and mustard greens *(Brassica juncea)*. **S. Bergeron**, D. Wayment
17--Bang for your bark: Comparative analysis of dog food by ICP-OES, mycotoxin testing, and SPME-GC-MS. **V.R. Costilow**
18--Changes in selected odorants in basil during growth and development. **W. Yang**, K.R. Cadwallader, K. Martin
19--Case study using California olive pomace for potential valorization strategy of olive oil industry by-products by the application in avocado oil based cosmetics. **Y. Cho**, H. Zhao, S. Wang
--Reevaluation of Ferrozine assay for rapid testing iron(II) chelation ability of phenolics in mole ratio: Case study by evaluating chelation of chemical standards of olive phenolics. **A. Mangubat**
--Development of a PCR assay for foodborne pathogens from soil. **L. Speaks**, N. Neff, I. Grabylnikov, K.M. Elkins
--Chemical composition of elderberry extract and its inhibitory effect on SARS-CoV-2 spike protein and

ACE2 binding, and radical scavenging properties. **M. Zeng**, Y. Li, U. Choe, L. Yu
--Maintenance of a kombucha starter preparation. **J. Scalia**, B. Watson, L. Stains, J.N. Richardson, J. Kegerreis
--Microbial transglutaminase improves the texture of surimi-like gels made with protein recovered from catfish by-products. **Y. Zhang**, S.K. Chang
--Recovery of fat from waste ice cream by destabilizing the emulsion using ethyl alcohol. **C. Lee**, R. Garcia, L. Bumanlag, C. Liang
--Stormwater runoff chemical contaminants and their effects on urban areas. **Y. Ahmadibeni**, S. Guha, Q. Hardy
--Phytochemical development over the ripening process of *Aronia mitschurinii*, elderberries, mulberries and haskap fruits. **E. Cable**, B. Green, D.G. Sauder, A.G. Ristvey, V. Volkis
--Effect of copper complexation on the chemical stability of beer. **M. Vincent**, A. Silakov, R. Elias
--Antifungal constituents from the fungus *Westerdykella multispora* against anthracnose disease of strawberries. **P. Tamang**, K. Meepagala
--Immunological characterization of peanut flour fermented with *Rhizopus oryzae*. **C.P. Mattison**, R. Dupre, K. Clermont, J. Yu
--Metabolism of condensed tannin by manganese peroxidase. **J. McLain**, A.E. Hagerman
--Computer-aided design and syntheses of novel flavanone derivatives for use as potential inhibitors of COVID-19 proteases. **A. Sigmon**, N. Yennawar, H. Yennawar, E. Margulis, H. Al Quaid
--Polyphenols in plant foods and their bioavailability. **Y. Zuo**, C. Wang, N. Ahmad, Y. Deng
--Fingerprinting of varietal honeys using nuclear magnetic resonance spectroscopy. **C.D. Emal**, G. Wilmes, M. Goodrich
--Comprehensive analysis of aromatic compounds in milk using GC-MS, SPME Arrow and Smart Aroma Database. **Y. Takemori**, M. Matsumoto
--Prebiotic potential of water-soluble non-starch polysaccharides from Barnyard millet grain. **S. Maji**, S. Dey
--Thermal stability of yeast alcohol dehydrogenase in the undergraduate teaching lab. K. Williams, A. Bates, **A.E. Hagerman**
--Zein nanoparticles coated with various types of tannin. J. Jefferson, S. Mallikarachchi, **A.E. Hagerman**
--Processing and characterization of biodegradable mulch films made of potato thermoplastic starch. **J. Staker**, K. Collier, R. Singh, A. Tovar, A. Siegel
--Probing the ripeness of berries rich by anthocyanin for food and nutraceutical markets with ripeness gauge. **R. Buzzetto More**, E. Cable, A.G. Ristvey, V. Volkis
--Development of starch based carriers for controlled release of Urea-ZnO nanoparticles. J.D. Palomino, L.T. Sanchez, **C.C. Villa**, A.F. Cañon-Ibarra
--Reducing the shrinkage and warpage of 3D-printed thermoplastic starch parts by freezing. **K. Collier**, J. Staker, R. Singh, E. Collier, A. Ansar, A. Siegel, A. Tovar
--Fast determination of total unbound fat in snack foods using a new fully automated parallel extraction system. **H. Yang**
--Evaluation of double stack sausages packaging. **D. Patterson**, K. Vorst
--Using Raman spectroscopy for non-destructive evaluation of carotenoids in *Cucumis melo* at different maturity stages. **G. Sah**, N. Goff, J. Singh, D. Kurouski, B.S. Patil
--Evolution of volatile flavor compounds produced during the fermentation of beer with genetically different yeast. **D. Roberts**, E.M. Diaz-Aceituno, J.M. Garcia, K.H. Moore, A.V. Lo Presti, V. Tirado, S.A. Morton, S. Harper, C.A. Hughey
--Natural products magnetic resonance database (NP-MRD): Comprehensive database and repository for natural products NMR data. **J.R. Cort**, A. Jystad, N. Govind, E. Knutson, V.Sullivan, L. Stillwell, M. Schutz, A. Maras, E. Poynton, P. Tavangar, v. yang, J.A. Van Santen, M. Pin, T. Jordan, J. Kim, B. Ledingham, R.G. Linington, R. Ghosh, S. Sarma, J. Koller, L.W. Sumner, Z. Sayeeda, Z. Budinski, A. Guo, B.L. Lee, M. Berjanskii, M. Rout, H. Peters, R. Dizon, R. Ma, E. Oler, D. Allen, X. Cao, V. Gautam, D.S. Wishart
--Quantifying estrone and β-estriol conjugates in dairy cattle manure and urine using sorptive stir Bar extraction and gas chromatography-mass spectrometry. **S. Ahmed**, S. Antle, J. Loughrin, E.D. Conte
--Lateral flow assay: Development of magneto-plasmonic nanosensors for the detection of E.coli O157:H7. **S. Santra**, N. Panchal, V. Jain, R. Elliott, Z. Flint, P. Worsley, C. Duran, T. Banerjee
--Influence of lutein content of marigold flowers on functional characteristics of baked flour products. **A. Anderson**
--Impact of ethanol and methanol on the betalains extraction of beetroot (Beta vulgaris Cv. Pablo). **A. Sani Ali**, W. Hayes, A. Tas, B. Onarinde

MONDAY MORNING March 27
Crown Plaza Downtown Union Square Penn Station B/C
Functional Ingredients in Food Processing
W. Dixon, Z. Li, X. Wu, *Organizers, Presiding*
Synopsis: This symposium provides the latest studies highlighting innovative functional ingredients used in food processing and how to use functional ingredients to produce safe, functional foods that offer an array of health benefits.
8:00 Introductory Remarks.
8:10 . Structural characterization of cocoa proanthocyanidins using three LCMS-based methods. **S. Navare**, B. Lam, M. Kwasniewski, R. Anantheswaran, J. Lambert

8:25 . Complexation of bark proanthocyanidins isolated from Western red cedar (*Thuja plicata* Donn) and food carbohydrates enhances colloidal stability. **G.M. Bautista**, S.E. Mhatre, O.J. Rojas
8:40 . Primary extraction methods of R-Phycoerythrin from dry biomass of marine macroalgae *Gracilaria corticata*. **V. Saraswat**, K. Raghavarao, V. Mantri
8:55 . Process intensification and integration for efficient downstream processing of bioactives from micro and macroalgae. **K. Raghavarao**
9:10 . Polysaccharide-based self-assembled smart hydrogel for *in vitro* delivery of co encapsulated probiotics and folic acid. **N. Srivastava**, A. Roy Choudhury
9:25 Intermission.
9:40 . Enzymatic hydrolysis of *makapuno* for production of potential prebiotics. A.A. Yanos, L. Go-Albia, **S.B. Arreola**, D. Haltrich, T. Nguyen
9:55 . Mechanism in improving solubility of pea protein isolates by high intensity ultrasound. **K. Gao**
10:10 . Potential of *Arachis hypogaea* testa as a functional food ingredient for the treatment of depression. **A. Patterson**, R. Donaldson, D. Davis, M. McKoy, W. Gallimore
10:25 . Effect of oat β-glucan on gut metabolism and health. **J. Bai**, L. Wang, L. Huang

Crown Plaza Downtown Union Sq. Grand Cent. Sta B
Agri-Food Sustainability at a Crossroads: Challenges of the Food, Energy, and Water Nexus Cospons AGRO M. Appell, L. Chen, V. Craver, Y. Tseng, *Organizers, Presiding*
Synopsis This symposium covers the merits and limitations of sustainability and green tech solutions in the Food/Energy/Water nexus.
8:00 Introductory Remarks.
8:05 . Complete analysis of the cashew nut (*Anacardium occidentale* L.) production and processing with later recovery of anacardic acid from vegetal residues. **R.A. Gómez Rodríguez**
8:35 . Grape marc as a potential feed additive to reduce enteric methane production in dairy cattle: Part I chemical composition analysis. **H. Zhao**, E. Kebreab, S. Wang
9:05 . Biodegradable polymer nanocomposites for controlled P release and nanocellulose hydrogels for efficient delivery of NPK fertilizers. **S. Vaidya**, L.R. Sigmon, C. Thrasher, S. Phillips, M.S. Peresin, C. Dimkpa, H. Fairbrother, J.C. White
9:35 Intermission.
9:50 . Foliar delivery of siRNA particles for treating viral infections in agricultural grapevines. **A. Avital**, A. Schroeder
10:20 . Use of bioconjugation and encapsulation approaches for delivery of cargo for agricultural applications. s. Dodard, Y. Liu, J. Lavertu, A. Parrott, S. Clark, **U. Hemraz**
10:50 . Nanobiotechnology-based strategies for enhanced crop stress resilience. **J.C. White**, L. Zhao, A.A. Keller, J.L. Gardea-Torresdey
11:20 Panel Discussion.

Virtual Session Section A Citrus Flavor in the Omics Era A.Plotto, Y. Wang, *Organizers, Presiding*
Synopsis: This symposium covers omics approaches used in the studies of citrus flavor (e.g., biosynthesis and metabolism of flavor compounds, quality assessment, pre- and post-harvest effects etc.). Omics technologies - metabolomics, proteomics, transcriptomics, genomics, metagenomics and/or their combinations (foodomics, nutriomics, flavoromics and sensomics) are powerful tools for these purposes. Rapid and accurate analyses of these components at different biological scales (metabolites, proteins, transcripts and genes) is critical to assess the quality of the products as well as to understand their biochemical mechanisms.
10:00 Introductory remarks.
10:05 . Identification of volatile sulfur compounds as key off-flavors in mandarin juice during processing and storage. **L. Huang**, Y. Cheng, R.L. Rouseff, H. Wu, H. Wang
10:25 . Five-year study of flavor and sensory evaluation of HLB-tolerant citrus hybrids. **K.A. Jeffries**, Z. Fan, X. Sun, E. Baldwin, J. Manthey, W. Zhao, E. Stover, M. Mattia, J. Bai, A. Plotto
10:45 . Evaluation of volatile profiles in *Poncirus trifoliata*-containing HLB-tolerant citrus hybrids. **Z. Fan**, K.A. Jeffries, X. Sun, E. Baldwin, J. Manthey, W. Zhao, G. Olmedo, E. Stover, M. Mattia, A. Plotto, J. Bai
11:05 . Effect of different rootstocks on metabolites of orange juices from HLB-affected trees. **X. Liu**, Y. Wang
11:25 Intermission.
11:40 . Natural sweeteners and sweetness-enhancing compounds identified in citrus using an efficient metabolomics-based screening strategy. **X. Tang**, Z. Wang, F.G. Gmitter, J.W. Grosser, Y. Wang
12:00 . Omics and sensorial analysis combinedly revealed characteristic aroma and consumer preference of novel citrus. Z. Hu, M. Chen, K. Zhu, Y. Liu, M. Chen, J. Kong, L. Cao, J. Ye, H. Zhang, X. Deng, **J. Chen**, J. Xu
12:20 . Using genome-wide association as a breeding tool for healthful flavonoids in mandarin accessions. **M. Mattia**, D. Du, Q. Yu, T.L. Kahn, M.L. Roose, Y. Hiraoka, Y. Wang, P.R. Munoz, F.G. Gmitter

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MONDAY AFTERNOON
Crown Plaza Downtown Union Sq. Penn Station B/C
Recent Advances in Analytical Strategies for Food Allergen Detection and Management
C. P. Mattison, Q. Rao, *Organizers, Presiding*

Synopsis: This symposium covers recent developments in detecting and managing food allergens and discusses analytical considerations for quantifying food allergens, global development trends, and the future availability of these technologies. Food allergies represent a significant and growing public health concern. Consumers with allergies must avoid foods containing allergens to prevent potentially fatal health consequences. Currently, the only widely accepted prevention method is complete avoidance of allergen-containing foods. Present analytical methods can be useful, but specific and sensitive detection of food allergens is often hindered by the effects of various treatment processes and food matrices on trace amounts of allergens.
2:00 Introductory remarks.
2:10 . Recommendations from the FAO/WHO expert consultation on food allergen risk assessment. **L. Jackson**
2:30 . Measurement challenges of quantifying milk protein allergens in foods. **D. Bunk**, A. Green, L. Kilpatrick, M.M. Phillips
2:50 . Mass spectrometric analysis of allergens from pecan protein extracts: Influence of pecan heating on observable peptides and modifications. **R. Dupre**, S. Patil, S.W. Lloyd, C.C. Grimm, B. Smith, C.P. Mattison
3:10 . Detection of finfish residues on contact surfaces by enzyme-linked immunosorbent assay. **X. Jiang**, Q. Rao
3:30 . Allergen Testing: How much is too much?. **G. Velasco Lopez**
3:50 Concluding Remarks.

Crown Plaza Downtown Union Sq. Grand Central Sta B
Agri-Food Sustainability at a Crossroads: Challenges of the Food, Energy, and Water Nexus Cospons AGRO M. Appell, L. Chen, V. Craver, Y. Tseng, *Organizers, Presiding*
2:00 Introductory Remarks.
2:05 . Date palm biochar and super hydrophobic sand mulching enhance tomato (*Solanum lycopersicum*) plants' yields in alkaline sandy soils. **N. Huve Musskopf**, K. Odokonyero, L. Oki Exposito, B. Albar, A. Gallo, H. Mishra
2:35 . Engineering cation exchange capacity of date palm biochar towards a sustainable soil amendment technology. **B. Albar**, N. Huve Musskopf, A. Gallo, H. Mishra
3:05 . Effect of biochar and superhydrophobic sand mulches on evaporation and water holding capacity in sandy soils. **L. Oki Exposito**, A.H. Al-Zu'bi, B. Albar, N. Huve Musskopf, A. Gallo, H. Mishra
3:35 Intermission.
3:50 . HPLC-UV determination of glyphosate, aminomethylphosphonic acid, and glufosinate using pre-column derivatization. **P.J. Martin**, K. He, L. Blaney, S.R. Hobbs
4:20 . Effects of superhydrophobic sand mulches on steady-state water evaporation fluxes. **A.H. Al-Zu'bi**, L. Oki Exposito, J. Zheng, A. Gallo, H. Mishra
4:50 Panel Discussion.

Virtual Session AGFD General Poster Session and Undergraduate Poster Competition
J. Beauchamp, K. Deibler, J. W. Soares, *Organizers*
12:00 . Screening and remodeling of enone oxidoreductase for high production of 2(or 5)-ethyl 5(or 2)-methyl-4-hydroxy-3(2H)-furanone in *Saccharomyces cerevisiae*. **X. Fu**, K. Hong, C. Zhang, W. Lu
12:00 . Effect and mechanism of *Citrus depressa* Hayata peel extract against acetaminophen induced liver injury in mice. **Z. Su**, P. Tsai, G. Wei, X. Chen
12:00 . Methodologies and strategic studies to estimation methods to reduce carbon emissions on climate change. E.J. Parish, **H. Honda**, S. Lee, G. Ren, W. Wang
12:00 . Polyphenolic antioxidants as inhibitors of the advanced glycation endproducts. **M. Atty**, J. Mehta, A. Vadapalli, Z. Afrasiabi, P. Reddy
12:00 . Capsaicin attenuates oleic acid-induced lipid accumulation via the regulation of circadian clock genes in HepG2 cells. **R. Li**, M. Lu, C. Ho
12:00 . Effects of moringa isothiocyanate-rich seed extract on muscle atrophy in C2C12 cells. **R. Farias-Pereira**, M. Ahmed, W. Bui, K. Thirunavukkarasu, I. Raskin
12:00 . Investigating secondary metabolites produced by a beneficial root endophyte for improving Canadian Prairie field crops. **K. Gill**

Innovative Technologies to Support 21st Century Agriculture Spons AGRO, Cospons AGFD, BIOT
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Advancing Agrochemical Regulation, Education, & Public Policy in an Age of Skepticism & Scientific Illiteracy Spons AGRO, Cospons AGFD, CHED, ENVR
Midwest Row Crop Revolution: Agrochemistry State of Affairs After a Quarter-Century of Biotech-Enabled Agriculture
Spons AGRO, Cospons AGFD, BIOT, ENVR

MONDAY EVENING 8:00pm Conv Ctr Hall F-H
AGFD Sci-Mix (note - see first 19 posters listed under SUNDAY EVENING AGFD General Poster Session and Undergraduate Poster Competition

TUESDAY MORNING March 28
Crown Plaza Downtown Union Sq Penn Station B/C
Biomarkers of Food or Drug Intake: Chemistry at the Intersection of Human Health Applications
J. Beauchamp, Y. Pham, *Organizers, Presiding*
Synopsis: This symposium explores biomarkers in non-invasive screening applications (e.g., breathalyzer tests to determine alcohol intake or the hydrogen breath test to diagnose lactase deficiency) relating to food intake and tolerance, and the pharmacokinetics of prescribed and recreational drug use. It covers novel approaches to

biomarker detection to identify foods, drugs and their metabolites in urine, feces and breath, with the goal of establishing non-invasive screening procedures or diagnostics.
8:00 Introductory remarks.
8:05 . GC saves lives! Determination of short chain fatty acids (SCFA) in human fecal samples. **L.N. Polite**, N.L. Polite, M.M. Freeman, A. Sandhu
8:25 . Effect of wholegrain particle size on breath metabolites in type 2 diabetes and normoglycaemia. C. Robinson, T. Perry, L. Te Morenga, J. Haszard, J. Mann, P. Silcock, **G. Eyres**
8:45 . Novel and efficient UHPLC/MS/MS method for assessing glucoraphanin and sulforaphane bioavailability in biological samples. W. Zhu, L.A. Lerno, E. Cremonini, P. Oteiza, A. Mastaloudis, G. Bornhorst, **A.E. Mitchell**
9:05 . Phytocannabinoids' therapeutic effects on endometriosis. **T. Melville**
9:25 . Coffee biomarker candidates – structures of conjugated atractyligenin metabolites. **R. Lang**, C. Czech, A. Beusch, S. Dirndorfer
9:45 . Biomarker detection using GC-ion mobility spectrometry. **W. Vautz**, C. Hariharan, S. Liedtke
10:05 Intermission.
10:20 . Methanol detection in exhaled breath, drinks and sanitizers with a handheld device. **A. Guentner**
10:40 . Use of exogenous compounds for monitoring human metabolic processes. F. Lochmann, F. Weiss, V. Stock, **V. Ruzsanyi**, C.A. Mayhew
11:00 . Washout of terpenes in breath following ingestion of a peppermint oil supplement. **Y. Pham**, R. Yu, J. Beauchamp
11:20 . Using exhaled nitric oxide to evaluate and quantify regional airway response to inhaled medications. J. Saunders, C. Clem, Y. Zhao, B. Gaston, **M. Davis**

Crown Plaza Downtown Union Sq Grand Central Stat B
General Papers
J. Beauchamp, J. W. Soares, *Organizers, Presiding*
Synopsis: This session is a platform for scientific discoveries and innovative developments in agricultural and food chemistry. The session spans the entire field of AGFD on topics not covered in the featured AGFD symposia.
8:00 Introductory remarks.
8:05 . Rapid identification of foodborne bacteria using single-cell Raman spectroscopic analysis combined with a conditional generative adversarial network. **K. Wang**, X. Ma, X. Lu
8:25 . Natural colorants in plant-based foods: Impact of colorant and droplet characteristics on optical properties of oil-in-water emulsions. **D. Wannasin**, D. McClements
8:45 . Detoxification of lipid peroxidation aldehyde, 4-hydroxynonenal, by flavonoids in apple and grapefruit. **R. Djorgbenoo**, Y. Zhu, W. Wang, S. Sang
9:05 . Phytochemical characterization of aronia, elderberries, hascaps, and mulberries: New generation of super fruits. A.G. Ristvey, **V. Volkis**
9:25 . Anti-proliferative properties of biologically active compounds extracted from bio-waste materials. M. Olkiewicz, A. Bajek, M. Maj, J. Montornes, **B. Tylkowski**
9:45 Intermission.
10:00 . Influence of chemical structure on the color, molar absorptivity, and stability of naturally derived pyranoanthocyanin pigments. **D.M. Voss**, G. Miyagusuku-Cruzado, L. Xun, M. Giusti
10:20 . Structural and compositional changes in the cell walls of cool-season pasture grasses for two growing seasons. **S. Newhuis**, M. Kunes-Agbana, B. Angeletti, H. Buecker, B. Harlow, I. Kagan, M. Flythe, R.R. Schendel
10:40 . Look at the residues not the emissions to understand chemical changes in waterpipe tobaccos during heating. **J.H. Lauterbach**
11:00 . Synthesis and characterization of 2-D Molybdenum-MOF/MXenes composite and their applications in sensing food contaminants. **G. Kaur**, S. Sharma, A. Deep
11:20 . Colorimetric assay of bacterial pathogens based on Co3O4 magnetic nanozymes conjugated with specific fusion phage proteins and magnetophoretic chromatography. **L. Pei**, L. Aihua

Virtual Session Agri-Food Sustainability at a Crossroads: Challenges of the Food, Energy, and Water Nexus Cospons AGRO M. Appell, L. Chen, V. Craver, Y. Tseng, *Organizers, Presiding*
10:00 Introductory Remarks.
10:05 . Microwave-induced specific aggregation behavior myofibrillar proteins. **X. Jiao**, D. Fan
10:35 . Plant nutrient delivery system for the enhancement of plant growth using an advanced coating on *Zea mays* seeds using modified hydroxyapatite nanoparticles. **L. Abeywardana**, C. Sandaruwan, S. Chathurika, V. Karunaratne, N. Kottegoda
11:05 . Using protein microgels as emulsion stabilizer, texture modifier, and bio-lubricant for designing fat-reduced food products. **Y. Chu**, L. Chen
11:35 . Impact of environmental change on the food water energy nexus: Can altering our diets help protect the global environment?. **J.W. Finley**
12:05 Panel Discussion.

Biomarkers of Food or Drug Intake: Chemistry at the Intersection of Human Health Applications
Cospons AGFD
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Midwest Row Crop Revolution: Agrochemistry State of Affairs After a Quarter-Century of Biotech-Enabled Agriculture
Spons AGRO, Cospons AGFD, BIOT, ENVR

TUESDAY AFTERNOON
Crown Plaza Downtown Union Sq Grand Central Stat B
Advances in Food Packaging and Preservation

M. Sarker, T. Yang, *Organizers, Presiding*
Synopsis: This symposium covers multidisciplinary aspects of packaging materials (e.g., films or coatings) and their applications to ensure the safe use of foods and improve the quality of foods. Packaging techniques include nanotechnology enabled, biopolymer-based, active, and intelligent packaging. Food/packaging material interactions are explored (e.g migration of substances from packaging to foods and its impacts on food safety and human health). This symposium provides information and innovative ideas regarding recently developed packaging techniques and their implications on food preservation.
2:00 Introductory Remarks.
2:05 . PHB/PLA/modified cellulose films, as packaging for chocolate and tropical fruits. **C.A. Sierra**, L. Bello-Rocha, V. Perez-Martinez, D. Castellanos, C. Zuluaga, O. Rodriguez, P. Yustres
2:40 . Development of bacteriophage added coating material to reduce *Escherichia coli* O157:H7 contamination in mushroom. **E. Evran**, E.K. Tayyarcan, I. Boyaci
3:15 . Sustainable ultra-high performance liquid chromatography method for analysis of carotenoids using GRAS solvents. **J. Singh, B.S. Patil**
3:50 Intermission.
4:10 . Photoactive films made from curcumin dopped ZnO nanoparticles and alginate. **C.C. Villa**, L.T. Sanchez, A.F. Cañon-Ibarra, J.A. Arboleda-Murillo
4:45 . Effect of gamma irradiation on vitamin D content in high fat finfish. **J.S. Brown**, P. Calvo, P. Julakanti, A. Khan, F. Mohiuddin
5:20 . Microbial valorization of industrial organic waste to biodegradable smart food packaging materials. **L. Jayakody**, L. Dissanayake, S. Kayastha, S. Jayasekara, B. Kolitha
5:55 Concluding Remarks.

Crown Plaza Downtown Union Sq Penn Station B/C
Chemistry of Alcoholic Beverages
N. O. Flynn, *Organizer, Presiding*
Synopsis: The global alcoholic beverage market share is valued at >1.5 trillion dollars presenting many opportunities for research and development. This symposium presents the latest research on the chemistry of alcoholic beverages.
2:00 . Introduction: Chemistry of alcoholic beverages. **N.O. Flynn**
2:10 . Effect of filtration and inclusion methods on rapid rapid wort analysis of malts. **N.O. Flynn**
2:30 . 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, K. Kingsbury, A. Brehm, **R.A. Quinlan**
2:50 . Dry hopping protocol has a limited influence on the chemical and sensory properties of India pale ale (IPA) beers. **B. Lam**, S.G. Ziegler, A.J. Ledley, S. Santan, H. Hopfer, J. Lambert
3:10 . Developing and analyzing the chemical fingerprint for popular whiskeys sold in the US. M. Hernandez, **J. Nevins**
3:30 . Required education and understanding in chemical kinetics, thermodynamics and sensory evaluation for distillers. **G. Spedding**
3:50 Intermission
4:00 . Investigation of the volatile composition of apple ciders from dessert apple cultivars with and without skin contact during fermentation using a metabolomics-based approach. **Y. Lin**, M. Warmund, M. Kwasniewski
4:20 . Chemical characterization and sensory evaluation of wine formulated with African black olive (*Canarium schweinfurthii* Engl) fruits. **O. Francis**, J. Okullo, S. Natukunda, R. Komakech, J. Agea
4:40 . Application of spectroscopy for quality screening in the production of pisco distillate. **Y. Wu**, L. Rodriguez-Saona
5:00 . Determination of key odorants in Chardonnay marc skins. **S. Warner**, J.P. Munafo
5:20 . Quantitative errors and analytical method improvement of volatile sulfur-containing compounds in Chinese Baijiu. **Z. He**, D. Zhao, J. Zheng, M.C. Qian
5:40 . Sensitive volatile phenol analysis in Chinese Baijiu using direct injection-on-line trapping coupled with gas chromatography-tandem mass spectrometry (LVI-Ttrap-GC-MS/MS). **K. Yang**, Z. He, J. Zheng, Z. Liu, D. Zhao, M.C. Qian

Virtual Session Panel Discussion: The Road to Successful Publishing
B. D. Guthrie, C. Osorio Roa, V. Somoza, *Organizers* J. Beauchamp, L. Yu, *Organizers, Presiding*
Synopsis: A discussion with editors from the division's flagship journal, Journal of Agriculture and Food Chemistry, ACS Food Science & Technology and ACS Agricultural Science & Technology. The editors present the current state of the journals and give tips for successful manuscript acceptance. The audience can submit questions during Q&A.
3:00 Introductory Remarks.
3:10 . Overview of ACS AGFD journals: Compare & contrast. **T. Hofmann**
3:20 . Editors' expectations for quality paper submissions. **V. Somoza**
3:30 Panel Discussion.
4:00 . Crash course in peer-review publishing. **J. Beauchamp**
4:10 . Case studies of acceptance/rejection of peer-reviewed publications. **F. Tomas-Barberan**
4:20 . Tips for successfully writing scientific research papers. **C. Osorio Roa**
4:30 Panel Discussion.

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WEDNESDAY MORNING March 29
Crown Plaza Downtown Union Sq Penn Station B/C
Advances in Food Packaging and Preservation
M. Sarker, *Organizer*, T. Yang, *Organizer, Presiding*, L. Jayakody, *Presiding*
8:00 Introductory Remarks.
8:05 . Effectiveness of bacteriophage-loaded edible coatings to control foodborne pathogens on fresh-cut apples. **E.K. Tayyarcan**, E. Evran, I. Boyaci
8:40 . Reusable and daylight induced antibacterial ethylene-vinyl acetate copolymer films. S.U. Islam, **G. Sun**, Z. Zhang
9:15 Intermission.
9:35 . Anthocyanin-based food packaging for monitoring the freshness of fresh cut fruits and vegetables. **P. Das**, P. Kalyani, M. Khandelwal
10:10 . Structure and properties of flexible starch-based double network composite films induced by dopamine self-polymerization. **H. Xu**, L. Chen, Z. Jin
10:45 Concluding Remarks.

Crown Plaza Downtown Union Sq Grand Central Stat B
General Papers
J. Beauchamp, J. W. Soares, *Organizers, Presiding*
8:00 Introductory remarks.
8:05 . Non-targeted identification of botanical origin markers for honeys. **L. Tian**, S. Bilamjian, T. Anumol, D. Cuthbertson, S. Bayen
8:25 . Water soluble vitamin analysis in feed using mass spectroscopy detection. **D.E. Clinton**, H.D. Inerowicz
8:45 . Inhibiting ice recrystallization with corn cob hemicelluloses. **M.W. Reeder**, T. Wu
9:05 . Proteolytic treatment of waste dairy ice cream to accelerate butterfat separation. **C. Liang**, R. Garcia, B. Plumier, C. Lee, F. Huynh, J. Uknalis
9:25 . Profiling the non-starch polysaccharides of hempseed cell walls. **M.K. Agbana**, B. Harlow, M. Bunzel, M. Flythe, R.R. Schendel
9:45 Intermission.
10:00 . Thermo-chemical decarboxylation kinetics study for cannabinoid acids in hemp (*Cannabis sativa* L.) by pressurized liquid system. **U. Urvashi**, J. Hatfield, S. Park, C.A. Kinney, J. Han, K. Olejar
10:20 . Bioprocess development to produce xylitol by *Escherichia coli* K12 from hemicellulosic hydrolysates. **R. Turner**, M. Racine, D. Demirjian
10:40 . Novel drug-delivery approach against infectious disease by using ovotransferrin nanoparticles. **H. Ibrahim**
11:00 . Longan pulp polysaccharides regulate gut microbiota and metabolites to protect intestinal epithelial barrier. **Y. Bai**

Virtual Session Before the Coffee Break: The Rich and Complex Chemistry of Coffee
J. Beauchamp, N. Buck, *Organizers, Presiding*
Synopsis: This symposium showcases the latest coffee-related chemistry, from bean to brew. Join us in enjoying some coffee chemistry before heading to the coffee break to savor the beloved brew first-hand. Studies explore different cultivars, examine cherry processing steps, beans undergoing all manner of roasting conditions, modes of brewing, and sensory impressions during consumption.
10:00 Introductory remarks.
10:05 . The physical chemistry of coffee brewing. **J. Melrose**
10:25 . Proton transfer reaction mass spectrometry analysis of coffee flavour compounds: A long story open to innovation. **F. Biasiol**
10:45 . It's all in the brew: How extraction parameters influence the aroma composition during espresso coffee brewing. **N. Buck**, A. Stenzel, J. Beauchamp
11:05 . Exploring unique coffee flavours of fermented high-end specialty coffee: Towards the fourth wave coffee. A. El Khouri, **S. Smrke**, S. Opitz, A. Mistretta, C. Yeretzian
11:25 . Sensory impact and changes in the volatile profiles of special coffees obtained by dry and wet processes. **W. da Silva Oliveira**, N. Buck, J. Beauchamp, C. Arcanjo, A. de Oliveira Garcia
11:45 Intermission.
12:00 . Chemistry and analysis of chlorogenic acids from coffee. **N. Kuhnert**
12:20 . Neglected coffee chlorogenic acids: *p*-coumaroyl-, sinapoyl- and di-acyl-quinic acid isomers in different coffee botanical species. **L. Navarini**, S. Colomban
12:40 . Anti-obesity and anti-aging effects of coffee components. **Y. Park**, R. Farias-Pereira, J Cho
1:00 . NMR-spectroscopic applications to control coffee authenticity. **V. Gottstein**, D.W. Lachenmeier, T. Kuballa, M. Bunzel

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NSF Funded Materials Innovation Platforms - MIP Overviews & Research Examples
Spons CELL, Cospons AGFD Westin Hotel
8:00-8:30 Rountable and Intro
8:35 NSF BioPACIFIC MIP J. Read De Alaniz
8:55 Degradable Polymers H. Maynard
9:10 Sequence controlled peptoids F. Kafer
9:25 Development & application of high input synthesis C. Hawher
9:40 PARADIM T. McQueen
10:20 Glycol MIP M. Roman
10:40 Carbohydrate-polymer conjugate synthesis C. Callman
10:55 Interaction of human Galectin-3 w/glycosaminoglycans T. Dam
11:10 Polysaccharide H2S donors A. Chinn
11:25 2D crystal consortium materials innovation platform J. Redwing

WEDNESDAY AFTERNOON
Crown Plaza Downtown Union Sq Penn Station B/C

Before the Coffee Break: The Rich and Complex Chemistry of Coffee
J. Beauchamp, N. Buck, *Organizers, Presiding*
2:00 Introductory remarks.
2:05 . Chemistry in your cup: Chemical characteristics of cold brew coffee. **N.Z. Rao**, E. Schwarzmann, M.P. Washington, M.D. Grim, M. Fuller
2:25 . Espresso bitterness and acidity: Influence of process parameters temperature, flow and coffee grind on non-volatile components. **B. Schmieder**, N. Buck, V. Pannusch, M. Minceva
2:45 . Multidimensional gas chromatography approach to elicit the odour-structure activity of chiral 2-methyltetrahydrothiophen-3-one in coffee. A. Pua, Y. Huang, V. Goh, L. Li, **M. Cornuz**, B. Lassabliere, L. Jublot, B. Yu
3:05 . NMR and sensory studies on interactions between odorants and melanoidins in coffee beverages. **M. Gigl**, T. Hofmann, O. Frank
3:25 . Electrochemical assessment of coffee qualities. **C.H.Hendon, R.Bumbaugh**
3:45 Intermission
4:00 . Using microwave energy for the rapid hydrolysis of coffee for amino acid profiling. **A.D. Douglas**, B. Liu, M. Swasy, C. Cashma
4:20 . Green chemical synthesis of various nanoparticle species using spent coffee grounds. **B.G. Yust**, N.Z. Rao, E. Schwarzmann
4:40 . Potential of near infrared spectroscopy and machine learning to predict volatile changes during coffee roasting. **B. Kebede**, S. Green, J. Sim
5:00 . Investigating the flavor of natural (dry process) coffee. M.R. Fernández-Alduenda, **P. Silcock**

Virtual Session Panel Discussion: Career Paths in Academia, Government and Industry
B. D. Guthrie, *Organizer* J. Beauchamp, A. E. Mitchell, *Organizers, Presiding*
Synopsis: A panel comprising senior scientists from industry, academia, and government will give a brief overview of their career journeys. The audience can submit questions in Q&A session. This is the second in a series as the first was well attended and enjoyed, especially by young chemists
3:00 Introductory remarks.
3:10 . Academia panelist biography - Keith Cadwallader, University of Illinois. **K.R. Cadwallader**
3:20 . Government panelist biography - Michael Appell, USDA. **M. Appell**
3:30 . Industry panelist biography: Mathias Sucan, Herbalife Nutrition Ltd.. **M. Sucan**
3:40 Discussion panel.
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THURSDAY MORNING March 30
Virtual Session General Papers
J. Beauchamp, J. W. Soares, *Organizers, Presiding*
10:00 . Bioactive phenolic compounds profiling of prairie berries. **C. Kodikara**, N. Bandara, T. Netticadan, S. Srinivas, C. Wijekoon
10:20 . Characterization of Cumberland rosemary, *Conradina verticillata,* essential oil. **C. Gorman**, J.P. Munafo
10:40 . Saltiness enhancement through the synergism of pyroglutamyl peptide mixtures. **O. Sahni**, J.P. Munafo
11:00 . Investigating the biodegradability of eco-friendly straws in prospective disposal environments. **A. Ali**, R.M. Santos, E. Chiang
11:20 . Myoglobin post-translational modifications in high- and normal-pH beef. **R. Ramanathan**, S. Suman, F. Kiyimba, S. Li, J. Chen, G. Mafi
11:40 . Development and validation of a food frequency questionnaire for adults in Fiji to estimate nitrate and nitrite intake. **A.A. Chetty**, J.J. Lal, S. Prasad
12:00 . *In silico, in vitro,* and *ex vivo* assessment to evaluate the antihyperglycemic, antioxidant and cytotoxic activity of *Carica papaya* L. leaf extract. **P. Prabhakar**
12:20 . Organophosphate esters in UK diet: Exposure and risk assessment. **G.R. Muideen**, S. Harrad, A. Mohamed
12:40 . Global GAP and harmonized MRL facilitating international trade study case. **D. Cerqueira**, J. Barnekow, C. Tiu
1:00 . Role of food science in forensic science. **A. Rajani**, **P.Y. Dave**
1:20 . Highly sensitive SERS-based tool made of gold nanosphere coated glass Petri dish for rapid detection of indole in shrimps and determination of freshness. A. DAS, **I. Terry**, H. Guo
1:40 . Classification of seaweeds based on tannin composition using differential sensing. **D. Garcia**, E. Yu, S. Kim, J. Richardson, M. Ledesma, M. Tran, D. Zamora-Olivares

AGFD ABSTRACTS

SUNDAY EVENING March 26 7:00 – 9:00 pm
AGFD General Poster Session and Undergraduate Poster Competition (note-first 19 posters listed below also presented at Monday Evening Sci-Mix)

01--Comparison of the amino acid metabolism of genetically different brewing yeasts Amanda R. Cicali[1], cicaliar@dukes.jmu.edu, Eliana M. Diaz-Aceituno[1], Samuel A. Morton[2], Steven Harper[2], Chrisi A. Hughey[1]. (1) Chemistry & Biochemistry, James Madison Univ., Harrisonburg, Virginia (2) Engineering, James Madison Univ., Harrisonburg, Virginia The selection of malt, hops, and yeast affects the quality and flavor of the final beer. Here a pale ale was brewed with a 2-row Briess malt and Cascade hops. The wort was transferred to five fermentation tanks and fermented with the following genetically different yeast: Belgian Saison, California ale, Czech pilsner lager, English ale, and Sake extreme fermentation. The aim of the work was to monitor amino acid metabolism during fermentation. Amino acids are extracted from the malt during mashing and utilized by the yeast to produce flavor compounds in various biochemical pathways, such as the Ehrlich pathway. In this pathway, amino acids are converted to a keto-acid via transamination. Decarboxylation, reduction and oxidation follow to produce an aldehyde, alcohol and ester, respectively. In order to monitor this pathway throughout fermentation, hydrophilic interaction liquid chromatography-mass spectrometry (HILIC-MS) was used to quantify sixteen amino acids. Reverse-phase (RP) LC-MS, using both positive and negative ion electrospray (ESI) modes, was collected to increase the likelihood of observing pathway intermediates. SPME Arrow and gas chromatography-mass spectrometry (GC-MS) data was collected to quantify the aldehydes, alcohols, esters and other flavor compounds. For each yeast, it can be shown that the amino acid concentration is highest halfway through mashing and decreases as fermentation progresses. The California ale yeast consumed each amino acid at the fastest rate with the exception of proline. Sake extreme fermentation consumed each amino acid at the slowest rate with the exception of proline, serine, and valine. To date, efforts to identify pathway intermediates have focused on reactions that produce 3-methyl butanol and phenylethyl alcohol. Excluding ethanol, these are the most abundant volatile compounds produced during fermentation. 3-methyl butanol arises from leucine in the Ehrlich pathway. The keto-acid 4-methyl-2-oxopentanoate has been putatively identified in the RP LC/MS data. Phenylalanine yields phenylethyl alcohol. The intermediates phenylpyruvate and phenylacetaldehyde have been putatively identified in the LC/MS and GC/MS data, respectively. Standards will be used to confirm these identifications and quantify the reaction intermediates, thus allowing the monitoring of important biochemical pathways that impact the flavor and aroma of the final beer.

02--Identification and quantification of carcinogen compounds in carotenoid foods through solid-phase microextraction gas-chromatography mass spectrometry Anna Pons, annaponsaguade@gmail.com, Maddie Tarrance, Karen Barnes. Chemistry, Univ. of West Florida, Pensacola Furan and benzene are highly volatile, non-polar aromatic compounds that can be formed in food, for example coffee. These compounds are formed via oxidative or thermally driven mechanisms and are toxic for humans since they can cause cancer. Furan is formed mainly in low acid canned and jarred foods containing carotenoids, such as baby foods that require high thermal processing for food safety concerns. Volatile carcinogens are often identified using a gas-chromatograph mass spectrometer (GC-MS), an analytical technique combining the properties of a gas-chromatography instrument and a mass spectrometer. The gas-chromatography column separates the molecules within a sample. Each molecule is then eluted off from the column at different rates which allows the mass spectrometer to ionize the molecules. Each ionized molecule is detected using a mass to charge ratio, allowing to identify the components of the sample. Recently, the solid phase microextraction, also known as SPME, has been combined with GC-MS to obtain more accurate results in the identification of specific molecules, such as furan. This technique involves a fiber coated with an extraction phase. The analytes of the sample are absorbed by the fiber and can be then transferred to a GC-MS for identification. Volatile compounds such as the carcinogens of this study will migrate into the headspace and can be captured on the SPME fiber. Sample preparation is dramatically simplified. After consolidating a sensitive and reproducible technique to identify furan and its derivatives, baby food will be studied to limit the formation of carcinogenic compounds, for example by adding antioxidants.

03--Hop (Humulus lupulus) phytochemical profiles as a function of growth region by HR-LCMS and GCMS analysis Celina Paoletta[1], celina.paoletta.18@cnu.edu, Christopher Balog[1], Adrienne Dew[1], Dmitry V. Liskin[1], Andrew Higgs[1], Kevin Kingsbury[2], Abbie Brehm[2], Ronald A. Quinlan[1]. (1) Molecular Biology and Chemistry, Christopher Newport Univ., Newport News, Virginia (2) 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 in hops also provide beer with other qualities such as flavor, foam, and microbial stability, as well as 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. Differences in the terroir can lead to alterations in the acid profiles of individual hop cultivars. Here we present our findings of phytochemical profiles from home-grown hops through a small-batch brewing process in collaboration with a local craft brewery using high resolution liquid chromatography mass spectrometry (HR-LCMS) and gas chromatography mass spectrometry (GCMS).

04--Effect of trans vaccenic acid on glucose homeostasis in a mouse model of diet-induced obesity and insulin resistance Christopher M. Prajogo, cmprajogo@ucdavis.edu, Yanqing Xu, Payam Vahmani. Dept. of Animal Science, Univ. of California Davis College of Agricultural and Envir. Sci. Recent government bans on industrial trans fatty acids (TFA) in developed countries

have left naturally occurring TFA from ruminant products (e.g., dairy and beef) as the sole source of TFA in the food supply. In contrast to industrial TFA, vaccenic acid (VA; trans11-18:1), the predominant TFA isomer in ruminant products, has been associated with a reduced risk of type 2 diabetes. This study addressed the hypothesis that supplementing a high-fat diet (HFD) with VA may help to improve glucose homeostasis by activating insulin signaling molecules. Thirty-six male C57BL/6J mice (7 weeks old) were fed either a low-fat diet (LFD, 10% kcal total fat), a HFD enriched with oleic acid (OA; cis9-18:1) (HFD-OA; 45% kcal total fat, 6% kcal from OA), or a HFD enriched with VA (HFD-VA; 45% kcal total fat, 6% kcal from VA) for 19 weeks. Following the dietary intervention, the metabolic phenotype was characterized using glucose tolerance test (GTT) and insulin tolerance test (ITT). Liver tissues (4 mice per group) were harvested and extracted for protein, which was analyzed for protein kinase B (Akt) and phosphorylated Akt (pAKT) by western blot using Vinculin as a loading control. The resulting band intensities were quantitated using the FluorChem 9900 program (Alpha Innotech). pAkt expression was normalized to Akt. Data were analyzed using one-way analysis of variance (ANOVA) followed by Tukey's test. Our GTT results suggest greater ($P < 0.01$) glucose intolerance in both HFD groups compared with the LFD group (Figure 1). Conversely, our ITT data suggest that the HFD-VA group was more insulin resistant ($P < 0.05$) compared to both LFD and HFD-OA groups. In agreement with the ITT results, we found lower ($P < 0.01$) level of Akt phosphorylation in the liver of the HFD-VA group compared to LFD. In conclusion, this work demonstrates that contrary to our initial hypothesis, a high dose of VA (6% of calorie intake) promotes glucose intolerance and insulin resistance in HFD-fed mice. Further studies using the typical intake of VA in humans (0.5-1% of calorie intake) are required to better understand VA effects on glucose homeostasis.

05--Evolution of kombucha in an air-permeable bag Emma Oberholtzer, e.oberholtzer26@gmail.com, Lieke Black, Jeb Kegerreis, John N. Richardson, Lauren Stains. Chemistry, Shippensburg Univ. of Pennsylvania, Shippensburg Kombucha brewing involves fermentation brought about by a symbiotic combination of bacteria and yeast (SCOBY). A major obstacle in the commercial brewing of non-alcoholic kombucha is maintaining an alcohol by volume (ABV) less than the legal limit, which is 0.5%. Many factors influence the production of alcohol, including the identity and abundance of bacteria and yeast, the food source for the microbes, the temperature of the brew, and the brewing vessel. Traditional brewing vessels that restrict exposure of the SCOBY to oxygen tend to produce ABV levels that are too large as the bacteria require the oxygen to convert ethanol to acetic acid. This project focused on small-scale brewing of kombucha in a vessel that maximizes exposure of the SCOBY to oxygen. Two batches of kombucha were brewed in different vessels using the same ingredients while the pH, sugar levels, ABV, and gluconic and acetic acid concentrations were monitored over time. One vessel was a silicone air permeable bag, which allowed for oxygen to enter from all sides. The second vessel was a traditional gallon-sized wide-mouth jar. We found that air permeability associated with the silicone bag enhanced the bacteria's activity relative to that of the yeast when measured against the control vessel. This observation was supported by the fact that the kombucha brewed in the air-permeable bag exhibited a decreased rate of alcohol production while also exhibiting a lower pH, higher titratable acidity, and higher concentrations of acetic acid and gluconic acid over the time of study. These preliminary results could act as a model for scale-up efforts by kombucha brewers as they strive to maintain a legal alcohol level in their brews.

06--Characterization of total antioxidant capacity in spent coffee ground extracts by roast and brewing method via UV-Vis spectrometry Brian G. Yust[2], Niny Z. Rao[1], Evan Schwarzmann[1], evan.schwarzmann@students.jefferson.edu. *(*1) College of Life Sciences, Thomas Jefferson Univ., Philadelphia, Pennsylvania (2) Physics, Thomas Jefferson Univ., Philadelphia, Pennsylvania Coffee is a commonly consumed beverage that is enjoyed by a large percentage of the world. However, it is a very diverse drink with each individual seeming to have a preference in the preparation of the beverage. Individuals and large corporations tend to dispose of spent coffee grounds (SCGs) after one extraction. Here, we show that SCGs that have already been used once in coffee brewing can be used to produce additional extracts containing similar compounds to the initial brew. Medium and dark roast SCGs from the same bean variety were acquired after extraction by hot brew, cold brew, and espresso methods. The total antioxidant capacity (TAC) and total caffeoylquinic acid concentrations of aqueous SCG extracts were investigated through HPLC analysis and five colorimetric assays including ABTS assay, total phenolic content, and FRAP assay. Results indicated SCG extracts from hot brew methods had the highest average TAC levels, while espresso SCG extracts had the lowest. SCGs extracts may be able to act as a substitute for standard coffee extracts in both syntheses and beverages as a part of greener chemistry.

07--Analysis of free, conjugated and insoluble-bound phenolics in buriti fruit shells as a potential source of functional dietary fiber Guillermo Guerrero, g.guerrerop@pucp.edu.pe, Eliana Esparza, Eric Cosio. Chemistry, Pontificia Univ. Catolica del Peru, Lima Buriti (Mauritia flexuosa L. f.) is an endemic palm in Amazon. The pulp is the main part of the buriti fruit that is consumed; as a result, other parts such as the shell are not used and are considered as a residue. Current investigations have found that conjugated and, overall, insoluble-bound phenolic compounds in dietary fiber in fruits have prebiotic effects and other benefits for the human health. In this context, research in our group was focused in the analysis of free (FP), esterified (EP), glycosilated (GP) and insoluble-bound phenolics (IBP) in shells of three buriti fruit morphotypes from Peruvian Amazon. The crude extract was obtained by ultrasound-assisted extraction with an initial cleanup by solid-phase extraction (SPE RP-18). In this step, degreased, bleached and freeze-dried shells were used. The FP fraction was directly extracted by liquid-liquid extraction, EP and IBP fractions were released after alkali hydrolysis, and the GP fraction was obtained by acid hydrolysis. These phenolics were analyzed using HPLC-DAD and GC-MS with 16 standards (phenolic acids and flavonoids). In addition, the separation of analytes was studied by means of normal phase TLC. Antioxidant capacity (ABTS) and total phenolic content, flavonoids, and tannins was estimated in each fraction. Furthermore, the total dietary fiber was measured by an enzymatic-gravimetric method. The results revealed that buriti fruit shells have an important conjugated and insoluble-bound phenolic component with a high antioxidant capacity. Nine phenolics were identified and quantified by reverse phase HPLC-DAD. GC-MS analysis using the trimethylsilyl derivatives corroborates these findings and it allows us to suggest the presence of other phenolics. Moreover, it was found that the shells are constituted mainly by insoluble fiber. These outcomes help provide a better understanding of the functionality of the buriti fruit shell as a potential healthy dietary fiber source for food supplementation.

08--Design of new, and environmentally safe herbicides using AI and molecular modeling Jerome A. Darsey, jadarsey@ualr.edu, Micah Shaver. Chemistry, Univ. of Arkansas at Little Rock Herbicides are biocidal chemical compounds or biological organisms used to kill weeds on plants. A herbicide

works primarily by inhibiting their growth. Herbicides can either be contact, translaminar, or systemic. Contact herbicides are not taken up into the plant tissue and protect only the plant where the spray is deposited. Translaminar herbicides redistribute the herbicide from the upper, sprayed leaf surface to the lower, unsprayed surface. Systemic herbicides are taken up and redistributed through the xylem. Few herbicides move to all parts of a plant. Some are locally systemic, and some move upwardly. Most herbicides can be bought in either the solid or a liquid form. Examples of herbicides are Glyphosate, Atrazine, Dicamba, Trifluralin, Beacon, Pinnacle, Harmony, etc. Herbicide residues have been found on food for human consumption, mostly from post-harvest treatments. The goal of this research is to take known herbicides and, using molecular modeling, modify these molecules in order to identify herbicides with more potent weed killing abilities but with reduced environmental impact. If successful, this could have a huge effect on the productivity of crops. Since Arkansas is a large agriculture state, this should have a great impact on the economy of Arkansas. We will use the parameters computed in the quantum mechanical molecular modeling, along with the known binding affinities (IC_{50}) and toxicology data found in the literature, to model these biological properties. The technique will be to use the trained data set from the AI program to predict the binding affinity and toxicity of new, modified herbicides. We will make approximately 200+ modifications to the known herbicides. This should provide several molecules that will have superior "weed-killing" properties but with much less environmental toxicity.

09--Quantification of nitrate in pomegranate extract using ion-pair reverse-phase HPLC Joanna Powell, joanna.powell@pepperdine.edu, Rachel Tan, Phillip M. Joyner. Pepperdine Univ., Malibu, California Pomegranate has been reported in some places in the scientific literature as a good dietary source of nitrate but there is a conspicuous absence of conclusive analytical confirmation of this assertion. While a variety of analytical methods exist for quantifying nitrate in foods and plant tissue, many of them use indirect measures of nitrate and appear likely to be susceptible to confounding matrix effects caused by the high quantity of flavonoids and other polyphenols in pomegranates. Previously we quantified nitrate in pomegranate extract using a reaction with salicylic acid in concentrated sulfuric acid to produce a color change that corresponds to the amount of nitrate in the sample; unfortunately, the spike recovery values for this method were very poor, leading us to search for more robust methods for making this measurement. In this study we used an ion-pair reverse-phase HPLC method to quantify the nitrate in pomegranate extract and fruit. Our method used isocratic aqueous 5 mM tetrabutylammonium chloride, 10 mM phosphate and 20 % (v/v) acetonitrile as the mobile phase with a 100 x 3.0 mm 3 µm C18 (100 Å) column and a flow rate of 0.4 mL/min. Nitrate absorbance was measured at 205 nm with a single-wavelength UV-Vis detector and quantified using integral values of the nitrate peak. Solid-phase extraction columns were used to remove flavonoids and polyphenols from the pomegranate samples prior to analysis by HPLC. Our results indicate that indirect measurements of nitrate in pomegranate appear to significantly overestimate the quantity of nitrate in this food compared to our direct measurement. Additionally, our results show that ion-pair reverse phase chromatography is an inexpensive and rapid method for quantification of nitrate in foods with complex matrices that may confound other analytical methods.

10--Beer processomics: Evolution of volatile and nonvolatile hop compounds throughout boiling and fermentation with genetically different yeast Juan M. Garcia[1], garci5jm@dukes.jmu.edu, Emma Nasipova[2], Samuel A. Morton[3], Steven Harper[3], Chrisi A. Hughey[1]. (1) Chemistry & Biochemistry, James Madison Univ., Harrisonburg, Virginia (2) Chemistry & Biochemistry, Northern Kentucky Univ., Highland Heights (3) Engineering, James Madison Univ., Harrisonburg, Virginia Hops are added to beer during brewing to impart flavor and to preserve the beer. Volatile terpenes impart hints on citrus, pine or medical flavors. Nonvolatile hop acids, like iso-α-acids, impart bitterness. Here we monitor the evolution of volatile and nonvolatile hop compounds in a pale ale throughout boiling and fermentation with five genetically different yeasts: Belgian Saison, California ale, Czech pilsner lager, English ale, and Sake extreme fermentation. Cascade hops were added at the beginning and end of the boil. Volatile hop compounds were quantified by SPME Arrow GC/MS with internal calibration. The evolution of nonvolatile compounds was monitored by reverse phase LC coupled to a triple quadrupole mass spectrometer (QqQ). Due to the lack of standards, compounds were putatively identified by matching MS/MS spectra to the literature and pseudo-quantified relative to an iso-α-acid standard. All samples were randomized for analysis. Eleven terpenes were identified and quantified. A ~90% decrease was observed for the most volatile terpenes (pinene, myrcene and limonene) between the first and second hop addition. The smallest loss (~20%) was observed for caryophyllene. An increase to ~75% of the initial concentration was observed after the second hop addition. Concentrations decreased rapidly after the second hop addition and then more slowing during the first few days of fermentation. A small increase in concentration was observed later in fermentation for terpene alcohols linalool and citronellol, especially for the Pilsner yeast. The α-acids exhibited trends similar to the terpenes between the first and second hop additions. The concentration of iso-α-acids, humulinones and prenylflavonoids exhibited a steady, rapid increase during boiling. The increase in the less soluble β-acids was more gradual. During fermentation, the concentration of all compound classes decreased, especially during the first two days. All compound classes exhibited periodicity where concentrations increased at days 5 and 10 of fermentation, which is likely due to the uptake/utilization by the yeast and subsequent release at the end of the yeasts' life cycle. Statistical analysis will be performed to determine if differences observed across yeast strains are significant. Collectively, the GC/MS and LC/MS data give a comprehensive look at the transformation of hop compounds throughout brewing and fermentation.

11--Plasticizing capabilities of glycerol: Acetic acid and choline chloride: Urea in potato thermoplastic starch film Kourtney Collier[1], kocollie@iu.edu, Riya Singh[1], riyasing@iu.edu, Jake Staker[2], jstaker@indy.rr.com, Eric Collier[3], escollie@iu.edu, Anum Ansar[3], aansar@iu.edu, Andres Tovar[1], Amanda Siegel[2]. (1) Dept. of Mechanical and Energy Engineering, Indiana Univ. Purdue Univ. Indianapolis (2) Dept. of Chemistry and Chemical Biology, Indiana Univ. Purdue Univ. Indianapolis (3) Dept. of Biology, Indiana Univ. Purdue Univ. Indianapolis Thermoplastic starch (TPS) is becoming increasingly popular for its potential to replace fossil-based plastic films. The fabrication of TPS film involves the reaction of four main components: starch, solvent, plasticizer, and initiator. The role of the plasticizer and initiator is critically important to provide the required mechanical properties of the film. The addition of a eutectic-based ionic liquid has potential to increase the mechanical properties for optimization. This research aims to evaluate the effect of two different plasticizers with their two corresponding initiators: (1) glycerol with acetic acid and (2) choline chloride with urea. Of particular interest is their effect on the strength and strain at fracture. The TPS film formulation in this work consists of 5 grams (g) of potato starch and 100 g of water (solvent). The molar ratio for the plasticizer and its corresponding initiator was 20:1 for glycerol: acetic acid and 1:2 for choline

chloride: urea following published reports. Test specimens are prepared and tested according to ASTM D882. Results show that glycerol and acetic acid have higher average elongation at break but lower average tensile strength. The replacement of a eutectic-based ionic liquid does in fact change the mechanical properties of potato thermoplastic starch films significantly, demonstrating the importance of specific binding characteristics within the plasticizer and its bio-polymer chain.

12--Isolation of monomeric anthocyanins from Vitis vinifera utilizing low-cost and high-throughput methodologies Luis Arce-Rosales, larcerosales@patriots.uttyler.edu. Chemistry, Univ. of Texas at Tyler College of Arts and Sciences Compositional analysis of grapes and wine are often performed using expensive HPLC and or UV Vis instrumentation. Quantification of anthocyanins (the primary red-pigment molecules found in red varieties of Vitis vinifera) is a common QA/QC method for grape and wine producers. This is primarily achieved through external calibration curves using certified standards. However, the approximate pricing for such standards is currently $37-$60/mg, making it an expensive purchase particularly for small scale operations. Development of a low-cost, high-throughput methodology for isolating anthocyanin standards from red grape sources would likely save many vintners and enologists on QA/QC costs. However, the majority of anthocyanins are found in a homogeneous mixture with sugars, organic acids, and other polyphenols in the vacuoles of skin cells, making isolation difficult. The following study aims to isolate monomeric anthocyanins from red wine pomace, a waste product of the wine making process. Utilizing simple solid-liquid extraction methods in conjunction with cost-effective, low-pressure, ion-exchange chromatography, grape-derived anthocyanins were successfully purified from the pomace matrix, and purity was verified via HPLC-VWD.

13--Determination and comparison of xanthophyll carotenoid content in age related macular degeneration vitamins versus vegetables through UV-visible spectrometry and high performance liquid chromatography Madison Tarrance, met36@students.uwf.edu, Anna Pons-Aguade, Karen W. Barnes. Chemistry, Univ. of West Florida, Pensacola The primary objective of this project is to extract the carotenoid content from different vegetables, plants and age related macular degeneration preventative vitamin brands. Age related macular degeneration is an ocular disease that targets the retina, the portion of the eye that converts light into electrical signals that are received by the brain to create the images we see. Age related macular degeneration is the leading cause of irreversible blindness in adults over 60 and affects millions of people across the world. Two of the main causes of age related macular degeneration are heredity and dietary deficiencies. There is no cure for this disease however, preventative vitamins are available and recommended to slow disease progression. Carotenoids play a significant role in the prevention of age related macular degeneration due to their ability to act as antioxidants and reduce oxidative stress in the retina. Lutein and Zeaxanthean are a specific type of carotenoid called xanthophylls which make up the macular pigment. Alongside the benefits aforementioned, these compounds reduce the effects of light scatter and chromatic aberration on visual performance, and protect against age related macular degeneration. The supplementation of these carotenoids is shown to increase macular pigment density to protect against degeneration. Many vitamin supplements are advertised to prevent or slow the progression of macular degeneration and contain varying contents of vitamins, minerals and carotenoids. Lutein and Zeaxanthean are consistently mentioned as main ingredients in these supplements. In a previous study, the mineral composition of these supplements was determined to explore differences between brands. Varying consistencies were found between brands for label claims versus experimentally determined concentrations. High levels of these advertised carotenoids are also found in varying food groups. After extraction, we plan to compare the available carotenoid content between different methods of supplementation in order to determine whether dietary or vitamin supplementation is likely to be more effective in terms of age related macular degeneration prevention. The carotenoid content of our samples will be extracted by using different organic solvents and solvent mixtures. Extracts containing carotenoids will be separated and determined by HPLC.

14--Induction of viable but nonculturable Campylobacter jejuni in various stress conditions Pierre-Luc Longchamps Longchamps, pierreluc.longchamps@gmail.com, Kaidi Wang, Xiaonan Lu. Food Science, McGill Univ. Faculty of Agriculture and Environment, Sainte-Anne-de-Bellevue, Quebec, Canada Campylobacter jejuni is one of the leading causes of foodborne diseases in Canada and the US. C. jejuni can enter a viable but nonculturable (VBNC) state under stressful conditions. In this dormant state, it maintains reduced metabolic activity but cannot be cultivated on media. VBNC C. jejuni retains pathogenic potential due to its ability to resuscitate under appropriate conditions. Food industry mainly applies physical and chemical stresses to inactivate bacteria that are highly likely to induce bacteria to enter VBNC state. The objective of this study was to investigate the formation of VBNC C. jejuni in food processing and storage-related environment. C. jejuni isolates were induced under different conditions mimicking various food treatments, including 1) room temperature (22 °C), 2) low-temperature (4 °C), 3) aerobic stress, 4) starvation (phosphate buffered saline (PBS)). The dynamics of VBNC population over time were monitored using the plating assay combined with quantitative polymerase chain reaction coupled with propidium monoazide (PMA-qPCR). All the conditions tested were able to induce C. jejuni into the VBNC state. It was found that increasing temperature increased the induction rate of the bacteria. Moreover, induction in nutrient broth led to shorter induction times and higher survival rates compared to that in PBS. Finally, C. jejuni F38011 required extended time to be completely induced to VBNC compared to C. jejuni ATCC 33560. The presence of VBNC C. jejuni were verified using LIVE/DEAD BacLight Bacterial Viability Kit combined with confocal fluorescence microscope. This study demonstrated that C. jejuni can enter into the VBNC state during transportation, processing and storage of food products, posing a health risk to agri-food system.

15--Evaluating the efficacy of smoke-water towards ripening of banana (Musa paradisiaca) Rameesha Khursheed, rameeshakhursheed@gmail.com, Sana Siddiq Baba. National and Physical Standards Laboratory, Islamabad, Pakistan Fruits are an important source of essential minerals, vitamins and nutrients required in our diet for proper growth and development. Naturally, fruits attain full maturity during ripening through a series of biochemical and physiological events that makes them more nutritious and palatable. Currently, the application of artificial ripening agents has become widespread due to economical and commercial uses. These agents have been reported to contaminate the fruits with toxic heavy metals and affect their nutritional quality. The present study was conducted to evaluate the effect of smoke-water derived from natural biotic products including rice husk, coconut shells and pines cones, on ripening of bananas in comparison to calcium carbide. Changes in biochemical composition were also investigated for each sample. The results revealed that application of smoke water extracts accelerated the ripening time of bananas in contrast to calcium carbide and naturally ripened fruits. Biochemical analysis indicated that fruits

administered with different concentrations of calcium carbide showed increased sugar content and TTA, whereas moisture content and vitamin C were found to decrease with increasing calcium carbide concentrations. Smoke water treatment resulted in higher composition of reducing sugars and vitamin C, however no significant difference was observed in TTA and moisture content. Antimicrobial activity of smoke water extracts was also assessed on three different bacterial strains including ATCC cultures of E. coli, Staphylococcus. aureus and Bacillus cereus respectively, which showed large inhibitory zones compared to standard sample. The quantitative analysis of different elements in calcium carbide and smoke-water treated bananas using Inductively coupled plasma mass spectrometry (ICP-MS) revealed increased concentrations of As, Pb and Ni in calcium carbide treated fruits, while all the heavy metals were found to be lower than the permissible levels set by FAO/WHO in smoke-water treated bananas.

16--Phytoremediation of toxic heavy metals from soils using sunflowers (Helianthus annuus), ferns (Nephrolepis biserrata) and mustard greens (Brassica juncea) Seth Bergeron, sbergeron55@nicholls.edu, Darcey Wayment. Chemistry and Physical Sciences, Nicholls State Univ., Thibodaux, Louisiana Phytoremediation is the use of vegetation to remove pollutants such as heavy metals from contaminated soil. In order to compare plants' effectiveness at removing heavy metals from soil, sunflowers, ferns, and mustard plants were grown in soils amended with arsenic, lead and copper at 0.01, 2 and 10 mg kg^{-1} soil respectively, and monitored for a period of 100d. For each plant, four soil samples were taken at different time intervals and assayed for the respective metals using Anodic Stripping Voltammetry (ASV) and the method of standard additions. Detection limits were determined to be 10 µg kg^{-1} for arsenic and 100 µg kg^{-1} for lead and copper. The amounts of metals in the plant biomass was also determined at the end of 100d. The results of the experiment will be presented along with conclusions as to each plant's effectiveness for potential use in phytoremediation of these metals.

17--Bang for your bark: Comparative analysis of dog food by ICP-OES, mycotoxin testing, and SPME-GC-MS Victoria R. Costilow, vrc9@students.uwf.edu. Chemistry, Univ. of West Florida, Pensacola The way that people care about their pets and what they feed them has grown and evolved over many years. Dog food in kibble form was made around 1950 by Nestle Purina, which is one of the oldest and most popular dog food companies in the world. People today are also willing to spend more than ever on pet food, with a global spend in the billions for dog food alone. Advertisements play into this spending by pushing people to believe that certain brands of dog food are better or worse for their dog in terms of ingredients, flavors, and processing. There is a widely believed notion in the present day that cheaper pet food will cause illnesses or even shorten life for pets. This experiment aims to analyze and compare dog foods from all price ranges for heavy metals and minerals, mycotoxins, and volatiles. Utilizing inductively coupled plasma-optical emission spectroscopy (ICP-OES) to analyze the mineral or heavy metal content, antibody test strips for mycotoxin content, and solid phase microextraction with gas chromatography - mass spectrometry (SPME GC-MS) for the flavor and aroma volatiles. As the dog food industry grows, the importance of analyzing the quality and safety of these products is of the utmost significance.

18--Changes in selected odorants in basil during growth and development Wenxi Yang[1], vince17@illinois.edu, Keith R. Cadwallader[1], Kevin Martin[2]. (1) Food Science and Human Nutrition, Univ. of Illinois Urbana-Champaign (2) Engineering Technology, Northern Illinois Univ., DeKalb Urban, indoor or vertical farming has great future potential for production of herbs, including microgreens. Basil is an essential herb in culinary applications and has become a popular microgreen option. Microgreens offer a more efficient way to produce biomass over production of mature plants. However, our initial studies on basil microgreens indicated that they lacked flavor intensity compared to mature basil. This study was conducted to better understand the impact of growth stage on basil flavor. Nine cultivars, including two specifically designated for microgreens production, were grown under controlled conditions (green house) and harvested at four stages of growth (microgreens, intermediate, mature and blooming). Contents of selected volatile compounds (eucalyptol, linalool, methyl chavicol, citral, methyl eugenol and eugenol) were determined by direct solvent extraction-gas chromatography-mass spectrometry. Results showed that the potent basil odorant eugenol was present at only trace levels in microgreens while methyl eugenol was the most abundant volatile constituent. On the contrary, eugenol accumulated during maturation of the plants along with a corresponding decline in methyl eugenol. This explains the much weaker flavor intensity of the microgreens compared to the mature basil. The potential for metabolic modulation to increase eugenol in microgreens to improve flavor quality will be discussed.

19--Case study using California olive pomace for potential valorization strategy of olive oil industry by-products by the application in avocado oil based cosmetics Yongju Cho, yoncho@ucdavis.edu, Hefei Zhao, Selina Wang. Food Sci. and Tech., Univ. of California Davis Olive oil production generates a considerable amount of olive pomace, presenting a major environmental hazard and disposal issue for the industry. Nevertheless, for its high phenolic content, there have been extensive valorization efforts to upcycle this byproduct into a functional ingredient. In light of rising interest in utilizing olive pomace, this project aims to assess the effectiveness of California olive pomace extract in an avocado oil-based cosmetic cream. Resin-purified olive pomace extract (RPOPE) with 303 mg gallic acid equivalents (GAE) was used as a natural antioxidant. Four groups of cream samples were formulated: negative antioxidant control without any antioxidants, positive antioxidant control with 70 ppm of EDTA, and two experimental groups ,respectively, with 400ppm and 800ppm GAE of RPOPE. All samples were subjected to the treatment of 1ppm ferrous iron as prooxidants. The cream samples were incubated in the dark at 35 oC for 2 weeks. Their L* a* b* color values were analyzed in the first week. As for the L* value, negative and positive control exhibited no significant difference ($p>0.05$), each with the average values of 91.23 and 90.95, whereas the value displayed an inverse relationship with the RPOPE concentration. In contrast, a* and b* values increased with RPOPE concentration, as indicated in the change of average a* value from 1.61 to 2.07 and that of b* value from 9.71 to 11.09. The antioxidant capacity of the extract is evaluated using DPPH free radical scavenging assay, suggesting that RPOPE has higher antioxidant activity than the control groups for both week 0 and week 2. Cream samples also demonstrated a significant ($p<0.05$) increase in antioxidant capacity from less than 0.121, to 1.722 and 3.922 Trolox equivalents µmol /g cream for the two control samples, 400ppm and 800ppm GAE of RPOPE, respectively. There was no significant difference between the antioxidant values from week 0 to week 2 for all cream sample groups, although antioxidant values minimally decreased. Overall, the research shows a promising valorization strategy of olive pomace as a value-added ingredient of cosmetic products, thus improving the sustainability of the olive agricultural industry.

Reevaluation of Ferrozine assay for rapid testing iron(II) chelation ability of phenolics in mole ratio: Case study by evaluating chelation of chemical standards of olive phenolics Archie Mangubat, abmangubat@ucdavis.edu. Univ. of California Davis Chelation studies have been underestimated among antioxidant activities evaluation and the measurement of chelation % is incomparable among published studies. There is limited data regarding chelation ability of olive pomace (OP). We evaluated Iron(II) chelation using chemical standards of olive phenolics to investigate olive phenolics chelation ability and to provide OP chelation data. Chemical standards of OP were analyzed for iron chelation ability in mM Iron(II)/ mM molecule through a Ferrozine-iron complex assay in pH 3.78 and 6.81 in triplicates and a phenolic concentration range of 0.04-0.5 mM. The standard curves showed no changes in absorption due to pH. A least significant difference (LSD) test at α=0.05 was performed to compare significant differences. High chelation OP phenolics were determined to include caffeic acid (0.9942 mM Iron(II)/ mM molecule) and verbascoside (1.047 mM Iron(II)/ mM molecule) both at pH 6.81 in which there is no significant difference as compared to gallic acid at pH 6.81 (0.9708 mM Iron(II)/ mM molecule). At pH 3.78, caffeic acid, verbascoside, and gallic acid had values of (0.123 mM Iron(II)/ mM molecule), (-0.113 mM Iron(II)/ mM molecule), and (-0.067 mM Iron(II)/ mM molecule) respectively. At pH 3.78, all the chelating ability significantly reduced. This assay would be used as a standardized protocol for the comparison of chelating ability among studies. The assay responsiveness to pH buffers allows for the potential for this method to be adopted in studies with different pH environments. Discovery of high chelation compounds in OP would allow repurposing and waste reduction of OP by-products as effective chelation reagents for inhibition of oxidative stress in both biological and oleaginous food systems as means of protection and preservation.

Development of a PCR assay for foodborne pathogens from soil Larissa Speaks, lspeaks1@students.towson.edu, Noelle Neff, Ilya Grabylnikov, Kelly M. Elkins. Towson Univ., Towson, Maryland Acinetobacter baumannii, Bacillus cereus, Escherichia coli, and Pseudomonas aeruginosa are foodborne pathogens found in soil and can be transmitted to crops and cause illness. The purpose of this project was to design and test new PCR assays to detect and identify these pathogens. The PCR primers were designed to be specific to each bacterium. Primers for A. baumannii were designed targeting the csuA/B, ompA, abaR, and oxa genes and primers for E. coli, B. cereus, and P. aeruginosa were designed to target the yedN, cmk, and lasR genes, respectively. The target DNA for each specie was obtained from ATCC and the primers were purchased from IDT. The primers were tested using real-time PCR using the LightScanner master mix and detecting the LC Green Plus fluorescent intercalating dye. The csuA/B and ompA primers were specific for A. baumannii and the sensitivity of each primer set was tested. An agarose gel was used to confirm the sizes of the amplicons. A duplex PCR assay was developed for A. baumannii and B. cereus and additional primer combinations and ratios are in testing.

Chemical composition of elderberry extract and its inhibitory effect on SARS-CoV-2 spike protein and ACE2 binding, and radical scavenging properties Melody Zeng, melmel3102@hotmail.com, Yanfang Li, Uyory Choe, Liangli Yu. Dept. of Nutrition and Food Science, Univ. of Maryland at College Park SARS-CoV-2 virus has caused a pandemic that has killed more than 6 million people worldwide. Studies have shown that inhibiting the binding between SARS-CoV-2 spike protein and the human ACE2 could reduce virus infection and the risk of COVID-19 disease. In this study, ethanol extract of elderberry was prepared and examined for its chemical composition by HPLC-MS/MS, potential in suppressing SARS-CoV-2 spike protein-ACE2 binding, ACE2 inhibition, total phenolic content, and scavenging capacities against HO, DPPH, and ABTS cation radicals. A total of 16 compounds were tentatively identified, including one (omubioside) with known antiparasitic activity. At concentrations of 3.3 and 0.8 mg dry botanical equivalents/mL, the inhibition on SARS-CoV-2 spike protein-ACE2 binding reached 100% and 60%, respectively, suggesting a dose-dependent matter. Elderberry extract contained 17.99 mg GAE/g TPC and the HO, DPPH, and ABTS cation scavenging capacities were 201.59, 1.18 and 2.71 µmol TE/g botanicals, respectively. This study provides important information about elderberry's chemical composition, as well as phenolic content and radical scavenging capacities. To our knowledge, this is the first report of elderberry's inhibitory effect on SARS-CoV-2 spike protein and ACE2 binding in vitro. Findings could be used to develop functional food and supplemental products for COVID-19 disease prevention in the future.

Maintenance of a kombucha starter preparation Jordan Scalia, jscalia001@gmail.com, Bret Watson, bw9157@ship.edu, Lauren Stains, John N. Richardson, Jeb Kegerreis. Shippensburg Univ. of Pennsylvania Kombucha is a complex fermented system of tea, sugar, water, and SCOBY (Symbiotic Culture of Bacteria and Yeast). The fermentation process allows for the different microorganisms to work together to produce unique acid profiles as well as ethanol. This process occurs through the breakdown of sucrose into glucose and fructose which are then consumed by the yeast and bacteria to generate primary end products of gluconic acid, acetic acid, and ethanol. The kombucha system has not been widely investigated, and its complexity is still not fully known. Consistency in brewing presents an ongoing challenge. To this end, we investigated starter preparations that could be maintained over long periods of time to produce reproducible batches of kombucha. In this experiment, we studied three separate starter preparations made with differing sugar concentrations, with the end goal of producing a consistent kombucha product. The brews were tracked in an initial two-week fermentation cycle, and then were maintained for an extended period. Acid, sugar, and ethanol concentrations, as well as titratable acidity and pH were measured using HPLC, brix, headspace gas chromatography, and titrimetric analysis, respectively, to track the fermentation process and subsequent maintenance of the starter. The ideal starter preparation is expected to produce a brew with a balanced acid profile that also falls below the 0.5% ethanol level required to commercially sell kombucha.

Microbial transglutaminase 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. Introduction. 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 microbial transglutaminase (MTGase). Methods. Protein isolate was extracted at pH 11 from catfish by-products including frames and heads. Microbial transglutaminase was applied at different levels (0, 0.1, 0.2, 0.3, 0.4, 0.5 and 0.6 unit/g) to make gels. Gels was also prepared with catfish fillet mince as control. Texture profile analysis, solubility (non-reducing and reducing), SDS-PAGE, and dynamic rheological analysis were conducted to determine the effects of disulfide bonds and MTGase induced cross-linking on the gel formation of protein isolate.

Results. All texture parameters were improved with the increase of MTGase added up to 0.5 unit/g. Springiness increased from 79 to 88%, deformation increased from 6.51 to 11.13 mm, and chewiness increased from 2200 to 12000 g. MTGase increased the elasticity of gels prepared from protein isolate and made them comparable to those made from fillet mince. The solubility of gels in both non-reducing and reducing buffers decreased with the increase of MTGase added, but the solubility in reducing buffer was at least 50% higher than that in non-reducing buffer, indicating both disulfide bonds and MTGase induced cross-linking played an important role in the gelling process. SDS-PAGE showed those MHC bands which were not observed in non-reducing gel showed up clearly in reducing gel, indicating the denatured proteins after alkaline extraction were prone to disulfide formation due to the exposure of sulfhydryl groups. With MTGase added, less low-molecular-weight bands showed up, which suggested that MTGase could inhibit proteolysis induced by endogenous enzymes to some extent. The temperature sweep showed protein isolate and fillet mince had different sol-gel transition patterns. Addition of MTGase did not change the color of the gels. Significance. This study solved the textural quality issues of gels made from recovered catfish protein and elucidated the molecular mechanism during gelation.

Recovery of fat from waste ice cream by destabilizing the emulsion using ethyl alcohol Changhoon Lee, changhoon.lee@usda.gov, Rafael Garcia, Lorelie Bumanlag, Chen Liang. USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania Ice cream manufacture typically results in some imperfect product that is discarded rather than being sent to retailers, resulting in human food loss. Ice cream may be seen as a dispersion of fat globules in water, stabilized by surfactant proteins. Addition of a water-miscible organic liquid will decrease the dielectric constant of the continuous aqueous phase, altering the solubility of ice cream components. In particular, proteins are expected to become less soluble, and fats are expected to become more soluble as the organic modifier concentration increases. In the present study, it is proposed that ethanol may be used to "break" the ice cream emulsion and facilitate the recovery of valuable components from waste ice cream. Melted ice creams with various concentrations of added ethanol (0 to 100 %, w/w) were kept at 4 or 40C overnight and centrifuged. Without the addition of ethanol, the ice cream did not separate into two layers; with addition of 40% or greater ethanol, a semi-solid, high-fat upper layer formed. The higher the ethanol concentrations added to the melted ice cream at 4C, the higher the purity of fat was observed. Whereas, at 40C, 70% ethanol showed the highest fat recovery rate. As increasing the melting temperature of ice cream, the emulsion becomes unstable and helps recover fat. Neither ethanol addition nor temperature increase had any effect on fatty acid oxidation. Based on these results, fat from waste ice cream can be recovered through the destabilization method using ethanol. Further study is needed to get a higher recovery rate and purity of fat from waste ice cream.

Stormwater runoff chemical contaminants and their effects on urban areas Yousef Ahmadibeni, bebinam9@gmail.com, Sujata Guha, Quianna Hardy. Dept. of Chemistry, Tennessee State Univ., Nashville Stormwater runoff is rainfall, that flows across the land. Stormwater may infiltrate into soil, and run directly into water sources, such as streams, lakes, rivers or drain inlets. When this happens, different types of waste, debris and contaminates get caught within the water from storm water runoffs. Originally these systems were used to prevent floods and didn't focus on the quality of water that would be produced. Because there is pollution in the storm water, the quality of water will be studied to understand what contaminates are most common in these systems. Identifying if there was injustice in the demographic based on cause and effects of stormwater runoff in different environments and living areas was a focal point in this project. Identifying what pollutants are in the Nashville area's water and understanding its quality was also important. After many contaminants; metals, oils, bacteria, and organic materials to name a few, were identified in the water of Davidson County in Nashville Tennessee, there was a focus on narrowing down contaminates, as well as comparing Davidson county's results to other areas. Through research and comparison, the contaminates that were chosen as a focus were a few heavy metals (Cd, Pb, Ni, Fe); Nitrates ($NaNO_3$, KNO_3) , Phosphates ($Ca_3(PO_4)_2$, $(NH_4)_3PO_4$), as they give a range of different sources and how they end up in the stormwater runoff. Nitrate at higher levels, can affect how blood carries oxygen. Phosphate can also affect oxygen delivery in cells, but mainly contribute to aquatic animals and plants. Cadmium naturally occurs in fossil fuels, and at high levels can cause severe illnesses. Based on stormwater pollution and location, the Nashville, TN area is compared to areas in San Diego CA, as they have larger risks considering their large populated urban areas.

Phytochemical development over the ripening process of Aronia mitschurinii, elderberries, mulberries and haskap fruits Ezra Cable[1], ezracable02@gmail.com, Breann Green[1], Deborah G. Sauder[1], Andrew G. Ristvey[2], Victoria Volkis[1]. (1) Dept. of Natural Sciences, Univ. of Maryland Eastern Shore, Princess Anne (2) Univ. of Maryland Extension, College Park A high demand for super fruit and nutraceuticals derived from these fruits has appeared in the market to address the need for products with high antioxidant contents. Aronia mitschurinii is a fruit which can satisfy the demand for one of highest known antioxidants content and low sugars. Research has been completed since 2006 studying the cultural management of aronia and antioxidant content per harvest, however in-depth phytochemical analysis over the ripening period has yet to be performed. The need for in-depth study of ripening arises from preliminary data for aronia that clearly shows peaks for both anthocyanins and soluble sugars, yet these two peaks may be up to 2-3 weeks apart, while the visual color of the berries is the same. It is important to harvest on the peak of anthocyanins for pharmaceutical needs, while for food production the harvesting should happen on the peak of brix. This project has two fundamental goals: (1) observe the ripening of aronia and find both laboratory and in-field methods to determine the optimal harvesting time; and (2) compare the data for four berries with almost same (and much higher than other known fruits) content of anthocyanins, to determine if they have the same or different ripeness patterns. The results for total content of anthocyanins, flavonoids, polyphenols tannins, and brix over the ripening period for aronia, elderberries, mulberries and hascaps is presented, along with phytochemical screening of juice from the berries.

Effect of copper complexation on the chemical stability of beer Morgan Vincent[1], m.vincent@setonhill.edu, Alexey Silakov[1], Ryan Elias[2]. (1) Chemistry, Pennsylvania State Univ., Univ. Park (2) Food Science, Pennsylvania State Univ., Univ. Park The worldwide brewing industry, which contributes more than $331 billion to the global gross domestic product, spends considerable time and effort optimizing and standardizing their product to meet the desired aroma and flavor profiles of their consumers. Beer, a product made from malted barley and/or non-barley cereal adjuncts, hops, water, and yeast, is a deceptively complex matrix and dynamic chemical system that is intrinsically unstable in its finished form. This chemical instability is largely due to deleterious oxidation reactions that are catalyzed by transition metals (e.g., Fe, Cu, Mn) in beer derived from brewing ingredients and metal-leaching from brewing equipment and packaging. Trace levels of Fe, Cu, and Mn (>50 μg/L) have been shown to catalyze reactions

in which reactive oxygen species (superoxide radical, singlet oxygen, hydrogen peroxide, and hydroxyl radical) are formed primarily via Fenton and the Haber-Weiss reactions. This project focuses on understanding how the environment of copper affects the chemical stability of finished beer. EPR spectroscopy was used to analyze a commercial pilsner fractionated into five molecular weight ranges with exogenous Cu^{2+} added. Results suggest that Cu is bound to a component that weighs less than 500 Da. Experiments use a phosphate buffer model beer matrix to explore how copper binds to components such as amino acids, hop compounds, and organic acids, all of which are contained in the smallest fraction. We determined that copper complexes bind with acids in three different ways: 1) Cu-hyperfine structure indicative of a mono-nuclear complex, 2) large groupings of nuclei that show spin-spin interactions, 3) a mix of the mono-nuclear and multi-nuclear complexes. Addition of thiols (like those from hop cones) are currently being added to the matrix for analysis. In the end, we hope to be able to provide brewers with some tools to combat oxidative staling in their finished products.

Antifungal constituents from the fungus Westerdykella multispora against anthracnose disease of strawberries Prabin Tamang, prabin.tamang@usda.gov, Kumudini Meepagala. USDA Agricultural Research Service, Washington, DC Fruit rot of strawberries caused by Colletotrichum spp. is an economically important disease worldwide. Chemical fungicides are primarily used to protect crop loss from this disease globally. However, Colletotrichum spp. has developed resistance to several commercial fungicides and poses a considerable threat to the strawberry industry, warranting a search for new and safer alternatives. Natural product-based fungicides are structurally diverse, environment-friendly, have fewer side effects and half-lives, and are thus considered a better alternative to synthetic fungicides. Here, we investigated the antifungal activity of the fungus Westerdykella multispora isolated from soil sampled from Sardis Lake in Mississippi. A single spore fungus isolate was prepared on a PDA plate as the stock culture. The fungus was cultured in potato dextrose broth (PDB) for four weeks, and the mycelia were separated from the culture broth by filtration through filter paper. The culture broth was extracted twice with 1:1 ratio of culture broth and ethyl acetate. The ethyl acetate crude extracts of the culture broth showed antifungal activity against C. fragariae in TLC-direct bioautography assay. The fractions retrieved from Biotage™ flash column chromatography fractionation using silica columns showed antifungal activity against C. fragariae. The bioassay-guided fractionation of the antifungal compounds will be presented. The present study will be the first step in studying the potential fungicides based on natural products in controlling the anthracnose diseases of strawberries.

Immunological characterization of peanut flour fermented with Rhizopus oryzae Christopher P. Mattison[1], chris.mattison@usda.gov, Rebecca Dupre[1], Kristen Clermont[1], Jae-Hyuk Yu[2]. (1) FPSQ, USDA-SEA-SRRC, New Orleans, Louisiana (2) Bacteriology, Univ. of Wisconsin-Madison Reactions to peanut allergens can be severe, and peanut allergens are resistant to several types of processing. Fermented foods are popular around the world and contain probiotics, enzymes, and other nutrients that can be beneficial to human health. Rhizopus oryzae is considered safe for human consumption and it is commonly used in the preparation of numerous foods. Peanut fermentation may be a useful processing method to generate novel foods with reduced allergen content that also contain microbial metabolites for improved human health. A commercial source of R. oryzae was used to characterize the effects of fungal fermentation on peanut allergens. SDS-PAGE analysis of soluble protein extracted from fermented peanuts indicated a clear reduction in numerous peanut proteins after 16 hours of fermentation. Mass-spectrometry confirmed the presence of peanut allergen peptides and an increased observance of R. oryzae proteins as fermentation progressed. Immunoblot and ELISA with rabbit anti-Ara h 1 and chicken anti-peanut polyclonal antibodies indicated a strong reduction in intensity of full-length Ara h 1 and Ara h 3 after eight hours. However, ELISA of soluble fermented peanut protein with peanut allergic IgE volunteer samples indicated only marginally reduced (10-40%) allergen binding even after 48 hours. The analysis presented here indicates that fermentation of peanut protein with R. oryzae can reduce allergen content, but not to an extent that it is suitable for those with peanut allergy.

Metabolism of condensed tannin by manganese peroxidase Jenna McLain, mclainjm@miamioh.edu, Ann E. Hagerman. Chemistry & Biochemistry, Miami Univ., Oxford, Ohio Tannin is a chemically stable phenolic compound found in plant leaves, fruits, and roots. It enters the soil from plant detritus, but what happens after it enters the soil is unknown. It has biological importance due to its action as an antioxidant and its ability to precipitate proteins. This unique ability to interact with proteins, however, may inactivate some enzymes, so the breakdown of this compound in soil is unclear. Manganese peroxidase is an enzyme from white-rot fungi that catalyzes the oxidation of Mn(II) to Mn(III), which can then diffuse away from the enzyme to oxidize other larger compounds. It has been known to oxidize lignin, another plant compound related to tannin. A method has been developed to confirm the breakdown of catechin and epicatechin monomers, as well as a dimer, by manganese peroxidase. This method combines a substrate, such as catechin, with manganese (II) sulfate, hydrogen peroxidase, oxalate buffer, and manganese peroxidase and allows oxidation of the components to occur. The products are then visualized by TLC and analyzed using ImageJ. In our study, we will optimize this method to visualize the greatest degree of disappearance of the substrates, and then apply that method to other polymers of tannin. The breakdown of sorghum tannin and cocoa tannin, a slightly smaller polymer, were not successfully seen using TLC, so we will employ the reaction with smaller polymers next, such as catechin trimer. Once a method is established to successfully metabolize the compounds, we can begin to identify the products and search for the mechanism by which tannins are degraded. The results of this project could provide valuable information about how large compounds and phenolics are metabolized in soils, with possible ramifications for human and animal digestion of dietary condensed tannin.

Computer-aided design and syntheses of novel flavanone derivatives for use as potential inhibitors of COVID-19 proteases Anna Sigmon[1], ajs8621@psu.edu, Neela Yennawar[2], Hemant Yennawar[3], Eleanora Margulis[1], Hamzah Al-Quaid[1]. (1) Penn State Brandywine, Media, (2) Pennsylvania State Univ. Huck Institutes of the Life Sciences, Univ. Park (3) Pennsylvania State Univ., Univ. Park A series of novel derivatives of plant-based flavanones were designed using in silico docking against the papain-like and main proteases of COVID-19. Initial docking results were obtained using a free and publicly available COVID-19 docking web server that utilizes AutoDock Vina as the docking engine. Those initial results were further evaluated using PRODIGY, a web server that evaluates the binding affinities of protein-ligand complexes. The docking results revealed that the most promising targets should comprise a naphthalenyl moiety linked to a flavanone core via a 4 or 5 atom linker. The most direct route to synthesize these compounds involved linking the naphthalenyl moiety to the flavanone core via a hydrazone functional group. The parent flavanones included naringenin, hesperetin, 7-hydroxyflavanone, 6-

hydroxyflavanone and 6-methoxyflavanone. Hesperetin and naringenin are both found in citrus fruits, 6-hydroxyflavanone is present in Crocus flowering plants, 7-hydroxyflavanone is derived from the stems of Spatholobus suberectus, and 6-methoxyflavanone is a synthetic derivative of 6-hydroxyflavanone. All compounds were made as racemic mixtures. The characterization and synthetic procedures for all compounds are described, along with the crystal structure of one of the naringenin-based compounds that reveals an E configuration of the hydrazone double bond, which is stabilized by an intramolecular hydrogen bond between the imino nitrogen of the hydrazone group and the neighboring hydroxy group.

Polyphenols in plant foods and their bioavailability Yuegang Zuo[1], yzuo@umassd.edu, Chengjun Wang[2], Naveed Ahmad[3], Yiwei Deng[4]. (1) Dept of Chemistry and Biochemistry, Univ. of Massachusetts Dartmouth (2) College of Resources and Environmental Science, South-Central Minzu Univ., Wuhan, Hubei, China (3) Dept of Chemistry, Univ. of Education, Lahore, Pakistan (4) Dept of Chemistry, Univ. of Michigan-Dearborn A number of epidemiological studies have given evidence that consumption of fruits and vegetables is correlated with reduced incidence of and mortality from cancer, and cardiovascular and neurological diseases. The protection that fruits and vegetables provide against these diseases has been attributed to the polyphenolic and other antioxidant phytonutrients contained in these foods. Therefore, it is important to isolate, identify and quantify polyphenolic compounds and their bioavailability in order to understand their critical roles in human health. In this presentation, the authors will report on the separation, identification and measurement of phenolic antioxidants in various fruits, vegetables, traditional Chinese medicines, tea and other plant-derived foods, and discuss the antioxidant, free-radical scavenger and anticancer capacity of polyphenols, and the bioavailability including absorption, subsequent distribution, metabolism and excretion of polyphenols in human fluids.

Fingerprinting of varietal honeys using nuclear magnetic resonance spectroscopy Cory D. Emal[1], cemal@emich.edu, Gregg Wilmes[1], gwilmes@emich.edu, Maria Goodrich[2]. (1) Chemistry, Eastern Michigan Univ., Ypsilanti (2) Biology, Eastern Michigan Univ., Ypsilanti The global market for varietal honeys, or honeys produced from a dominant botanical source, has grown dramatically in recent years. Certain varietals are prized by meadmakers for the organoleptic qualities that they lend to fermented honey wines, while other varietals are purported to convey specific health benefits to the consumer. Given the economic pressures that impact the cost and availability of high-demand varietals, there is an ongoing need for the development of analytical techniques that can validate that the labeling of honey varietals is accurate and that the honeys are free from adulteration by less desirable varietals or non-honey sugar sources, such as rice or corn syrup. We have made efforts towards using nuclear magnetic resonance spectroscopy (NMR) to create 'fingerprints' of specific varietals by identifying unique collections of molecular markers specific to particular varietal honeys of interest. This rapid, non-destructive technique provides the ability to sense multiple chemical compounds simultaneously with minimal sample preparation, unlike most other analytical techniques in use in the honey industry. By combining this technique with multivariate analysis, we are able to distinguish between different honey varietals based on the differences in the minor chemical constituents that emanate from the original botanical source.

Comprehensive analysis of aromatic compounds in milk using GC-MS, SPME Arrow and Smart Aroma Database YusukeTakemori[1], takemori@shimadzu.co.jp, Mitsuharu Matsumoto[2]. (1) Shimadzu Corp., Kyoto, Japan (2) Kyodo Milk Industry Co.,Ltd, Nishitama, Japan The aroma component of milk is one of the important factors that determine the taste, and it is said that it would greatly depends on the production area, feed, sterilization method, storage method, and so on. The authors comprehensively analyzed the flavor compounds of milk. A wide-scope target analysis was used for the comprehensive analysis of aromatic compounds. Acquired data were processed by multivariate data analyses to calibrate and visualize milk qualifications. In this study, six types of milk were used as samples for aromatic analysis. However, the concentration of aromatic compounds in milk is very low, so comprehensive analysis is difficult. In this experiment, solid phase microextraction (SPME) was used for high sensitivity analysis of aromatic compounds. SPME is a method used to adsorb compounds into a fiber to concentrate them before injection into a GC unit. That offers the advantage of much higher sensitivity. In this case, new SPME, know as SPME Arrow, was used. The SPME Arrow enables analysis at high sensitivities due to approximately 5 to 20 times more sorption phase than conventional SPME fibers. After extraction of the concentrated aromatic compounds by SPME Arrow, they were analyzed by GC/MS. Based on the analysis data, aroma compounds were analyzed using a special aroma database, and 45 aroma compounds could be identified The data obtained from the analysis of aroma was finally processed by Principal Component Analysis (PCA). By PCA, there was a significant difference between Milk-2 and the others. The loading plot of PCA confirmed that Milk-2 contains higher amount of several aromas, such as hexanal, 1-hexanol , delta-dodecalactone and so on, than the others.

Prebiotic potential of water-soluble non-starch polysaccharides from Barnyard millet grain Sachin Maji, sachinmaji0906@gmail.com, Satyahari Dey Biotechnology, Indian Institute of Technology Kharagpur, West Bengal, India Increasing awareness of millet among the general public due to its high nutraceutical value is encouraging. The year 2023 being declared the 'International Year of Millet', draws attention to focus research endeavours to explore the potential of various millet polysaccharides with high nutritional values. High nutraceutical value and cost-effectiveness make Barnyard millet a potential candidate for extracting polysaccharides. Water-soluble non-starch polysaccharides were obtained from the residual part of Barnyard millet after ethanol extraction of low molecular weight sugar and treatment with water at a 1:2 sample solvent ratio for 2 hours at 40 °C. Its yield was found to be approximately 2-3% (w/w). On subjecting the dialyzed and lyophilised residue to gastric acidity, salivary and pancreatic amylases it was found to be non-digestible. Interestingly, in presence of various Lactobacilli strains, positive prebiotic scores of water-soluble non-starch polysaccharides indicated the prebiotic potential of barnyard millet.

Thermal stability of yeast alcohol dehydrogenase in the undergraduate teaching lab KatieMei Williams, Alison Bates, Ann E. Hagerman, hagermae@miamioh.edu. Chemistry & Biochemistry, Miami Univ., Oxford, Ohio The enzyme yeast alcohol dehydrogenase (YADH) is used in the undergraduate biochemistry lab class at Miami Univ. to teach students essential biochemical methods and concepts. Specifically, the students compare wild type enzyme to overexpressed His-tagged YADH. An experiment was designed for students to monitor protein stability over time using recently "upcycled" HP 8453 UV/vis spectrophotometers. The instruments were equipped with Peltier cell holderss and new software by Olis (Athens, GA). A 927 nM YADH solution in a 50 mM phosphate buffer at pH 7.0 was incubated at temperatures of 10, 25, 37, and 55 °C. The

denaturation of the protein was accompanied by aggregation and turbidity, which was monitored by collecting absorbance readings at 310 nm every 20 minutes for 3 hours and 20 minutes. The experiment worked well in graduate student hands, but several issues without a clear source became apparent once the experiment was performed in the lab. Discrepancies in the students' showed problems with the reproducibility of the data. Additionally, the starting absorbance of the protein solution was very high in certain experimental runs when it should have always been close to zero. I am optimizing the previous method for this experiment so as to solve these issues and make any other improvements in the protocol for using the thermally controlled UV-Vis. I have been focused on improving the conditions of the initial YADH solution to keep the starting absorbance measurement low as well as preventing unwanted precipitate from forming throughout the experiment. In doing this research, I hope to provide valuable information about the protocol using the upcycled instruments that can be standardized across instruments and improve students' data collection.

Zein nanoparticles coated with various types of tannin Jules Jefferson, Sadeepa Mallikarachchi, Ann E. Hagerman, hagermae@miamioh.edu. Chemistry & Biochemistry, Miami Univ., Oxford, Ohio Zein, a protein found in corn, can form nanoparticles that can be utilized in drug delivery systems. Condensed tannin and hydrolyzable tannin are high molecular weight plant polyphenols that interact strongly with protein, presumably by crosslinking via phenol-peptide hydrogen bonds. Adding a tannin "coat" to zein nanoparticles may protect the particles so they provide a stable drug delivery system. Our study sought to better understand how the chemical composition of the tannin preparation affected its interactions with zein nanoparticles. The nanoparticles were assessed using Dynamic Light Scattering to describe the size and dispersity of particles. Because zein has unusual solubility features, we first compared sonicating vs. gentle mixing to dissolve the zein in 70% ethanol. Sonication was quicker and produced smaller, more monodisperse particles. We then prepared nanoparticles using several different types of tannin, including condensed tannin from several sources and hydrolyzable tannins with different degrees of esterification. Our results suggest that the molecular weight and type of the tannin influence the Size of the nanoparticles, with coated particles smaller than uncoated particles. Surprisingly, hydrolysable tannins destabilized the particles to digestion in an in vitro system.

Processing and characterization of biodegradable mulch films made of potato thermoplastic starch Jake Staker1, jstaker@indy.rr.com, Kourtney Collier2, Riya Singh2, Andres Tovar2, Amanda Siegel1. (1) Chemistry and Chemical Biology, Indiana Univ. Purdue Univ. Indianapolis (2) Indiana Univ. Purdue Univ. Indianapolis Mulch film made of petroleum-based black plastic has effectively helped to increase crop yields for many agricultural products worldwide; however, it creates plastic waste and leaves microplastics in the soil and increases water runoff. Bio-based mulch film is gaining popularity as a suitable alternative, but commercially viable compounds require synthetic or polylactic acid-derived additives. In this work, studies are done regarding the processing and characteristics of thermoplastic starch (TPS) extracted from potato scraps for applicability as a mulch film. Our proposed potato starch based TPS comprises of 1.0 grams (g) of acetic acid, 1.5 g of glycerol, 100 g of water, and 5 g of potato starch (PS). The materials are heated to 60 °C, where the mixture then is poured onto a flat receptacle to form the film size desired. The film is dried at room temperature for ~24 hours. The plastic biodegradability is assessed using ASTM (American Society of Testing and Materials) D6400. The product obtained survives over 3 weeks with minimal structure loss or degradation when exposed to the open environment. Sheets fabricated with less acetic acid degraded more rapidly, demonstrating the importance of this starting reagent for mulch longevity. The mulch sheets have been tested on flora/soils while also being exposed to over 15 mL of rainwater, retaining their structure. They are also stable for 14 days fully immersed in 20 °C deionized (DI) water, though fully degraded when exposed to DI water at 100 °C for 22 minutes. The plastics formed are fully compostable and safe for all organic life. This is an advance toward the goal of developing fully compostable, plant safe material of customizable physical structure.

Probing the ripeness of berries rich by anthocyanin for food and nutraceutical markets with ripeness gauge Ryan Buzzetto More1, rrmore@umes.edu, Ezra Cable1, Andrew G. Ristvey2, Victoria Volkis2. (1) Natural Sciences, Univ. of Maryland Eastern Shore, Princess Anne, Maryland (2) Wye Research and Education Center, Univ. of Maryland Extension, Queen's Town Aronia mitschurinii is a crop obtained by crossbreeding 25% of Mountain Ash with 75% of Aronia Melanocarpa. Aronia has been known as a fruit having highest known antioxidant contents, making it a superfood. Recently we have shown that elderberries, mulberries and hascaps have anthocyanin content similar to aronia. We found for aronia that both anthocyanins and brix reach peaks over the ripening period, yet those peaks occur 2.5-3 weeks apart. Harvesting at the peak of anthocyanins is important for nutraceutical applications, while for food applications harvesting at the peak of brix is required. However, the color is the same at both peaks, presenting a challenge for farmers to decide on harvesting dates. Current laboratory methods for brix are relatively simple, while measuring anthocyanins requires expensive lab equipment that is out of reach for farmers. This creates a need for a cheap, simple, portable testing kit to test both brix and anthocyanins in the field. Anthocyanins in berries are in glucoside form, with cyanidin-3-glucoside (C-3Glu) being the major one. Glucoside bonds can be hydrolyzed at acidic pH. We have observed that at neutral pH, the measurement made with glucometer gives readings proportional to the brix content observed with refractometer, whereas at acidic pH, when glucoside bonds are hydrolyzed, glucometer measures both soluble glucose and the hydrolyzed glucoside from C-3Glu, giving readings proportional to anthocyanin content measured by UV/Vis. The glucometer can only read values in a certain range, requiring to dilute juice from smashed berries with a buffer. Here we present the comparison of UV/Vis and refractometer measurements of aronia juice over the entire ripening period, from the time berries are green and until they are over-ripened, in comparison with glucometer reads of same samples diluted by buffers of pH 7 and pH 3.5. As well, prototypes of cartridge for dilution of aronia samples in the field and comparison of these prototypes with manual sample preparation will be presented.

Development of starch based carriers for controlled release of Urea-ZnO nanoparticles Juan D. Palomino1, Leidy T. Sanchez2, Cristian C. Villa1, ccvilla@uniquindio.edu.co, Andres F. Cañon-Ibarra1,2. (1) Chemistry, Univ. del Quindio, Armenia, Colombia (2) Food Engineering, Univ. del Quindio, Armenia, Colombia Controlled release of nutrients and pesticides has been one of the main topics on agrochemical research, as it diminish soil contamination and makes for more efficient agriculture. One of the most common problems that can be solved by using controlled release systems it related to Zinc (Zn), which is applied to soils in the form of poorly bioavailable complexes. One of the alternatives to improve the absorption of this mineral is the use of zinc oxide nanoparticles (ZnO Nps). These types of nanomaterials have shown that they can increase plant growth, since they dissolve easily in soils with acid pH, which increases its bioavailability. On the other

hand, ZnO Nps can be easily modified, with organic molecules such as urea. This would allow them to be used as vehicles for other nutrients necessary for plant growth. The synthesis of the ZnO Nps was carried out by controlled precipitation of zinc acetate, followed by a calcination process. Finally, the modification with urea, introducing it directly in the coprecipitation process of the ZnO Nps, carrying out a follow-up by UV-Vis where the functionalization of these was evidenced. Modified ZnO Nps were then incorporated into starch based films and their mechanical and water sorption properties were studied.

Reducing the shrinkage and warpage of 3D-printed thermoplastic starch parts by freezing Kourtney Collier1, kocollie@iu.edu, Jake Staker2, jstaker@indy.rr.com, Riya Singh1, riyasing@iu.edu, Eric Collier3, escollie@iu.edu, Anum Ansar3, aansar@iu.edu, Amanda Siegel2, Andres Tovar1. (1) Dept. of Mechanical and Energy Engineering, Indiana Univ. Purdue Univ. Indianapolis (2) Dept. of Chemistry and Chemical Biology, Indiana Univ. Purdue Univ. Indianapolis (3) Dept. of Biology, Indiana Univ. Purdue Univ. Indianapolis Due to its compostability, thermoplastic starch (TPS) is considered an alternative to traditional plastics in 3D-printing applications, i.e., extrusion-based additive manufacturing. However, due to the need for a relatively high volume of solvent (water) during TPS fabrication, the 3D-printed parts shrink and warp as they dry. This work aims to establish the effect of freezing on shape (the shrinkage and warpage) and material properties (hardness, strength, and flexibility) of the 3D-printed part. The TPS material contains 40 grams (g) of water (solvent), 5 g of potato starch, 3 g of glycerol (plasticizer), and 1.9 g of 5% acetic acid (initiator). Parts are 3D printed via liquid deposition modeling (LDM) on an Eazao Zero 3D printer. Specimens for tensile strength analysis are prepared according to the ASTM D638 by extruding several layers of plastic to reach a thickness of 10 mm. The samples are dye-cut and frozen at a temperature of -20 C for two days. Then, the samples are brought to room temperature. The warpage, shrinkage, and hardness are measured daily for five days. Results show that freezing the plastic results in significantly less visual warpage in the 3D parts. The hardness of the frozen TPS is increased compared to the samples that were not frozen.

Fast determination of total unbound fat in snack foods using a new fully automated parallel extraction system Hua Yang, hua.yang1@thermofisher.com. Thermo Fisher Scientific Inc Santa Clara, Sunnyvale, California Food manufacturers need a reliable, fast, and accurate process control method for the determination of fat content to maintain food product quality. The traditional fat determination methods, AOAC Methods 983.23 and 945.16 use Soxhlet extraction, which determines fat gravimetrically following solvent extraction. In previous report, it has been shown that replacing a Soxhlet system with a pressurized liquid extraction (PLE) system combined with a separate evaporator system significantly saves solvent and time. Here we demonstrate application of a new fully automated parallel PLE extraction system to determine total unbound fat in snack foods. This new system is based on the proprietary gas assisted solvent delivery technology. It combines the extraction and evaporation capabilities in one instrument and can extract up to 16 samples (4 in parallel at one time). It is shown that the result using the new system is comparable to the result from the validated PLE plus evaporator method.

Evaluation of double stack sausages packaging Diallo Patterson1, pattersonda@comcast.net, Keith Vorst2. (1) Chemistry, Tuskegee Univ., Alabama (2) Polymer and Food Protection Consortium, Iowa State Univ., Ames Double stack ready-to-eat smoked sausage packages (28oz, 793g) experience low vacuum seal and excess purge (moisture) when shipped domestically to international markets. Root cause analysis was determined for the product/package system to understand failure while the product is being frozen, shipped and slacked resulting in low vacuum appearance and excess purge. Product is packaged in film on a horizontal wrapper at a Midwest facility and packed into cases, 8pkgs/case (2x4). Cases are then frozen at -40 °F for 24hrs. Results of this study suggest that a low-quality seal on the zipper is causing the low vacuum appearance/excess purge. Storage conditions remained constant at 35-37°F throughout the study. All samples were inspected daily for evidence of failure. Between day 7 and day 14 of the study, it was evident that the size of air pockets found in the film increased as seen in Figures 8 and 12. In addition, an overall decrease in burst pressure of 0.116(psi) on day 7 and 0.203(psi) on day 14 compared Day 1 was observed using the Lippke leak and seal strength tester (Mocon Inc. Minneapolis, MN). Data suggests differences in adhesive strength and dimensional stability of packaging film during product sealing resulted in loss of vacuum after prolonged storage.

Using Raman spectroscopy for non-destructive evaluation of carotenoids in Cucumis melo at different maturity stages Ganga Sah1, g-sah@tamu.edu, Nicolas Goff2, Jashbir Singh3, Dmitry Kurouski2, Bhimanagouda S. Patil2. (1) Food Sci. and Tech., Texas A&M Univ. System, College Station (2) Texas A&M Univ. System, College Station Cucumis melo. L. var cantalupensis belongs to the Cucurbitaceae family and is popular among consumers for its sensory and functional attributes. Melons have many health-promoting compounds such as carotenoids, vitamin C, sugars, volatiles, phenolics, and flavonoids. Cantaloupes have high concentrations of carotenoids, especially β-carotene, which is a precursor of vitamin A and acts as an antioxidant. Accumulation of health-promoting compounds in fruits varies with developmental stage. Conventionally, maturity in cantaloupe is determined based on visual cues such as changes in color of the fruit from green to pale or creamy, and slipping of the stalk from the fruit. The present study explored the feasibility of using handheld Raman spectroscopy to assess cantaloupe maturity using carotenoid as a biomarker. Two commercial varieties (Infinite Gold and Da Vinci) and three breeding lines (TH5, TH6, and TH16) were grown in College Station, Texas. Flowers were tagged on the day of anthesis, and cantaloupes were harvested at 13, 26, and 39 days after anthesis. Raman spectra were acquired from intact cantaloupes using surface scan mode, and analysis of carotenoids using HPLC was conducted to validate the results. Our chemometric analysis achieved an average accuracy of 95% in determining the maturity in cantaloupe via surface scan mode. In conclusion, Raman spectroscopy can be a potential non-destructive technique to determine cantaloupe maturity.

Evolution of volatile flavor compounds produced during the fermentation of beer with genetically different yeast Drew Roberts1, robe24am@dukes.jmu.edu, Eliana M. Diaz-Aceituno1, Juan M. Garcia1, Kayla H. Moore1, Angelina V. Lo Presti1, Viridiana Tirado2, Samuel A. Morton3, Steven Harper3, Chrisi A. Hughey1. (1) Chemistry & Biochemistry, James Madison Univ., Harrisonburg, Virginia (2) Physical Sciences, Bakersfield College, Bakersfield, California (3) Engineering, James Madison Univ., Harrisonburg, Virginia Beer is a complex mixture of volatile and nonvolatile compounds that arise from malt, hops, and fermentation. A pale ale wort brewed from a 2-row malt and Cascade hops was equally divided between five fermenters. A genetically different yeast was pitched in each: WLP 001 California Ale, WLP 002 English Ale, WLP 566 Belgian Saison, WLP 800 Czech Pilsner Lager, Wyeast 4347 Extreme Fermentation. While

samples were collected during mashing and boiling, this work focuses the production of flavor compounds during fermentation and the differences across yeast strains. Ten milliliter samples were collected in triplicate at each time point and immediately frozen. Samples were spiked with internal standards prior to extraction and quantitation by SPME Arrow GC/MS. Data collection was randomized. ABV was also measured for each final beer by GC-FID: Sake (4.0%), Pilsner (4.4%), California and English (5.3%) and Belgian (5.5%). Not only did the Belgian have the highest ABV, it also had the highest concentration of the most abundant fermentation products including ethyl acetate, 2- and 3-methyl butanol, 2- and 3-methylbutyl acetate, phenylethyl alcohol, phenylethyl acetate and ethyl hexanoate. With the exception of the California yeast, the Belgian yeast also began production of these compounds faster than other strains (e.g., within 12 hours of pitching). The Extreme Fermenter also produced relatively high concentrations of flavor compounds, especially fatty acid esters, but began production around 20 hours. The English ale and Pilsner did not start to produce flavor compounds until ~30 hours into fermentation. It should be noted that all fermentation tanks were held within each yeast's optimal temperature range (20-23C), with the exception of the Pilsner, which is a lager yeast. While not the primary focus of this work, compounds that were present in the wort prior to fermentation, such as aldehydes, furans, aromatic hydrocarbons and terpenes, were also monitored. Hexanal, for example, was present in malt, decreased during boiling and was then produced in varying amounts by the yeast during fermentation. Aromatic hydrocarbons, which were also present in the malt, were not utilized by the yeast as evidenced by a constant concentration throughout brewing and fermentation. Collectively, this research will help brewers better understand how the impact of yeast strain selection impacts flavor and aroma development throughout the brewing process and in the final product.

Natural products magnetic resonance database (NP-MRD): Comprehensive database and repository for natural products NMR data John R. Cort1,2, john.cort@pnnl.gov, Amy Jystad1, Niranjan Govind1, Eleanor Knutson1, Victoria Sullivan1, Lillian Stillwell1, Mischelle Schutz1, Andrew Maras3, Ella Poynton3, Pegah Tavangar3, vera yang3, Jeffrey A. Van Santen3, Matthew Pin3, Tamara Jordan3, Jonghyeok Kim3, Benjamin Ledingham3, Roger G. Linington3, Rajarshi Ghosh4, Saurav Sarma4, Jay Koller4, Lloyd W. Sumner4, Zinat Sayeeda5, Zachary Budinski5, AnChi Guo5, Brian L. Lee5, Mark Berjanskii5, Manoj Rout5, Harrison Peters5, Raynard Dizon5, Robert Ma5, Eponine Oler5, Dana Allen5, Xuan Cao5, Vasuk Gautam5, David S. Wishart5. (1) Pacific Northwest National Laboratory, Richland, Washington (2) Washington State Univ., Pullman (3) Simon Fraser Univ., Burnaby, British Columbia, Canada (4) Univ. of Missouri, Columbia (5) Univ. of Alberta, Edmonton, Canada NMR spectroscopy is essential to natural products and specialized metabolite research: for example, in novel structure determination and dereplication, characterization of functions and interactions, or analysis of mixtures. However, these critical activities are hindered by inaccessibility to NMR data for known natural products. Currently, chemical shift assignments are scattered throughout decades of published scientific literature and a few valuable, but incomplete, chemical shift databases. Moreover, nearly all raw data (FIDs) used to determine structures of natural products is not archived and is likely unrecoverable. To address these inadequacies, the Natural Products Magnetic Resonance Database (NP-MRD, np-mrd.org) has been established with a goal to become a comprehensive, searchable, connected, and open database and repository for all natural products NMR data. The mission of NP-MRD is to benefit research through engagement and partnership with the worldwide natural products community. With derived (eg. chemical shift assignments), raw (FID), predicted, and simulated NMR data, as well as tools and links to other databases, NP-MRD facilitates dereplication, supports correction of erroneous or missing chemical shift assignments, and enables structure validation or structure revision. Furthermore, NP-MRD creates opportunities for developing new artificial intelligence-based approaches for structure determination and chemical shift or spectral prediction, among other presently unforeseen applications of such a database resource.

Quantifying estrone and β-estriol conjugates in dairy cattle manure and urine using sorptive stir Bar extraction and gas chromatography-mass spectrometry S M Istiak Ahmed2, istiak.a.shuvo@gmail.com, Stacy Antle1, stacy.antle@usda.gov, John H. Loughrin1, john.loughrin@usda.gov, Eric D. Conte2, eric.conte@wku.edu. (1) Food Animal Environmental Systems Research,, USDA Agricultural Research Service, Bowling Green, Kentucky (2) Chemistry, Western Kentucky Univ., Bowling Green The environmental presence of compounds with estrogenic properties has become a major subject of worldwide concern. Endocrine-disrupting compounds (EDCs) are environmental contaminants that interfere with the function of the endocrine system of wildlife and humans. Among the wide range of substances with endocrine-disrupting properties, estrogens are of particular interest due to their high estrogenic potency and fate in the environment. A large source of these naturally occurring estrogens, such as estrone and β-estriol that enter the environment originate from dairy wastes. These lipophilic compounds may accumulate within livestock's fat tissues and thus enter the human food chain. Estrone and β-estriol conjugates (i.e., sulfated forms), being more water soluble, have greater mobility and are more persistent in the environment than free, non-conjugated forms. This persistence may result in a greater degree of estrogenic activity in the environment and more significant potential for human endocrine disruption than non-conjugated estrogens. Free estrogen forms in the environment are heavily studied; however, their conjugate forms have not. A Gas-Chromatography-Mass-Spectrometry (GC-MS) method for determining estrone and β-estriol and their conjugates will be presented. In this method, estrogen conjugates are converted to their respective free form (i.e., estrone or β-estriol) using acid hydrolysis. This method will be applied to quantify estrogen conjugates, contained in dairy cattle waste and surrounding dairy farm samples, for monitoring their spread in the environment.

Lateral flow assay: Development of magneto-plasmonic nanosensors for the detection of E.coli O157:H7 Santimukul Santra1, ssantra@pittstate.edu, Nilamben Panchal1, Vedant Jain1, Rebekah Elliott1, Zachary Flint2, Paul Worsley1, Caine Duran1, Tuhina Banerjee2. (1) Chemistry, Pittsburg State Univ., Pittsburg, Kansas (2) Chemistry and Biochemistry, Missouri State Univ., Springfield Increasing foodborne illnesses have led to global health and economic burdens. E. coli O157:H7 is one of the most common disease-provoking pathogens and known to be lethal Shiga toxin-producing E. coli (STEC) strains. With a low infection dose in addition to person-to-person transmission, STEC infections are easily spread. As a result, specific and rapid testing methods to identify foodborne pathogens are urgently needed. Nanozymes have emerged as enzyme-mimetic nanoparticles, demonstrating intrinsic catalytic activity that could allow for rapid, specific and accurate pathogen identification in the agrifood industry. In this study, we developed a sensitive nanoplatform based on the traditional ELISA assay with the synergistic properties of gold and iron oxide nanozymes, replacing the conventional enzyme horse radish peroxidase (HRP). We designed an easily interchangeable sandwich ELISA composed of a novel, multifunctional magneto-

plasmonic nanosensor (MPnS) with target antibodies (MPnS-Ab). Our experiments demonstrate a 100-fold increase in catalytic activity in comparison to HRP with observable color changes within 15 minutes. Results further indicate that the MPnS-Ab is highly specific for E. coli O157:H7. Additionally, effective translatability of catalytic activity of MPnS technology in the lateral flow assay (LFA) platform is also demonstrated for E. coli O157:H7 detection. As nanozymes display more stability, tunable activity and multi-functionality than natural enzymes, our platform could provide a customizable, low-cost assay that combines high specificity with rapid detection for a variety of pathogens in a point-of-care setup.

Influence of lutein content of marigold flowers on functional characteristics of baked flour products Alfred Anderson, a.anderson@ku.edu.kw. Dept. of Food Science and Nutrition, Kuwait Univ. Lutein, a yellow plant pigment belonging to the Xanthophyll family of carotenoids and widely present in marigold flower, acts as an effective antioxidant and may be utilized in foods as a natural pigment and functional food ingredient. The present study was undertaken to evaluate the effect of lutein in two types of marigold flowers belonging to the Tagetes erecta and Tagetes patula species on functional properties of baked pan bread. Lutein-rich marigold flowers dried by three different methods, namely, freeze-drying, oven-drying, and vacuum-drying, were incorporated into wheat flour (WF) and whole wheat flour (WWF) bread recipes at the levels of 0%, 1.5%, 3.0%, and 4.5% marigold flower powder (MFP). Bread loaf texture, specific loaf volume (cm3g-1) and baking loss (%) of WF and WWF breads were determined. The stability of lutein content during bread making was also estimated. Data indicated that Tagetes erecta marigold flower produced significantly higher amount of lutein, and freeze-drying process was found to be the best technique for preserving lutein in the flowers. The results showed the lutein concentration in WF and WWF bread significantly increased as the level of MFP level was increased. The addition of marigold MFP resulted in decreased baking loss, soft bread texture, and lower specific loaf volume both in the WF and WWF pan bread. The data suggest that ground marigold flower may be used as a functional ingredient in baked food products to enhance physical properties, color, as well as antioxidant properties in view of their rich lutein content.

Impact of ethanol and methanol on the betalains extraction of beetroot (Beta vulgaris Cv. Pablo) Abubakar Sani Ali, 25441118@students.lincoln.ac.uk, William Hayes, Aylin Tas, Bukola Onarinde. Dept. of Food Chemistry, Univ. of Lincoln, Lincolnshire, United Kingdom The current study was designed with the main purpose to determine the impact of ethanol and methanol on the betalains extraction of beetroot (Beta vulgaris Cv. Pablo). Beetroot was purchased from Lidl supermarket, Lincolnshire, UK. The Pablo beetroot was trimmed and cut into slices. The slices are cut into 1/4 pieces. 10g of fresh beetroot was blended with 200ml of water (control), methanol, and ethanol at a concentration of 25,50, 75, and 100%. The mixture of the beetroot cut sample with different concentrations of solvents was blended using a KENWOOD blender (TYPE: FDP30), Hampshire, the United Kingdom for 3 minutes. The blended extract was Filtered using (Whatman 1) and diluted 10 times with deionised water and the absorbance of the diluted juice was read at 538 and 476nm for betacyanin and betaxanthin respectively and corrected absorbance was used at 600nm using an Eppendorf Bio Spectrometer basic UV-VIS Spectrometer and glass cuvette with a water blank. The results indicate higher extraction of betacyanin and betaxanthin at 50, 25, 75%, control, and 100% of methanol of which are (1.053 and 0.944), (0.959 and 0.814), (0.734 and 0.584), (0.622 and 0.543), and (0.538 and 0.506) respectively. Ethanol extraction was observed to have lower extraction of betalains as compared with methanol. The highest extraction of ethanol was observed at 50, 25, 75 and 100% of which are (0.673 and 0.654), (0.671 and 0.620), (0.514 and 0.534), and (0.003 and 0.023) respectively. Further research will be needed with various solvents to optimise the extraction process of betalains in beetroot.

MONDAY MORNING March 27
Functional Ingredients in Food Processing
8:10 Structural characterization of cocoa proanthocyanidins using three LCMS-based methods Sawali Navare, sawali.navare@gmail.com, Bethany Lam, Misha Kwasniewski, Ramaswamy Anantheswaran, Joshua Lambert. Food Science, Pennsylvania State Univ., Univ. Park Proanthocyanidins (PACs) are present as monomers and oligomers in cocoa beans and have been reported to have anti-inflammatory and digestive-enzyme-inhibitory effects. Previous studies have suggested that high temperature roasting can cause PAC polymerization. It is difficult to characterize these polymers by direct quantification using LC-MS due to lack of available standards and chromatographic challenges due to increased PAC polymerization. This study compared three LC-MS-based methods to characterize PACs, one of which is applied to cocoa for the first time. The goal was to compare the information provided by each method to study the effect of roasting on PAC composition. Cocoa beans were roasted under different time-temperature combinations. Method 1 used six cone voltages to fragment oligomers of increasing size. PAC-terminal and extension units were identified by their unique fragmentation in the MS. The terminal-to-extension-units ratio was used as an indicator of chain length. Method 2 used thiolytic cleavage of PAC chains into monomers and thiolytic derivatives, and the ratio of these products, to compute the mean degree of polymerization (mDP). Method 3 was a direct quantification of PACs using standards up to (DP)5. Method 1 showed that some roasting treatments had a lower ratio of terminal-to-extension units than the unroasted control indicating greater PAC polymerization. Higher cone voltages could fragment larger PAC chains more effectively as indicated by the increased mDP with increasing cone voltage. Method 2 showed that the mDP increased (~27%) for some roasting treatments compared to unroasted control, confirming findings from method 1. Method 3 revealed a decrease (50-70%) in oligomer (DP2-5) concentration and an increase in monomer concentration (~100%) with longer roasting treatments. Oligomer concentrations were unaffected by shorter roasting treatments at the temperatures studied. Each method gave unique structural information about the effect of roasting on cocoa PACs in addition to validating findings from other methods.

8:25 Complexation of bark proanthocyanidins isolated from Western red cedar (Thuja plicata Donn) and food carbohydrates enhances colloidal stability Gio Ferson M. Bautista1,2, gio62@student.ubc.ca, Sameer E. Mhatre2, Orlando J. Rojas2,3. (1) The Univ. of British Columbia Dept. of Chemistry, Vancouver, Canada (2) The Univ. of British Columbia, Bioproducts Institute, Departments of Chemical and Biological Engineering, Chemistry, and Wood Science, Vancouver, Canada (3) Aalto Univ., School of Chemical Engineering, Dept. of Bioproducts and Biosystems, Espoo, Finland Carbohydrate aggregation results in undesirable turbidity and haziness of colloidal food suspensions. Industries commonly use proteins to overcome this problem but they also bring unwanted changes during food processing, such as formation of new aroma (leading to undesired flavor), denaturation (leading to loss of stabilization), and production of glycotoxins, especially upon heating. Therefore, new generation stabilizers of food carbohydrates are highly desirable, such as proanthocyanidins, as proposed in this study. Proanthocyanidins are polyphenols with a

unique structure composed of flavonoid monomers that vary in hydroxylation and branching patterns. These structural features influence the interactions with other biomolecules and the stability of the complexes they form, making them good candidates for colloidal stabilization. This study used western red cedar bark proanthocyanidins (1.65%, oven-dried basis), with the majority being water-soluble at room temperature, RT (~60%) and the remaining extractable only at high temperature, HT (~40%). Based on mass spectrometry analyses, the RT fraction is rich in branched structures with a low degree of polymerization. In contrast, the HT fraction is rich in linear structures with a high degree of polymerization. The RT and HT fractions were tested for their colloidal stabilization of representative food carbohydrates (cellulose, starch, pectin, chitin). RT proanthocyanidins are shown to form stable carbohydrate complexes that withstand coalescence and settling. On the other hand, HT proanthocyanidins promote bridging and aggregation, leading to carbohydrate complexes that easily settle. In addition to the already well-known health-promoting activities of proanthocyanidins, this study highlights the potential of western red cedar bark proanthocyanidins as ingredients of functional foods, to modify the texture and guarantee consumer acceptance.

8:40 Primary extraction methods of R-Phycoerythrin from dry biomass of marine macroalgae Gracilaria corticate Vaishali Saraswat1, ch21s502@iittp.ac.in, KSMS Raghavarao1, Vaibhav A. Mantri2. (1) Chemical Engineering, Indian Institute of Technology Tirupati, Andhra Pradesh (2) CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat, India
Phycobiliprotein, namely R-Phycoerythrin, is a fluorescent red pigment. Being water soluble, its importance in diagnostics, cosmetics, therapeutics, and food processing (as nutraceutical cum colorant) is on a rise. The cell wall contains a complex matrix of (agar, cellulose, etc.) polysaccharides, making not only the cell disruption but also the extraction very difficult. Drying makes it more difficult. However, it helps in the shelf-life extension. This eliminates the significant space requirement for cultivation, benefiting small-scale industries. The present study aims at developing an efficient primary extraction protocol of R–PE from the dry biomass of macroalgae Gracilaria corticata. A biomass pre-soaking step (180 min) before subjecting it to extraction was observed to improve the degree of extraction irrespective of the method employed. In addition to ultrasonication, conventional primary extraction by freezing and thawing, maceration, and homogenization have been performed individually and also in integrated mode with ultrasonication. The ratio of solid to liquid (1:6, 1:8, and 1:10), maceration time (10–35 min), homogenization time (1–7 min, 15000 rpm), amplitude (10–70%), and time (0–3.5 minmin) of ultrasonication are major process parameters that are standardized in the study. A significant synergy was observed when ultrasonication was used in an integration mode employing conventional protocols of primary extraction. Ultrasonication followed by freezing and thawing was observed to result in a maximum degree of extraction out of all protocols employed (81.7%). Maceration followed by ultrasonication resulted in the second highest (67%). Spectrophotometric analysis of recording the absorbance maxima (564nm, 618nm, and 730nm) in order to estimate the R–PE content.

8:55 Process intensification and integration for efficient downstream processing of bioactives from micro and macroalgae Ksms Raghavarao, raghava@iittp.ac.in. Chemical Engineering, Indian Institute of Technology Tirupati, Andhra Pradesh, India
Production aspects (fermentation and cultivation) were well studied and reported in the international literature. However, Downstream Processing (DSP) received scanned attention with an assumption that whatever is produced can be isolated and purified. In fact, many of the lab scale processes do not see the light of the day due to high cost of DSP. Algae (micro and macroalgae) are rich natural sources of many important bioactive compounds (proteins, pigments, lipids, carbohydrates, and polyphenols). They are becoming popular post-pandemic owing to their numerous applications in diagnostics, therapeutics, nutraceuticals, and functional foods. Our group has been active in the research area of DSP. Process intensification and integration enable increased productivity and in turn, increase economic viability. The efforts in this direction are presented in the current study. Most of the work is reported on wet algal biomass which is highly perishable, and very few reports are available on dry microalgal biomass. While, practically none found on dry macroalgae. Biomass cultivation requires a lot of space which is a major obstacle for industries especially those located in urban and metropolitan places. On the other hand, macroalgae is cultivated in sea water along the coastline making it imperative to have the processing units in its vicinity. Drying of micro and macroalgae alleviates these constraints. In this context, biomass drying increases the shelf life and it also helps in eliminating the significant space requirement for cultivation, benefiting small-scale industries. Therefore, our study focuses on the process intensification and integration for efficient downstream processing of biomolecules from dry micro and macroalgae. All these aspects are discussed in this presentation.

9:10 Polysaccharide-based self-assembled smart hydrogel for in vitro delivery of co-encapsulated probiotics and folic acid Nandita Srivastava, nansri2501@imtech.res.in, Anirban Roy Choudhury. Bioprocess Engineering Research and Process Development, CSIR - Institute of Microbial Technology, Chandigarh, Punjab, India
The biologically active platforms such as hydrogels are three-dimensional hydrophilic porous structures capable of supporting bioactive components attachment to their surface. By providing a physical barrier between encapsulated biomolecules and the harmful environment, hydrogels can enhance their viability and stability. They can serve as cargos for sustainable and controlled delivery of bioactive compounds to the site of action through reversible sol-gel transitions by responding to external triggers. Thus, it is crucial to develop a hydrogel matrix with smart or intelligent properties that can undergo structural and volume changes in response to different stimuli. Here, we have fabricated a self-assembled, stimuli-responsive, novel tri-composite polysaccharide-based hydrogel of chitosan, gellan, and κ-carrageenan devoid of toxic chemical cross-linkers. Although there are several reports on the encapsulation of probiotics and bioactive compounds, however maintaining the viability of loaded probiotics, stability of folate, and their bioavailability is still a challenge. We utilized this hydrogel to facilitate the co-encapsulation of folate (vitamin B9) and probiotic spores. Its encapsulation with folate, while increasing nutritional value of system, also allows maintaining the viability of spores. The studies on hydrogel revealed that it had remarkable encapsulation efficiency and exhibited sustainable release. The release rate studies at different pH suggested maximum release in alkaline conditions, which correlates with in vitro release in the simulated intestinal phase. Moreover, microscopic and FE-SEM analysis depicted the conversion and colonization of bacterial spores to vegetative cells in the intestinal phase. Overall, this study paves the way to develop a green matrix for co-encapsulating various functional foods with controlled delivery at the targeted site.

9:40 Enzymatic hydrolysis of makapuno for production of potential prebiotics Adonis A. Yanos1, Louelle Sheryl Go-Albia1, Sheryl Lozel B. Arreola1, sbarreola@up.edu.ph, Dietmar Haltrich2, Thu-Ha Nguyen2. (1) Institute of Chemistry, Univ. of the

Philippines Los Banos, Laguna, Calabarzon (2) Dept. of Food Sci. and Tech., Institute of Food Technology, Univ. fur Bodenkultur Wien, Austria Human gut microbiota has been gaining more interest because of its influence on one's health. Several approaches for modulating the composition of gut microbiota include incorporation of prebiotics and/or probiotics to one's diet. Probiotics are microorganisms which beneficially affect the host animal by improving its intestinal microbial balance. On the other hand. prebiotics are non-digestible food ingredients that selectively stimulate the growth and metabolism of beneficial bacteria in host digestive systems and, consequently, limit the colonization of potentially harmful bacteria. Some of the food ingredients that meet the prebiotic criteria are inulin, lactulose, galacto-oligosaccharides, and fructo-oligosaccharides. Recently, several studies have shown the potentially prebiotic activity of manno-oligosaccharides (MOS). MOS are products of hydrolysis reaction of the mannan component of the lignocellulosic biomass by β-mannanase (EC 3.2.1.78, mannan endo-1,4-β-D-mannosidase). Galactomannan, a type of mannan, consists of β-1,4-linked D-mannose units with random side chains of α-1,6-linked D-galactose units. Different sources of galactomannan give variable distribution of D-galactose residues along the main chain, thus affecting the by the number of hydrophilic galactose attached to the main chain. In the Philippines, makapuno endosperm locally known as makapuno, is widely used as sweetened dessert. Its endosperm galactomannan ranges from 3 - 8% making it a good substrate of β-mannanase for production of MOS. In our study, purified β-mannanase from prebiotic Bifidobacterium adolescentis DSM 20083 successfully hydrolyzed galactomannan from makapuno into MOS with varying length. The major products observed were mannobiose, 61-α-D-galactopyranosyl-β-1,4-mannobiose and 61-α-D-galactopyranosyl-β-1,4-mannotiose. After 24 hours of reaction, 20% of makapuno galactomannan was hydrolyzed to MOS. This study shows that β-mannanase from B. adolescentis can be used to produce potential prebiotic MOS.

9:55 Mechanism in improving solubility of pea protein isolates by high intensity ultrasound Kun Gao, kun.gao@ndus.edu. North Dakota State Univ., Fargo Although plant-based proteins potentially provide merits for long-term global food security, their poor functionality particularly solubility has hampered the utilization as functional biopolymers in the industry. High intensity ultrasound (HIUS, 20 kHz) has been researched extensively for its possible application in modifications of protein functionality. We applied a series power of HIUS (100, 150, 200, 300, 400 W) to sequentially treat a same commercial pea protein isolate (PPI) solution for 5 min. After each treatment, the water-soluble fraction (WPPI) from supernatant of the HIUS treated PPI was collected while the total volume was fixed at 25 mL by supplementing water. The structure and morphology of each WPPI was characterized. Here, we show that the solubility of commercial pea protein isolate (PPI) is drastically improved from 7.2 to 58.4 mg/mL at an intermediate power (150 W) after a sequential HIUS treatment. Quantifying nonproteinaceous constituents (dietary fiber and β-glucan) and observing the morphological changes of the resultant pea protein solution have served as a critical step toward understanding the mechanism of action of HIUS in improving protein solubility. The investigation unravels that the formation of soluble aggregates between pea proteins and soluble complex between pea protein and indigenous dietary fiber is the underlying reason that HIUS improves the solubility of poorly soluble pea protein. Our findings offer unprecedented insights into the fundamental role of HIUS on structure modification of plant protein, thus paving the way for their industrial applications as green technique in fabricating plant proteins with improved solubility.

10:10 Potential of Arachis hypogaea testa as a functional food ingredient for the treatment of depression Akenio Patterson1, ampathens@gmail.com, Rushardo Donaldson2, Doleasha Davis1, Marsha-Lyn McKoy2, Winklet Gallimore1. (1) Dept. of Chemistry, Univ. of the West Indies at Mona, Saint Andrew, Jamaica (2) Dept. of Basic Medical Sciences, Univ. of the West Indies at Mona, Saint Andrew, Jamaica Arachis hypogaea (peanut) testa, a rich source of bioactive compounds, is produced as waste from peanut production. In Jamaican folklore, the testa is purported to "improve mood" when it is brewed as a tea; however, there is a lack of scientific evidence to support this claim. The goal of this study was to investigate the potential of the testa as a functional food ingredient for the treatment of depression. Ethyl acetate and ethanol extracts of the testa were obtained and fractionated. The Tail Suspension Test (TST) and the Forced Swim Test (FST) were used to investigate the antidepressant effects of the testa. Chemical analyses were conducted using Gas Chromatography Mass Spectrometry (GC-MS) to investigate the bioactive compounds in the testa. Both extracts increased mobility time in the TST and FST in mice, thus demonstrating antidepressant activity and validating the folklore use for depression. Of the seven (7) fractions tested in the TST, five (5) showed increased mobility time at 10 mg/kg ($p < 0.05$). Pindolol (10 mg/kg), a 5HT1A receptor antagonist, reversed the antidepressant effects of C9-C3, an efficacious medium polarity fraction ($p < 0.001$). This indicates that the serotonergic pathway is involved in the antidepressant mechanism of action of the testa. Compounds with antidepressant activity, such as phloroglucinol and protocatechuic acid, were detected in the testa using GC-MS. Utilizing Thin Layer Chromatography sprays determined that C9-C3 may contain a catechol or a terpene. Lead was detected in the testa at 4.88 ppm and a qualitative pesticide screening detected the presence of chlorflurenol and o-hydroxybiphenyl. This study confirms that Arachis hypogaea testa has the potential for commercial value as a functional food ingredient for the treatment of depression; however, heavy metals, biocides and pesticides are a food safety concern.

10:25 Effect of oat β-glucan on gut metabolism and health Junying Bai1,2, baijunying@swu.edu.cn, Li Wang2, Linhua Huang1. (1) Citrus Research Institute, Southwest Univ., Chongqing, Sichuan, China (2) School of Food Sci. & Tech., Jiangnan Univ., Wuxi, Jiangsu, China Firstly, in vitro gastrointestinal tract digestion model was used to examine the changes of relative molecular weight and spatial structure of oat β-glucan in simulated stomach and small intestine. The results showed that oat β-glucan was not hydrolyzed by digestive enzymes but partially degraded by gastric acid environment, and the triple-stranded helix structure of oat β-glucan was also influenced. Next, gut microbial fermentation model was constructed to study the effect of oat β-glucan on gut microbiota and the metabolism of oat β-glucan in the gut. The results showed that Lactobacillus was the main microbe enriched by oat β-glucan in simulated mice colon while Bacteroides was the primary microbe enriched by oat β-glucan in simulated human colon. Moreover, oat β-glucan degradation was both accompanied by amino acid metabolism and fatty acid biosynthesis. Then, these microorganisms that primarily metabolize oat β-glucan were isolated and LPS-induced Raw264.7 cells model was used to assess the effect of the metabolites produced by gut microbial fermentation of oat β-glucan on inflammation. The results suggested that the metabolites produced by 4 species of Lactobacillus partially inhibited LPS-induced inflammatory responses and the metabolites produced by 9 species of Bacteroides all significantly suppressed LPS-induced inflammatory responses. Finally, DSS-induced colitis mice model was further established to systematically analyze the effect of oat β-

glucan metabolism on colitis mice. The results showed that intragastric administration of oat β-glucan remarkably ameliorated clinic symptoms, regulated gut microbial community structure, significantly increased SCFAs contents, and caused changes in gut metabolic profiles and pathways in colitis mice. Our findings revealed that oat β-glucan ameliorated DSS-induced colitis in mice simultaneously through regulating gut-derived short-chain fatty acids and gut microbial metabolism.

Agri-Food Sustainability at a Crossroads: Challenges of the Food, Energy, and Water Nexus

8:05 Complete analysis of the cashew nut (Anacardium occidentale L.) production and processing with later recovery of anacardic acid from vegetal residues René Alejandro A. Gómez Rodríguez, A01570550@tec.mx. Instituto Tecnologico y de Estudios Superiores de Monterrey, Nuevo Leon, Mexico The cashew tree (Anacardium occidentale L.) produces several products, nevertheless the cashew nut (CN) is by far the most commercialized. The CN needs to undergo two mandatory stages to reach commercial quality: the production and processing. However, most reported Life Cycle Assessments (LCA) focus only on CN production resulting in an underestimation of the environmental impacts (EI). For determination of the process EI, a quantification was realized following ISO 14040/14044 and added to the production outcomes found in literature. As a result, the production accounts for 91% while processing represents at least 9% of total EI. In production, there are great opportunities to improve practices that can reduce EI. Therefore, a comparison of an organic against a conventional crop was accomplished. Particularly, the studied farm that is located at Chiapas Mexico avoids the use of any fertilizer or pesticide. Results show that the organic crop improves mainly in climate change, eutrophication, and human toxicity impacts, but the production yield is 21% lower. Consequently, can be concluded that the CN as an organic production can be a great option to a small scale, but challenging at a large scale. Besides the LCA analysis, it was observed that the cashew shell, one of main residues, contains high amounts of anacardic acid (AA), which has high commercial value due its antioxidant properties. However, it was detected that boiling the CN with water, transforms AA to cardanol and cardol through decarboxylation, losing 99.99% of commercial value. Nevertheless, other processing methods avoid this step since its only purpose is to soften the cashew shell for its removal. To study the transformation of AA, three methods were compared: supercritical fluids, thin layer maceration/chromatography and Soxhlet, making emphasis on green chemistry principles. Results obtained by GC-MS confirms the decarboxylation. By removing boiling, one liter of water is saved per each kilogram of CN, avoids 14% of EI of the process and the AA is preserved. Hence the recovery of AA in the cashew shell can lead to new economic opportunities and human development to the people involved in the production line.

8:35 Grape marc as a potential feed additive to reduce enteric methane production in dairy cattle: Part I chemical composition analysis Hefei Zhao1, hefzhao@ucdavis.edu, Ermias Kebreab2, Selina Wang1. (1) Food Sci. and Tech., Univ. of California, Davis (2) College of Agriculture and Envir. Sci., Univ. of California, Davis Background. About 27% of methane emissions comes from the enteric fermentation of ruminant livestock. Although methane accounts for only 11% of total greenhouse gas (GHG), it is 28 times more powerful than carbon dioxide in the warming effect over 100 years. Previous studies showed that plant tannins, and organic and fatty acids could reduce methane emissions from livestock. The US produces 1.5 million tons of grape pomace (GP) per year, however, limited studies focused on the use of grape pomace as a source of anti-methanogenic compounds. Method. In this study, the chemical compositions related to the methane emission reduction effect of three types of grapes were evaluated. Result. Results showed that the oil content of wet GP (WGP from red grape), dry GP (DGP from red and white grape mix), and ground dry GP (DGGP from red and white grape mix) were 4.33, 5.73 and 4.57% (wt/wt dry basis), respectively, but there was no significant difference ($p< 0.05$) among them. WGP contained the highest moisture (62.8%) among the three GPs. Both total phenolic content (10.2 mg/g defatted dry base, DDB), extractable (12.5 mg/g) and non-extractable (37.7 mg/g) condensed tannins of WGP were about twice as much as that of dry GPs. There was no significant difference in total organic acids (106-115 mg/g), but the malic acid and succinic acids of dry GP were slightly higher than the WGP. Therefore, the WGP would be a good candidate for reducing enteric methane emissions. Significance. This study provides a pivotal data foundation for both upcycling value-added by-products from the US wine industry and reducing methane emissions for a sustainable and eco-friendly agriculture and food supply chain.

9:05 Biodegradable polymer nanocomposites for controlled P release and nanocellulose hydrogels for efficient delivery of NPK fertilizers Shital Vaidya1, shitalravaidya@gmail.com, Leslie R. Sigmon2, Corey Thrasher2, Savannah Phillips2, Maria S. Peresin3, Christian Dimkpa1, Howard Fairbrother2, Jason C. White1. (1) Analytical Chemistry, Connecticut Agricultural Experiment Station, New Haven (2) Analytical Chemistry, 2Johns Hopkins Univ., Baltimore, Maryland (3) Auburn Univ. System, Alabama Worldwide increased food requirements and challenges with existing fertilizers are affecting the environment negatively. With each application of traditional NPK fertilizers, most soluble N and P fails to reach the intended target and demands repetitive application of fertilizers for acceptable crop yield. To reduce the environmental impact of traditional fertilizers, we are combining benefits of nanotechnology by developing biodegradable polymer nanocomposites and nanocellulose hydrogels for controlled release and targeted delivery of nutrients. In initial greenhouse studies with tomato, polymer nanocomposites (PNCs) containing polyhydroxyalkanoate (PHA) and calcium phosphate nanoparticles were shown to produce equivalent tomato vegetive growth and fruit quality as compared to conventional phosphorus amendments but exhibited an 80% reduction in P loss from the soil. Furthermore, we also studied response of different conventional P fertilizers, calcium pyrophosphate, hydroxyapatite nanoparticles with and without PHA nanocomposites. We observed reduced P loss, efficient P uptake, and slow release of P with PHA nanocomposites of calcium phosphate dibasic, hydroxyapatite, and calcium pyrophosphate nanoparticles. In another study, we immersed nanocellulose hydrogel beads in NPK solution and coated with beeswax or densified with maleic anhydride. Water release profile suggest nanocellulose based NPK fertilizers show less loss of nutrients and enhance efficiency. Collectively these strategies show great potential for more sustainable nutrient delivery and use in agriculture

9:50 Foliar delivery of siRNA particles for treating viral infections in agricultural grapevines Aviram Avital, aviramavital@campus.technion.ac.il, Avi Schroeder. Chemical Engineering, Technion Israel Institute of Technology, Haifa, Israel Grapevine leafroll disease (GLD) is a globally spreading viral infection that causes major economic losses by reducing crop yield, plant longevity and berry quality, with no effective treatment. Grapevine leafroll associated virus-3 (GLRaV-3) is the most severe and prevalent GLD strain affecting wine production. Here, we evaluated the ability of RNA interference (RNAi), a non-GMO gene-silencing pathway, to treat GLRaV-3 in infected Cabernet

Sauvignon grapevines. We synthesized lipid-modified polyethylenimine (lmPEI) as a carrier for long double-stranded RNA (dsRNA, 250-bp-long) that targets RNA polymerase and coat protein genes that are conserved in the GLRaV-3 genome. Self-assembled dsRNA-lmPEI particles, 220 nm in diameter, displayed inner ordered domains spaced 7.3±2 nm from one another, correlating to lmPEI wrapping spirally around the dsRNA. The particles effectively protected RNA from degradation by ribonucleases and showed to increase uptake rate into plant cells as a result of the lipid component comprising the RNA carrier. In three field experiments, a single dose of foliar sprayed treatment of the RNA-particles knocked down GLRaV-3 titer, and multiple doses of the treatment kept the viral titer at baseline and triggered recovery of the vine and berries. This study demonstrates RNAi as a promising platform for treating viral diseases in agriculture.

10:20 Use of bioconjugation and encapsulation approaches for delivery of cargo for agricultural applications Sabine Dodard, Yali Liu, Jean-Danick Lavertu, Ashlyn Parrott, Shawn Clark, Usha Hemraz, Usha.Hemraz@cnrc-nrc.gc.ca. National Research Council Canada, Ottawa, Ontario There is currently an increased demand for food production arising from the growing human population, climate change and decrease in arable land. Traditional crop management technologies that often use agrochemicals to increase yields or fight pests are starting to lose their appeal due to their negative impact on human health and the environment, and their inability to continuously increase agricultural productivity. As such, there is a need to design environmentally-friendly methods to increase yields and/or provide protection against pathogens. Herein, we present different approaches that make use of bioconjugation and encapsulation to deliver cargo using nanomaterials and polymers for agricultural applications.

10:50 Nanobiotechnology-based strategies for enhanced crop stress resilience Jason C. White1, jason.white@ct.gov, Lijuan Zhao2, Arturo A. Keller3, Jorge L. Gardea-Torresdey4. (1) Connecticut Agricultural Experiment Station, New Haven (2) Nanjing Univ., Jiangsu, China (3) Univ. of California Santa Barbara (4) The Univ. of Texas El Paso College of Liberal Arts Low use and delivery efficiency of conventional agrichemicals is a significant impediment to maintaining global food security, particularly given that a 60-70% increase in food production is needed by 2050 to support the projected population. Further confounding these efforts is a changing climate, which may force increased cultivation of crops under more marginal and stress-inducing conditions. Thus, novel and sustainable strategies for enhancing food production are needed all along the "farm-to-fork" continuum. Nanobiotechnology approaches to engineer crops with enhanced stress tolerance may be a safe and sustainable strategy to increase crop yield. Under stress conditions, cellular redox homeostasis is disturbed, resulting in the over-accumulation of reactive oxygen species (ROS) that damage biomolecules (lipids, proteins, and DNA) and inhibition of crop growth and yield. However, delivering ROS-scavenging nanomaterials (NMs) at the appropriate time and place can alleviate abiotic stress. Importantly, ROS-production in living cells carries both costs and benefits. When present below a threshold level, ROS can mediate redox signaling and defense pathways that foster plant acclimatization against stress. We find that many NMs are ROS-triggering, such as nanoscale Cu, Fe, S, and CuS, but these materials have the potential to be judiciously applied to crop species to stimulate defense systems, prime stress responses, and subsequently increase the biotic and abiotic stress resistance of crops. This knowledge can be used to engineer climate-resilient crops. It is also clear that the ability to effectively tune nanoscale material structure and composition will be critical to maximizing positive impacts, including significantly reduced amounts of agrichemical use while simultaneously enhancing yield.

Citrus Flavor in the Omics Era - Virtual Session

10:05 Identification of volatile sulfur compounds as key off-flavors in mandarin juice during processing and storage Linhua Huang1,2, Huanglh@cric.cn, Yujiao Cheng1,2, Russell L. Rouseff1,2, Houjiu Wu1,2, Hua Wang1,2. (1) Citrus Research Institute, Southwest Univ., Chongqing, China (2) National Citrus Engineering Research Center, Southwest Univ., Chongqing, China From factory to consumer, the flavor quality of mandarin juice decreases as being exposure to thermal treatment, storage temperature and light. The produced mandarin juice off-flavors resulting in quality deterioration restricted its potential as commercial citrus juice. Sulfur volatiles are highly potent off-flavors which may alter juice flavors even at ultra-trace levels. Sulfur volatiles in mandarin juice were investigated by headspace solid-phase microextraction multidimensional gas chromatography−mass spectrometry/olfactometry (MDGC-MS/O) and a GC−MS/pulsed flame photometric detector (GC−MS/PFPD). Eleven volatile sulfur compounds (VSCs) have been identified in mandarin juice. Methanethiol (putrid-smelling), s-methyl thioacetate (cabbage-like), dimethyl disulfide (onion, garlic), 2-methylthiophene (green, metal, sulfur), 3-methylthiophene (astringent, burnt, plastic), dimethyl trisulfide (onion, cabbage), and ethyl(methylthio)acetate (green odor) have been identified for the first time in mandarin juices. The concentration of 5 VSCs showed significant changes during storage or shelf-life. Three VSCs (methanethiol, dimethyl trisulfide, and methional) were confirmed as key off-flavor compounds in Ponkan mandarin juice based on addition/omission experiments. The flavor deterioration marker dimethyl sulfide was identified based on off-flavor contribution and variable importance in projection (VIP) (score >1) values in the PLS-DA model. Furthermore, heat treatment, storage time and light irradiation accelerated the degradation of sulfur precursors (methionine and S-methylmethionine), as well as the formation of VSCs, which lead to an increase in off-flavor intensity of mandarin juice.

10:25 Five-year study of flavor and sensory evaluation of HLB-tolerant citrus hybrids Kristen A. Jeffries1, kristen.jeffries@usda.gov, Zhen Fan2, Xiuxiu Sun3, Elizabeth Baldwin1, John Manthey1, Wei Zhao1, Ed Stover1, Matthew Mattia1, Jinhe Bai1, Anne Plotto1. (1) USDA, ARS, Fort Pierce, Florida (2) Horticultural Sciences, Univ. of Florida Institute of Food and Agricultural Sciences, Wimauma (3) USDA, ARS, Hilo, Hawaii In an effort to combat citrus greening disease, which has devastated Florida citrus agriculture, the USDA, Agricultural Research Service (ARS) is studying a collection of hybrids showing disease tolerance. These citrus hybrids are introgressed with Poncirus trifoliata and are part of a unique breeding program that has used P. trifoliata as a source of disease and cold tolerance. P. trifoliata has an undesirable flavor, however, after several generations of crossing with Citrus, some hybrids have acceptable flavor. In order to identify hybrids with disease resistance and acceptable flavors, sensory and chemical data were collected. Citrus juice is a very complex matrix, several variables were analyzed for around 50 hybrids with multiple harvests over 5 years. With over two hundred harvest/genotype combinations, the use of tree-based modeling has identified key components for predicting orange or mandarin flavors. Compounds with strong predictive value for orange in comparison to mandarin flavor included most esters, (E)-2-hexenal, carvone and sesquiterpenes. Soluble solids over titratable acidity ratio, as well as sucrose, were strong predictors for mandarin flavor. Additionally, a broadly targeted analysis of flavonoids and limonoids adds to our understanding of

undesirable bitterness in orange juice. Taken all together, large data sets like the one described herein, will lead to the selection of disease-tolerant hybrids with good flavor quality for a stand-alone variety or for use in orange-like juice blends and a better understanding of chemical compounds important for orange flavor.

10:45 Evaluation of volatile profiles in Poncirus trifoliata-containing HLB-tolerant citrus hybrids Zhen Fan2, fanzhen@ufl.edu, Kristen A. Jeffries1, Xiuxiu Sun3, Elizabeth Baldwin1, John Manthey1, Wei Zhao1, Gabriela Olmedo1, Ed Stover1, Matthew Mattia1, Anne Plotto1, Jinhe Bai1. (1) Horticultural Research Laboratory, USDA-ARS Southeast Area, Fort Pierce, Florida (2) Horticultural Sciences Department, Univ. of Florida, Wimauma (3) Pacific Basin Agricultural Research Center, USDA-ARS, Hilo, Hawaii Orange juice (OJ) is a popular fruit juice thanks to its high nutritional value and distinctive flavor. However, OJ production has been severely impacted by the Citrus greening disease, Huanglongbing (HLB). OJ is narrowly defined by the Food and Drug Administration (FDA) as the juice from the sweet orange, Citrus sinensis. However, recent genomic analysis has revealed that sweet orange is not a true species but rather an introgression of mandarin (C. reticulata) and pummelo (C. maxima). Some hybrids from C. reticulata, and Citrus x Poncirus trifoliata, a related species, are showing greater tolerance to HLB than sweet oranges. There is now interest in using these hybrids as parents for their potential sweet orange-like flavor properties. Therefore, this study analyzed over 50 hybrids of C. reticulata, C. sinensis and Citrus x P. trifoliata over 5 years in search of an individual that would produce fruit with flavor similar to sweet oranges. Volatile compositions revealed distinct groups for oranges, mandarins and C. x P. trifoliata hybrids based on principle components analysis (PCA) and cluster analysis (CA). After multiple generations of backcrossing Citrus Sp., some P. trifoliata hybrids showed similar chemical profiles to oranges, while still retaining high levels of tolerance against HLB. A chemical correlation analysis revealed three clusters for terpenes and one cluster for esters, implying that there are shared underlying biosynthetic pathways among volatiles belonging to the same cluster. RNA was extracted from fruit juice of genotypes with extreme concentrations of terpenes and esters. Bulk segregation analysis is underway to identify key biosynthetic genes responsible for producing different groups of terpenes and esters, and natural genetic variation leading.

11:05 Effect of different rootstocks on metabolites of orange juices from HLB-affected trees Xin Liu, xin.liu@ufl.edu, Yu Wang. Citrus Reserch and Education Center, Univ. of Florida, Lake Alfred Citrus greening disease, Huanglongbing (HLB), has been causing large economic damage in the citrus industry worldwide. In this study, untargeted and targeted metabolomics strategies were used to investigate the effect of six different rootstocks (CH, Blue, 1804, FG, SW, and Volk) on metabolites of orange juices from HLB-affected trees. Untargeted metabolomics analysis showed that a total of 2531 ion features were detected using UHPLC-Q-Orbitrap HRESIMS, and 54 metabolites including amino acids, amines, flavonoids, coumarins, fatty acids, and glycosides were definitely or tentatively identified as the differential markers based on the random forest algorithm. Furthermore, 24 metabolites were verified and semi-quantified using authentic standards. Notably, the presence of specific amino acids and amines especially polyamines indicated that different rootstocks might affect glutamate, aspartate, proline, and arginine metabolism to regulate the physiological response against HLB. Meanwhile, the production of flavonoids and prenylated coumarins suggested that rootstocks influenced phenylalanine and phenylpropanoid metabolism. The possible metabolic pathways were proposed, and the important intermediates were verified by authentic standards. In addition, targeted metabolomics approach combined with flavor sensory test was employed to elucidate some key flavor compounds. Chemical profile analysis demonstrated that orange juices from different rootstocks were discriminated on the basis of orthogonal projections to latent structures discriminant analysis (OPLS-DA). Canonical correlation analysis indicated that sugar and sugar alcohols including raffinose, xylose, rhamnose, glucose, sorbitol, and myo-inositol presented strong contribution to sweetness, and amino acids such as alanine, glutamic acid, proline, arginine, serine, asparagine and aspartic acid were responsible for positive flavor quality. Limonin, adenosine, and uridine made positive contribution to bitterness. These results provide new insight on effect of rootstocks on metabolomics of HLB-affected orange juices.

11:40 Natural sweeteners and sweetness-enhancing compounds identified in citrus using an efficient metabolomics-based screening strategy Xixuan Tang, tangxx1991@ufl.edu, Zhixin Wang, Fredrick G. Gmitter, Jude W. Grosser, Yu Wang. Citrus Research & Education Center, Univ. of Florida Institute of Food and Agricultural Sciences, Gainesville Increasing demand from consumers for healthy and flavorful food has driven the exploration and development of a series of taste modulators including natural sweeteners. Preliminary studies on citrus have indicated that citrus is a good potential source of natural sweeteners or sweetness enhancing compounds. However, it is challenging to efficiently identify potential sweeteners from citrus considering the chemical complexity and relatively low abundance of sweetness associated compounds compared to sugar content in fruits. To address the challenge in exploration of potential sweeteners and sweetness enhancers from citrus fruits, a strategy combining targeted and untargeted metabolomic analyses based on an in-house database was proposed to efficiently screen and identify sweeteners or sweetness enhancing compounds from citrus. Through the examination and screening of 11 cultivars of citrus fruits, in total of eight natural sweeteners or sweetness enhancing compounds were identified, including eriodictyol, hesperetin, 3-Acetoxy-5,7-dihydroxy-4′-methoxyflavanone (ADMF), dihydroquercetin-3-acetate-4′-methyl ether (DAME), Hernandulcin, 4β-hydroxyhernandulcin, Perillaldehyde, and oxime V. Except for eriodictyol, the other seven compounds were identified from citrus for the first time. Notably, oxime V, an artificial sweetener, was identified firstly and naturally in citrus. The contents of five sweeteners or sweetness enhancing compounds in 11 cultivars of citrus obtained from two production years were also determined and compared. These findings provided insights for future agricultural practices in citrus breeding to produce cultivars with low sugar content while maintaining sweetness. The proposed strategy offered an efficient solution in the exploration and identification of taste modulators with low content in natural sources. Promisingly, it also expanded opportunities for industry to develop sugar substitute from natural products for food and beverage application.

12:00 Omics and sensorial analysis combinedly revealed characteristic aroma and consumer preference of novel citrus Zhehui Hu1,2, Mengjun Chen1,2, Kaijie Zhu1, Yuan Liu1,2, Minghua Chen1,2, Jiatao Kong1,2, Lixin Cao3, Junli Ye1, Hongyan Zhang1,2, Xiuxin Deng1, Jiajing Chen1,2, chenjiajing@mail.hzau.edu.cn, Juan Xu1,2. (1) Key Laboratory of Horticultural Plant Biology (Ministry of Education), College of Horticulture and Forestry, Huazhong Agricultural Univ., Wuhan, Hubei, China (2) Sensory Evaluation and Quality Analysis Centre of Horticultural Products, Huazhong Agricultural Univ., Wuhan, Hubei, China (3) Citrus Variety Propagation Centre, Yichang,

Zigui County, China Natural occurred novel citrus with pleasant flavor are precious to citrus industry, which could be applied as important gene donor, pollen parents or essential oil supplier plant material. Mangshanyegan (Citrus mangshanensis), C. reticulata 'chachiensis' and a brown 'Zong Cheng' navel orange (ZC) (C. sinensis Osbeck) are novel and potentially highly profit with pleasant odor. In the study, directional difference test and flash profile analysis was applied to investigated the significant differences in aroma sensorial attributes of the novel citrus fruits, combined with metabolomic analysis on volatile profiles throughout fruit development by using Gas chromatography-mass spectrometry (GC-MS), odor active substances identification via solvent-assisted flavor evaporation (SAFE), aroma extract dilution analysis (AEDA) on Gas chromatography-Olfactometry (GC-O), followed by omission experiment. As the result, β-myrcene, valencene and trans-β-ocimene was found as characteristic aroma components to ZC, which was more preferred by consumers. Finally, integrated transcriptomic analysis and gene characterization screened out two genes of TPS18 and LO1, which play important roles in valencene and linalool oxidates biosynthesis, respectively. The study lay a foundation for the flavor citrus breeding by identify the specific metabolites that satisfying consumers' preference, and will benefit the future regulatory mechanism research on flavor related volatiles biosynthesis in citrus.

12:20 Using genome-wide association as a breeding tool for healthful flavonoids in mandarin accessions Matthew Mattia1, Matthew.Mattia@usda.gov, Dongliang Du2, Qibin Yu2, Tracy L. Kahn3, Mikeal L. Roose3, Yoko Hiraoka3, Yu Wang2, Patricio R. Munoz2, Fredrick G. Gmitter2. (1) USDA-ARS US Horticultural Research Laboratory, Fort Pierce, Florida (2) Citrus Research & Education Center, Univ. of Florida Institute of Food and Agricultural Sciences, Gainesville (3) Dept. of Botany and Plant Sciences, Univ. of California Riverside Mandarins have many unique flavonoids with documented health benefits including preventing chronic human diseases. Flavonoids are difficult to measure and cannot be phenotyped without the use of specialized equipment; consequently, citrus breeders have not used flavonoid content as selection criteria to develop cultivars with increased benefits for human health or increased tolerance to diseases. In this study, peel, pulp, and seed samples collected from many mandarin accessions and their hybrids were analyzed for the presence of selected flavonoids with documented human health benefits. A genome-wide association study (GWAS) was used to identify single nucleotide polymorphisms (SNP) associated with biosynthesis of flavonoids in these mandarin accessions. There were 420 significant SNPs associated with 28 compounds in peel, pulp, or seed samples. Four candidate genes involved in flavonoid biosynthesis were identified by enrichment analysis. SNPs that were found to be associated with compounds in pulp samples have the potential to be used as markers to select mandarins with improved phytonutrient content to benefit human health. Mandarin cultivars bred with increased flavonoid content may provide value to growers and consumers.

MONDAY AFTERNOON

Recent Advances in Analytical Strategies for Food Allergen Detection and Management

2:10 Recommendations from the FAO/WHO expert consultation on food allergen risk assessment Lauren Jackson, Lauren.Jackson@fda.hhs.gov. Division of Food Processing Sci. & Tech., US FDA/CFSAN, Bedford Park, Illinois Food allergies are a global public health issue and their prevalence appears to be increasing. The labelling of food allergens in pre-packaged foods plays a key role in protecting consumers with food allergies as there are no preventative clinical treatment is currently available. Complete and accurate disclosure of allergenic ingredients on food labels is essential for consumers to make safe choices regarding the foods they purchase and consume. However, unintended allergen presence (UAP) is a major cause of packaged food recalls in the U.S. and elsewhere. In 2020, the Food & Agriculture Organization (FAO) of the United Nations and the World Health Organization (WHO) organized an ad hoc Joint Expert Consultation on Risk Assessment of Food Allergens. From 2020 – 2022, the expert panel convened on several occasions to develop recommendations on the global priority list of allergenic foods, thresholds/reference doses, and labeling strategies using thresholds/reference doses, and exemptions from allergen labeling. This presentation will summarize the recommendations from the Expert Committee. As analytical methods will be essential for implementation of thresholds/reference doses, this presentation will also discuss current analytical capabilities as well as deficiencies.

2:30 Measurement challenges of quantifying milk protein allergens in foods David Bunk1, david.bunk@nist.gov, Ashley Green1, Lisa Kilpatrick1, Melissa M. Phillips2. (1) Biomolecular Measurement Division, National Institute of Standards and Technology, Gaithersburg, Maryland (2) Chemical Sciences Division, National Institute of Standards and Technology, Gaithersburg, Maryland Existing methods for quantification of protein allergens are primarily based on immunoassay and are linked to a commodity (e.g., total milk protein, total egg protein). Quantitative methods using liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) also exist. Between methods, and often within the same method, food allergen concentration measurement equivalence is rarely observed. The lack of measurement equivalence for milk protein allergens stems from many difference sources. Potentially, the largest contribution to a lack of measurement equivalence between routine milk allergen assays is fundamental differences in the assays themselves: they aren't measuring the same things. Given that milk allergens are comprised of more than a dozen different protein species, the antibodies used in immunoassays can target any or all allergen proteins. Even for LC-MS/MS measurements, when antibodies aren't used, different target peptides from different milk proteins are frequently used in different LC-MS/MS methods, potentially leading the differences in what is being measured. Measurements that target different measurands can only be compared after conversion to a common reporting unit. A lack of measurement traceability is likely to be another significant contributor to the lack of measurement equivalence between milk allergen assays. No reference materials exist with certified values related to allergen concentration. Without reference materials to provide a target for measurement traceability, assay manufacturers assign values to their calibration materials using any means at their disposal. Reporting units for milk allergen concentrations are not standardized. Conversion between concentration units involved uses conversion factors from the scientific literature which frequently have not been validated, frequently are offered without measurement uncertainty, and are used without consensus from the food allergen measurement community. These potential sources of measurement variability will be discussed as will potential solutions to achieving measurement equivalence across assays.

2:50 Mass spectrometric analysis of allergens from pecan protein extracts: Influence of pecan heating on observable peptides and modifications Rebecca Dupre, rebecca.dupre@usda.gov, Shaina Patil, Steven W. Lloyd, Casey C. Grimm, Brennan Smith, Christopher P. Mattison. FPSQ, USDA-SEA-SRRC, New Orleans, Louisiana Due to the potential severity of nut-induced allergenic reactions, reliable and accurate methods for detection are essential.

Pecans, along with other popular tree nuts, are a widely consumed food that commonly cause serious allergic reactions. Consumers affected by nut allergies depend upon accurate food testing to make informed choices about their diets. Heat treatments during nut processing have been demonstrated to alter the IgE-reactivity of nut allergens. Differing degrees and durations of heating may induce a variety of changes in protein structure; modifications of allergen proteins during heating may hinder detection of allergens if analytical methods are not carefully developed. To account for this, arginine and lysine modifications that would be expected to block trypsin digestion were considered in heated samples. To assess the changes in observable peptides from heated samples, pecans from four commercial sources were heated at 300 °F for 12, 20, and 24 minutes. Protein extracts were digested with trypsin and separated by reverse phase liquid chromatography prior to introduction into the mass-spectrometer (MS) by electrospray. Peptide cations from pecan allergens were detected and fragmented using MS/MS to produce peak lists, which were then searched against a pecan allergen library. The peptides identified in the unheated and heated samples were systematically compared to identify robust marker peptides for each allergen. More than five candidate marker peptides from Car i 2 and Car i 4 were identified in all pecan samples, while only one distinct peptide from Car i 1 was found in all heated and unheated samples.

3:10 Detection of finfish residues on contact surfaces by enzyme-linked immunosorbent assay Xingyi Jiang, xj15@my.fsu.edu, Qinchun Rao. Florida State Univ., Tallahassee Undeclared allergenic residues are one of the leading reasons for food recalls in the US. More than 90% of undeclared allergens are caused by cross-contact, defined as unintentionally incorporating allergens from sharing storage space or production equipment. Cross-contact allergens induce potential health risks and economic loss. Finfish is one of the major allergenic foods, affecting 0.9% of adults in the US, and must be disclosed in packaged foods. Parvalbumin has been recognized as a key allergen and is responsible for 90% of finfish allergies. This study aims to establish a competitive enzyme-linked immunosorbent assay (cELISA) to quantify parvalbumin from cross-contact surfaces. Parvalbumin from four finfish species (Atlantic cod, Atlantic salmon, striped mullet and tilapia) was purified using size exclusion and anion exchange chromatography. Its conformation was investigated using reducing, non-reducing and native gel electrophoresis. The immunoaffinity, selectivity and epitope of one anti-parvalbumin antibody were investigated using non-competitive ELISA, Western blot and dot blot, respectively. One cELISA for the detection of finfish parvalbumin was developed and validated. Two surfaces, stainless steel and plastic, were used for cross-contact allergen sampling. First, the purity of parvalbumin from each finfish species was above 97%. Native parvalbumin is a mixture of monomers and oligomers, exhibiting different mobility. The covalent and non-covalent interactions in parvalbumin oligomers can be dissociated by reducing agent and detergent, respectively, leaving only the monomer under the reducing condition. Second, one anti-finfish parvalbumin antibody was characterized. It showed high immunoaffinity with finfish parvalbumin without cross-reaction with non-finfish species. One calcium-dependent epitope was identified. Third, one cELISA was established with sensitivity (limit of detection: 0.58 ppm) and reproducibility (coefficient of variance (CV) < 20%). In addition, the swabbing process showed good recovery (80-120%) and repeatability (CV < 10%) at low levels of purified parvalbumin protein (5 µg) and cod fish protein extracts (125 µg) on stainless steel (316 and 430) and plastic (polycarbonate and high-density polyethylene) surfaces. This assay demonstrated the ability to detect trace amounts of finfish proteins to minimize the risk for finfish allergic consumers and the potential for allergen risk management in the food industry.

3:30 Allergen Testing: How much is too much? Gabriella Velasco Lopez, Glopez@neogen.com. Neogen Corporation, Lansing, Michigan, Over the years awareness of food allergy has increased in the society due to its clear impact on public health. Today, most food manufacturers worldwide have implemented risk management strategies to control allergens during food production to minimize the risk of unintentional contamination of processed foods with allergenic ingredients. The effectiveness of these strategies is monitored with allergen testing methods in the manufacturing environment for raw materials and finished products. A big challenge for method developers of allergen testing technologies, is to determine what is an adequate limit of detection that is relevant to food processors. Ultimately, it is food processors who finally make critical decisions about the safety of a finished product before it is commercialized using data generated through allergen testing techniques. An important gap is the lack of established regulatory thresholds levels to define how much of an allergen is safe if present in a product. Today we are seeing advances in the application of risk assessment to add tools which intend to add health-risk information to analytical results enabling food processors to make more and consistent informed decisions based on data. In this session we will review: a) available analytical methods to the food industry; b) the value of analytical methods as verification tools to assess allergen risk management strategies; c) current guidelines and recommendations related to thresholds for allergenic foods; and d) the use of the Voluntary Incidental Trace Allergen Labelling Program as a risk assessment tool which connects the use of analytical results and its impact to allergic population.

Agri-Food Sustainability at a Crossroads: Challenges of the Food, Energy, and Water Nexus

2:05 Date palm biochar and super hydrophobic sand mulching enhance tomato (Solanum lycopersicum) plants' yields in alkaline sandy soils Nayara Vivian Huve Musskopf1,2,3, nayara.huvemusskopf@kaust.edu.sa, Kennedy Odokonyero1,2,3, Lisa Oki Exposito1,2,3, Batool Albar1,2,3, Adair Gallo1,2,3, Himanshu Mishra1,2,3. (1) Environmental Science and Engineering, King Abdullah Univ. of Sci. & Tech. Biological and Envir. Sci. & Eng., Thuwal, Makkah, Saudi Arabia (2) King Abdullah Univ. of Sci. & Tech. Water Desalination and Reuse Research Center, Thuwal, Makkah, Saudi Arabia (3) Center for Desert Agriculture, King Abdullah Univ. of Sci. & Tech., Thuwal, Makkah, Saudi Arabia Plant growth in hot and dry regions such as the Middle East suffers from water stress, heat stress, and low-fertility soils. In particular, the soils in the western Saudi Arabia are characterized by high sand content, alkalinity, salinity, and low organic matter content. In response, we have developed the following soil-amendment technologies: (1) Superhydrophobic Sand (SHS) mulch – common sand grains coated with nanoscale paraffin wax layer, and (2) date palm biochar – derived from the pyrolysis of locally abundant organic waste. SHS prevents the evaporative water loss from the topsoil, while date palm biochar enhances soil's ion-exchange capacity. We investigated the effects of these technologies on tomato (Solanum lycopersicum) plants in a field trial; also, the effects of super water absorbent polymer (SAP), consisting of potassium polyacrylate and polyacrylamide. Specifically, we probed the effects of the following soil treatments on plant growth: (i) only NPK fertilizer (control); (ii) NPK fertilizer with 1 cm-thick layer of SHS on the top; (iii) NPK fertilizer with SAP; (iv) 300 g of nutrients-loaded biochar (37% lesser N and 103% higher P content than the NPK fertilizer, plus micronutrients, including copper, manganese, sulfur, and zinc); and

(v) the combination of SHS, SAP and nutrients-loaded biochar. Remarkably, in comparison to the control (i), the soil treatments enhanced the tomato fruit yields as follows: (ii) 81%, (iii) 38%, (iv) 700%, and (v) 679%. To understand these results, we performed soil analysis that revealed higher bio-availability of some of the nutrients, such as ammonium, phosphorus, and manganese, with positive correlation with fruit yield enhancement. We will explain how the addition of biochar facilitated the nutrients exchange and accessibility in the highly alkaline soil (pH 9.2), such as the water-soluble form of phosphorus. These findings underscore the potential of date palm biochar and SHS in realizing food security in Middle East.

2:35 Engineering cation exchange capacity of date palm biochar towards a sustainable soil amendment technology Batool Albar, batool.albar@kaust.edu.sa, Nayara Vivian Huve Musskopf, Adair Gallo, Himanshu Mishra. Environmental Science and Engineering Program, Interfacial Lab, Water Desalination and Reuse Center, Center for Desert Agriculture, Biological and Envir. Sci. & Eng., King Abdullah Univ. of Sci. & Tech., Thuwal, Makkah, Saudi Arabia Biochar is derived from the pyrolysis of organic biomass, such as crop residue and food waste; and it is characterized by a dehydrated porous scaffold that is chemically stable in the soil. In fact, a number of studies world-over have demonstrated that biochar can improve soils' organic matter content, cation exchange capacity (CEC), and water holding capacity, while also facilitating long-term carbon sequestration. We will present the results of our investigation of the CEC of various biochar blends derived from the pyrolysis of date palm residues in Saudi Arabia. Given the abundance of this feedstock in the Middle East, our long-term goal is to recruit date palm biochar to enhance sandy soils' fertility in hot and dry regions. In this study, we compared the effects of post-pyrolysis oxidative modification of date palm biochar via two chemical reactions across a wide range of temperatures and durations. Remarkably, we have established protocols for enhancing biochar CEC by up to 700%. The quantitative analysis was performed by the following two independent methods: (i) saturation of the ion-exchange sites with hydronium ions; and (ii) summing up the cations extracted from biochar using the Mehlich-3 protocol. We also tracked the changes in the biochars' pH, the O/C elemental mass ratios, and surface area as a function of the post-pyrolysis treatments. Curiously, prolonged oxidative stress caused mechanical degradation of biochar, thereby releasing water-soluble acidic substances. We will describe in depth analytical and materials characterization of these materials and also comment on their potential in mitigating soil alkalinity in arid lands and the scalability of this approach for food production and greening efforts.

3:05 Effect of biochar and superhydrophobic sand mulches on evaporation and water holding capacity in sandy soils Lisa Oki Exposito1,3,4, lisa.okiexposito@kaust.edu.sa, Amr H. Al-Zu'bi1,3,4, Batool Albar1,3,4, Nayara Vivian Huve Musskopf1,3,4, Adair Gallo1,2,3, Himanshu Mishra1,3,4. (1) Environmental Science and Engineering, King Abdullah Univ. of Sci. & Tech. Biological and Envir. Sci. & Eng., Thuwal, Makkah, Saudi Arabia (2) Terraxy Corporation, Thuwal, Makkah, Saudi Arabia (3) King Abdullah Univ. of Sci. & Tech. Water Desalination and Reuse Research Center, Thuwal, Makkah, Saudi Arabia (4) Center for Desert Agriculture, King Abdullah Univ. of Sci. & Tech., Thuwal, Makkah, Saudi Arabia Realizing high irrigation efficiency in hot and arid lands is a daunting challenge due to the significant percolation and evaporation losses. Sandy soils exacerbate the situation due to their low water holding capacity that also leads to nutrients leaching. In response, we have developed two soil amendment technologies, namely SandX and Biochar, for boosting soil's water-holding capacity and curtailing evaporative losses, respectively. Specifically, SandX is a superhydrophobic material comprised of silica sand grains coated with ~20 nm-thick paraffin wax, and the biochar was derived from the pyrolysis of date palm leaves at ~500 °C. We investigate the effects of these materials on the hydraulic properties of a sandy soil (A3 - fine sand ASTM D3282) via pot studies. Experiments revealed that when SandX is applied as a 5-10 mm-tick mulch over the sandy soil in pot studies (transient state; initial soil moisture 22wt%; final soil moisture 10wt%), the evaporation loss was reduced by 54% and 70% respectively relative to the sandy soil (8.35 mmH2O/day) under an average of 40 °C and 60% relative humidity. Pot-holding capacities (PHC) for water were determined gravimetrically for sandy soil (23.63% gH2O/g of dry soil) and BC at (a) 2 and (b) 5wt% in sandy soil. PHC increased by (a) 11% and (b) 51%, respectively for the biochar treatments. The synergic effects of SandX and biochar as a function of biochar particle size and mass fraction in the soil will be presented. Our presentation will demonstrate the potential of SandX and datepalm biochar in curtailing high evaporation rates and percolation, respectively, in sandy soils in arid lands.

3:50 HPLC-UV determination of glyphosate, aminomethylphosphonic acid, and glufosinate using pre-column derivatization Pedro J. Martin1, pedro.martin@uci.edu, Ke He2, Lee Blaney2, Shakira R. Hobbs1. (1) Univ. of California Irvine (2) Univ. of Maryland Baltimore County, Baltimore Derivatization enhances analytical sensitivity and enabling the use of conventional detectors for measurement of these emerging contaminants. Typically, derivatization involves attachment of a chromophore or fluorophore to the amino moiety in the herbicide. Pre-column derivatization is preferred to post-column processes due to the simplified logistics, enhanced separation, and high sensitivity. The detection of glyphosate, glufosinate, and aminomethylphosphonic acid (AMPA) in environmental samples is crucial to understanding ecotoxicity and threat to human health. It is difficult to develop a reliable analytical approach for assessing the environmental presence of glyphosate, glufosinate, and AMPA because of inadequate knowledge on the effects of different derivatizing techniques on detecting these compounds. This study reports a reproducible analytical method for glyphosate and glufosinate using pre-column derivatization, high performance liquid chromatography (HPLC) separation, and ultra-violet (UV) detection. The sensitivity of the pre-column derivatization with 9-fluorenylmethylchloroformate (FMOC-Cl) was reliant on reaction duration, EDTA concentration, and borax buffer strength. The addition of EDTA to the reaction medium minimized the occurrence of metallic complexation. Increased concentrations of FMOC-Cl and EDTA resulted in significantly higher response ($p < 0.05$). The lower concentration of the derivatizing agent and borax shortened the reaction time from 24-h to 4-h. The borax buffer ensured the alkaline conditions necessary for the complete reaction of the target analytes and the FMOC-Cl. The conditions for successful derivatization involved a 4-h derivatization period after addition of 2.5 mM FMOC-Cl, 5% (w/v) borate buffer, and 1% (w/v) EDTA. This study fills knowledge gaps in the development of sensitive analytical methods for detecting glyphosate, glufosinate, and AMPA at low concentrations. The limits of detection were 0.60 μg/L, 0.15 μg/L and 0.37 μg/L for glyphosate, glufosinate, and AMPA respectively. This method has the potential to enable herbicide measurements for environmental science due to instrument accessibility and cost, simplicity and high reproducibility. Furthermore, this analytical technique can provide practical solutions for protecting vulnerable ecosystems and human health and advancing agroecosystem management.

4:20 Effects of superhydrophobic sand mulches on steady-state water evaporation fluxes Amr H. Al-Zu'bi4,1,3, amr.alzubi@kaust.edu.sa, Lisa Oki Exposito4,1,3, Jiaqi Zheng2, Adair Gallo4,1,3, Himanshu Mishra4,1,3. (1) Environmental Science and Engineering Program,Interfacial Lab, Water Desalination and Reuse Center., King Abdullah Univ. of Sci. & Tech. Biological and Envir. Sci. & Eng., Thuwal, Makkah, Saudi Arabia (2) Tongji Univ. College of Electronic and Information, Shanghai, China (3) Center for Desert Agriculture, Biological and Envir. Sci. & Eng., King Abdullah Univ. of Sci. & Tech., Thuwal, Makkah, Saudi Arabia (4) King Abdullah Univ. of Sci. & Tech. Biological and Envir. Sci. & Eng., Thuwal, Makkah, Saudi Arabia Food–water security is a matter of great concern in regions endowed with hot and arid climates, e.g., the Middle East, California, western Australia, and northwestern India. Under these conditions, the evaporation of water from the topsoil can be as high as 60% of the total evapotranspiration budget for some cultivars; consequently, irrigation efficiencies are abysmal . In response, our team has pioneered SuperHydrophobic Sand (SHS) mulch technology to reduce the evaporative water loss from the topsoil. Here, we have developed an experimental setup to systematically measure and compare the evaporation fluxes of bare and SHS-mulched soil columns in a steady-state regime as a function of water table depth, surface heat flux, soil-type, and water-retaining materials. Evaporative losses of water were quantified from bare (0 mm) and mulched (5 and 10 mm-thick SHS layers) soils comprised of (i) fine sand , and (ii) silica sand with larger grain size. Remarkably, the use of 10 mm-thick SHS layer reduced the evaporative flux ≈80% in comparison with the bare soil. An image analysis software was developed to realize a simple and inexpensive method to analyze results of multiple experiments in parallel. This experimental design and image analysis software present a simple but realistic platform to study heat and mass transfer across soils as a function of soil-amendment technologies. A heat and mass transfer model will also be presented to provide mechanistic insight into these experiments.

AGFD General Poster Session and Undergraduate Poster Competition – Virtual Session - Noon

Screening and remodeling of enone oxidoreductase for high production of 2(or 5)-ethyl-5(or 2)-methyl-4-hydroxy-3(2H)-furanone in Saccharomyces cerevisiae Xiaomeng Fu, 1019207099@tju.edu.cn, Kunqiang Hong, Chuanbo Zhang, Wenyu Lu. School of Chemical Engineering and Technology, Tianjin Univ., Tianjin, China 4-Hydroxy-2(or 5)-ethyl-5(or 2)-methyl-3(2H)-furanone (HEMF), also called homo furaneol or 2 (or 5)-ethyl-4-hydroxy-5 (or 2)-methyl-3(2H)-furanone, is an important industrial aromatic compound that exhibits the unique characteristic of keto–enol tautomerism. HEMF is a safe edible flavoring agent approved for use by the American Flavor and Extract Manufacturers Association of the US (FEMA) and has been developed as a raw flavoring material. Owing to its unique fragrance, HEMF is widely used as a food flavoring agent and has high demand. Enone oxidoreductase is a vital enzyme involved in HEMF production. In this study, an enone oxidoreductase from Naumovozyma dairenensis CBS 421 (NDEO) was used for HEMF production for the first time. The mutant NDEOT183W, K290W was obtained through semirational protein engineering, which increased HEMF yield by 75.2%. Finally, the engineered strain BM4 produced the highest HEMF yield, 194.42 mg L-1 in 132h, this yield was 7.2-fold higher than that of BY4741. Very few studies have reported on microbial production of HEMF. We believe that our proposed strategy will be helpful in accelerating the industrial production of HEMF and realizing the commercialization of more high-value natural products in the future.

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) Dept. of Bioscience Technology, Chung Yuan Christian Univ., Taoyuan City, Taiwan (2) Institute of Food Safety and Health Risk Assessment, 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 APAPinduced liver injury in Balb/c mice. The mice were randomly divided into control, APAP (400 mg/kg), APAP+N-acetylcysteine (NAC) as a positive control, APAP+CD-EE (250 and 500 mg/kg bw), APAP+Nob (50 mg/kg bw), and APAP+Tan (50 mg/kg bw). The mice were oral administrated with NAC, CD-EE, Nob or Tan once daily for nine weeks, and injected intraperitoneally (i.p.) with APAP 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.

Methodologies and strategic studies to estimation methods to reduce carbon emissions on climate change Edward J. Parish3, Hiroshi Honda1, chrishonda@yahoo.com, Shwn-meei Lee2, Gui Ren4, Wei-Ping Wang5. (1) Bioengineering, Northwestern Polytechnic Univ., Fremont, California (2) International Management, Hsiuping Univ. of Sci. & Tech., Dali, Taiwan (3) Chemistry, Auburn Univ., Auburn, Alabama (4) Economics, Shanghai Univ., Shanghai, China (5) Hotel and Management, Overseas Chinese Univ., Taichung, Taiwan Novel approaches to the application of estimation methodologies to reduce carbon emission on climate change.

Polyphenolic antioxidants as inhibitors of the advanced glycation endproducts Manal Atty1, matty@soka.edu, Jatin Mehta2, Avinash Vadapalli2, Zahra Afrasiabi1, Prakash Reddy2. (1) Soka Univ. of America, Aliso Viejo, California (2) Missouri Univ. of Sci. & Tech., Rolla Advanced glycation endproducts (AGEs), which are formed through Maillard reactions of reducing sugars with proteins, are implicated in various pathophysiological effects. The AGEs formed during food processing and storage control food quality parameters, including taste, aroma, color, and flavor. Toward attenuating the formation of the AGEs in the Maillard reactions, in the present research we have investigated the effects of various polyphenolic antioxidants from natural resources on the Maillard reactions of D-glucose with L-leucine, using NMR and fluorescent spectroscopy. Our data show that polyphenolic antioxidants are effective antiglycating agents.

Capsaicin attenuates oleic acid-induced lipid accumulation via the regulation of circadian clock genes in HepG2 cells run li1, runli677@163.com, Muwen Lu1, Chi-Tang Ho2. (1) College of Food Science, South China Agricultural Univ., Guangzhou, Guangdong (2) Dept. of Food Science, Rutgers, The State Univ. of New Jersey, New Brunswick Obesity and overweight have become a serious health problem in the world, which are linked to a

variety of metabolic disorders. Phytochemicals with weight-loss effect have been widely studied for past few decades. Capsaicin is the major bioactive component in red chili peppers with many beneficial functions. Its anti-obesity effects have been evaluated extensively using different model systems, including cell models, animal models and human subjects. The attenuation effect of capsaicin on oleic acid (OA)-induced lipid accumulation in HepG2 cells was evaluated in respect of circadian clock gene expressions. Lipid profiles, including triacylglycerols, total cholesterols, high-density lipoproteins, low-density lipoproteins and aspartate aminotransferase content were measured using enzymatic assay kits. The mitochondrial membrane potential, cellular redox status and lipid droplet morphology were also determined by different assay kits and staining methods. The mRNA and protein expressions of core circadian clock genes and major lipometabolism-related factors were assessed using RT-qPCR and western blotting. Results showed that 50 μM capsaicin alleviated the circadian desynchrony and inhibited OA-induced ROS overproduction (from 166.44 ± 12.63% to 119.90 ± 5.43%) and mitochondria dysfunction from (0.60 ± 0.08 to 0.83 ± 0.09, represented by the red/green fluorescence ratio) in HepG2 cells. The amelioration effect of capsaicin on OA-induced lipid accumulation was weakened after Bmal1-knockdown, demonstrating that the rhythmic expression of circadian clock gene is involved in the regulation process of capsaicin in lipid metabolism.

Effects of moringa isothiocyanate-rich seed extract on muscle atrophy in C2C12 cells Renalison Farias-Pereira, r.fariaspereira@rutgers.edu, Malia Ahmed, William Bui, Keerthana Thirunavukkarasu, Ilya Raskin. Plant Biology, Rutgers The State Univ. of New Jersey, New Brunswick Moringa isothiocyanate-1 (MIC-1, also known as moringin) is an isothiocyanate that composes up to 40% of moringa seed extract (MSE). Previously it was shown that MIC-1 inhibited lipopolysaccharide-induced inflammation in skeletal muscle, however little it is known about the MSE and MIC-1's effects on muscle atrophy-related pathways. To investigate the beneficial effects of MSE and MIC-1, muscle atrophy was induced by dexamethasone or lipopolysaccharide as models. MIC-1 (1 μM) and MSE (at equivalent dose of 1 μM MIC-1) did not reduce viability of muscle cells at different stages. Dexamethasone and lipopolysaccharide reduced myotubes size by upregulating the muscle atrophy-related molecular targets, the E3 ubiquitin ligases Trim63 (a.k.a. Murf1) and Fbxo32 (a.k.a. Atrogin1). However, MIC-1 and MSE partially prevented the muscle atrophy. The reduction of muscle atrophy markers by MSE and MIC-1 were strongly associated with the downregulation of Trim63, rather than Fbxo32. Furthermore, Trim63 was identified as a molecular target for MSE and MIC-1's improvements on skeletal muscle health in C2C12 cells. These results suggest that Moringa oleifera extracts and their related isothiocyanates may improve skeletal muscle health at different conditions.

Investigating secondary metabolites produced by a beneficial root endophyte for improving Canadian Prairie field crops Krista Gill, krista.gill@agr.gc.ca. Saskatoon Research and Development Centre, Agriculture and Agri-Food Canada, Saskatoon, Saskatchewan Root endophytic fungi are often a critical component of the plant root microbiome. Piriformospora indica is an axenically cultivable endophytic basidiomycete that was originally isolated from the Indian Thar desert. This fungus can colonize the roots of a broad range of plants and provides many beneficial effects including increasing resistance to biotic and abiotic stresses, nutrient uptake and yield. We explored the secondary metabolites produced by this fungus and their involvement in these beneficial effects to host plant systems. To achieve this, P. indica was cultured on 7 different solid media, extracted, and analyzed for in vitro production of secondary metabolites. The extracts were evaluated for their impact on the growth of the model plant Arabidopsis thaliana. Characterization of the secondary metabolite profile of this beneficial endophyte can lead to an improved understanding of these fundamental plant-microbe interactions and can lead to development of bioproducts that can improve crop production and contribute to sustainable crop production.

MONDAY EVENING 8:00pm
AGFD Sci-Mix
See first 19 abstracts from the Sunday evening AGFD General Poster Session and Undergraduate Poster Competition (above)

TUESDAY MORNING March 28
Biomarkers of Food or Drug Intake: Chemistry at the Intersection of Human Health Applications
8:05 GC saves lives! Determination of short chain fatty acids (SCFA) in human fecal samples Lee N. Polite1, lee@axionlabs.com, Nikolas L. Polite1, Morganne M. Freeman2, Amandeep Sandhu2. (1) Axion Analytical Laboratories Inc, Chicago, Illinois (2) Dept. of Food Science and Nutrition, Institute of Food Safety and Health, Illinois Institute of Technology, Chicago Short Chain Fatty Acids (SCFA's) may be best known for their unpleasant odors, but they are also key indicators of serious human digestive disorders such as colorectal cancer and celiac disease. Unfortunately, the SCFA's are not easy to measure and the matrix is...poop! Current methods involve extensive sample preparation: pH adjustments, water / ether extractions, filtering, etc. The excessive sample manipulation leads to a sacrifice in precision and sensitivity. Fortunately, this can all be mittigated by applying modern chromatography technology to legacy methods. The first method improvement involved reducing sample preparation from 6 steps to just one: water extraction. Historically, water is not injected into GC's due to its excessive expansion coefficient (1200x). However, modern GC's can handle direct water injections by using a pressure-pulsed injection to dramatically reduce the volume of water vapor. The next method simplification employs headspace GC to eliminate the one remaining step of sample preparation: dissolving the sample. Headspace is best suited for the determination of volatile compounds in a complex matrix. There is no question as to the volatility of the analytes (they smell!) and the complexity of the sample "matrix". The raw sample is placed into a headspace vial, and just the volatile compounds (SCFA) are injected into the GC. This approach leaves behind all of the non-volatile extractables and keeps the GC inlet much cleaner. The latest method improvement takes advantage of Solid Phase Micro Extraction (SPME). In this case, a fiber coated with an adsorbent is introduced to the vapor surrounding the sample: the volatile analytes stick to the fiber and release when inserted into the hot injection port. Imagine a method where the analyst simply waves their "magic wand" (SPME fiber) around the sample and then inserts it into the hot GC. These method improvements will allow medical researchers to analyze more samples on simpler equipment with greater sensitivity and precision…while reducing the amount of time the analyst has to spend with the malodorous samples!

8:25 Effect of wholegrain particle size on breath metabolites in type 2 diabetes and normoglycaemia Caleb Robinson1,2, Tracy Perry1, Lisa Te Morenga2,3, Jill Haszard1, Jim Mann1,2, Patrick Silcock1, Graham Eyres1, graham.eyres@otago.ac.nz. (1) Univ. of Otago, Dunedin, New Zealand (2) Centre of Research Excellence, Riddet Institute, Palmerston North, New Zealand (3) Research Centre for Hauora and Health, Massey Univ., Palmerston North,

Manawatu-Wanganui, New Zealand Consumption of wholegrains are associated with reduced risk of type 2 diabetes and a lower glycaemic response compared to consumption of refined wholegrains. However, the effects of wholegrain particle size on the volatile metabolites in exhaled breath are currently unknown. The aim of this study was to evaluate the dynamic changes in exhaled breath metabolites and glycaemic response following consumption of food samples containing 50 g of available carbohydrate. People with normal glucose tolerance (NGT) and type 2 diabetes participated in a randomised crossover study. Volatile metabolites were measured in end tidal breath over 3-6 hours using proton transfer reaction mass spectrometry (PTR-MS) following consumption of three test foods. These included: a glucose drink and two types of wholegrain breads differing only in wheat grain particle size one made with finely milled wholegrain wheat, the other with a mixture of intact, kibbled and finely milled wheat. PTR-MS distinguished different patterns in the volatile metabolites in exhaled breath post-consumption between test foods and between subjects with and without type 2 diabetes, demonstrating significant differences in metabolism following consumption of wholegrain foods of differing intactness. Analysis of volatile metabolites in exhaled breath thus provides a novel approach to understand how foods are digested and metabolised in real time.

8:45 Novel and efficient UHPLC/MS/MS method for assessing glucoraphanin and sulforaphane bioavailability in biological samples Wei Zhu1, Larry A. Lerno3, Eleonora Cremonini1, Patricia Oteiza1, Angela Mastaloudis5, Gail Bornhorst2,4, Alyson E. Mitchell2, aemitchell@ucdavis.edu. (1) Nutrition and Environmental Toxicology, Univ. of California Davis (2) Food Sci. and Tech., Univ. of California Davis (3) Viticulture and Enology, Univ. of California Davis (4) Biological and Agricultural Engineering, Univ. of California Davis (5) Brassica Protection Products, Baltimore, Maryland The health benefits associated with the consumption of cruciferous vegetables (Brassicaceae family) are largely attributed to glucoraphanin (GR), which must be enzymatically hydrolyzed into its bioactive form sulforaphane (SF). SF is absorbed and metabolized primarily in intestinal epithelial cells to sulforaphane-glutathione (SF-GSH), sulforaphane-cysteine (SF-CYS) and sulforaphane-N-acetyl-cysteine (SF-NAC); each have been shown to have therapeutic effects. Clinical investigations of GR, SF and SF metabolites however, require a robust, sensitive and high throughput method that can be applied to a range of biological tissues (plant, digesta, culture medium, cell lysates). Currently-available methods require sample pre-treatment with solid phase extraction (SPE); increasing analysis time and reducing sensitivity. To address this, a novel UHPLC-QQQ-MS/MS method without SPE pre-treatment was developed and used for the simultaneous determination of GR and SF metabolites in a range of biological materials. The LODs for this 9 min method ranged from 0.03 to 1.95 µg L-1 and the LOQs ranged from 0.06 to 3.90 µg L-1. The intra- and inter-day variation was ≤ 15 %. Linearity ranged from 3.90-1000 µg L-1 (GR), 0.06-500 µg L-1 (SF), 3.90-1000 µg L-1 (SF-NAC) and 31.25-1000 µg L-1 for SF-CYS and SF-GSH. The matrix recoveries ≥ 85 %. The method was validated by determining transport and metabolism of SF in Caco-2 monolayers and in broccoli seed powder. Results indicate that 70% of SF was absorbed, transported, and metabolized (SF-CYS, SF-GSH, SF-NAC) in the Caco-2 monolayers after 4 h incubation. This is a robust, time- and cost-efficient method for measuring GR, SF and its metabolites in biological samples and is suitable for high throughput application in clinical trials.

9:05 Phytocannabinoids' therapeutic effects on endometriosis Taylor Melville, tayloremelville1@gmail.com. Graduate School of Biomedical Sciences and Professional Studies, Drexel Univ. College of Medicine, Philadelphia, Pennsylvania The Endocannabinoid System is responsible for maintaining homeostasis by regulating processes such as chronic pain and stress through the Cannabinoid Type 1 and 2 Receptors. These receptors can be activated by phytocannabinoids, such as Delta-9-tetrahydrocannabinol (Δ9-THC) and Cannabidiol (CBD), which are plant-derived molecules from the Cannabis Sativa plant that produce medicinal effects or euphoria. Cannabinoid receptors have been implicated in the amelioration of disease symptoms such as those of endometriosis. Endometriosis is a common disease in individuals assigned female at birth (AFAB) and is characterized by the presence of endometrial tissue outside of the uterine cavity, commonly associated with chronic pelvic pain and infertility. Roughly 176 million AFAB individuals around the world endure the symptoms of endometriosis throughout their reproductive years. Therefore, this research asks whether phytocannabinoids can effectively treat symptoms of endometriosis. A literature review of numerous studies on phytocannabinoid use to treat endometriosis was conducted. Based on an analysis of these studies, phytocannabinoids relieved feelings of pain and cognitive impairment in patients with endometriosis. In addition, the size of the extrauterine tissue was reduced in endometriosis subjects treated with THC. The use of mouse models and self-reported data were strong limitations of the studies; therefore, the results are not completely generalizable. In the future, it will be important to conduct clinical trials to provide clearer evidence on the translatability of these results to AFAB individuals with endometriosis.

9:25 Coffee biomarker candidates – structures of conjugated atractyligenin metabolites Roman Lang, r.lang.leibniz-lsb@tum.de, Coline Czech, Anja Beusch, Sebastian Dirndorfer. Leibniz Institute for Food Systems Biology at the Technical Univ. Munich, Freising, Bayern, Germany Consumption of roasted coffee is a daily pleasure for many people around the world. Assuming coffee affects human health due to the abundance of bioactive compounds, its short- and long-term impact is investigated in nutritional studies. Such studies need the participants to self-report their diet in questionnaires, but these data are often biased. Coffee specific biomarkers could help objectify the data eg. in terms of compliance control during wash-outs or intervention periods. Conjugated urinary metabolites of the diterpenoid atractyligenin have been suggested as coffee specific biomarker candidates, but the conjugates' structures have been elusive so far. We conducted a MS-guided fractionation of pooled coffee drinkers' urine to isolate three conjugated metabolites. NMR and ToF-MS investigation revealed the conjugated compounds as atractyligenin-19-O-β-D-glucuronide (M1), 2β-hydroxy-15-oxoatractylan-4α-carboxy-19-O-β-D-glucuronide (M2), and 2β-hydroxy-15-oxoatractylan-4α-carboxylic acid-2-O-β-D-glucuronide (M3). Further, free atractyligenin was isolated from urine. Knowledge of the structures enables the development of dedicated methods to investigate how long and how sensitive coffee consumption can be detected.

9:45 Biomarker detection using GC-ion mobility spectrometry Wolfgang Vautz, w.vautz@ion-gas.de, Chandrasekhara Hariharan, Sascha Liedtke. ION-GAS GmbH, Dortmund, Germany Ion mobility spectrometry (IMS) is a very sensitive and rapid analytical tool for trace gases, first applied for military and security purpose (chemical warfare, explosives and drug detection). In the last 2 decades, in particular by coupling IMS with gas-chromatographic (GC) pre-separation, thus enabling the rapid (seconds - few minutes), sensitive (down to the pptV level) and selective analysis of extremely complex and humid samples, more and more civil

applications have been developed. It is obvious, that those characteristics make the method attractive for the detection of biomarker compounds. In recent years, we furthermore implemented a MEMS-based pre-concentration system, thus obtaining sensitivities down to the ppqV concentration range. Thus, mobile GC-IMS systems are available which is broadening the fields of application. After a brief introduction into the analytical method and instrumentation, particular examples focused on biomarker detection in various fields will be addressed e.g., biomarker detection in exhaled breath for diagnosis, therapy control and drug level monitoring, including medication as well as drugs of abuse. Moreover, microbial volatiles were detected from cultivated bacteria for their rapid identification via their characteristic biomarker patterns (after 4—6 h of incubation) from medical samples to enable an early specific antibiotic therapy and from food samples to detect microbial contaminations. Last but not least, bio-process control was developed detecting biomarkers from yeasts and fungi during fermentation processes.

10:20 Methanol detection in exhaled breath, drinks and sanitizers with a handheld device Andreas Guentner1,2, Andreas.Guentner@ptl.mavt.ethz.ch. (1) Eidgenossische Technische Hochschule Zurich, Switzerland (2) UniversitatsSpital Zurich, Switzerland Methanol poisoning outbreaks after consumption of adulterated alcohol or sanitizers frequently overwhelm health care facilities in developing countries. Here, we present how a recently developed low-cost and handheld breath detector can serve as a non-invasive and rapid diagnostic tool for methanol poisoning [1]. The detector combines a separation column and a micromachined chemoresistive gas sensor [2] fully integrated into a device that communicates wirelessly with a smartphone [3]. The performance of the detector is validated with methanol-spiked breath of 20 volunteers (105 breath samples) after consumption of alcoholic beverages. Breath methanol concentrations were quantified accurately within 2 min in the full breath-relevant range (10 – 1000 ppm) in excellent agreement (R2 = 0.966) with benchtop mass spectrometry (PTR-TOF-MS). Bland-Altman analysis revealed sufficient limits of agreement (95% confidence intervals), promising to indicate reliably the clinical need for antidote and hemodialysis treatment. This simple-in-use detector features high diagnostic capability for accurate measurement of methanol in spiked breath, promising for rapid screening of methanol poisoning and assessment of severity. It can be applied readily by first responders to distinguish methanol from ethanol poisoning and monitor in real time the subsequent hospital treatment. The device can also be applied as analysis tool to screen alcoholic beverages [4] and sanitizers [5] by head-space analysis to prevent poisoning cases.

10:40 Use of exogenous compounds for monitoring human metabolic processes Franziska Lochmann, Florentin Weiss, Valentina Stock, Veronika Ruzsanyi, Veronika.Ruzsanyi@uibk.ac.at, Chris A. Mayhew. Institute for Breath Research, Univ. Innsbruck, Tirol, AT, Academic, Austria In recent years, there has been a growing realization that exogenous compounds and their resulting metabolic volatiles provide ideal probes to metabolic processes. We are undertaking in vitro and in vivo studies to enhance the potential of exogenous compounds for use in non-invasive breath tests. In vitro. Extensive polymorphisms in a major group of drug-metabolizing enzymes, the cytochrome P450 family (CYPs), cause differences in metabolism influencing the therapeutic efficacy of drugs. The use of biomarkers as predictors to drug response provides insight into a patient's ability to metabolise a given medication. A patient's drug tolerance is often just estimated, based on reported side effects or a subjective evaluation by the patient. The use of metabolic volatile biomarkers that can be detected in exhaled breath would enable fast non-invasive screening tests to be developed for determining drug tolerability. In our current research, we focus on potential specific CYP substrates that result in unique volatile metabolites. Substrates are being tested using cell cultures. Currently, we are investigating HepG2 cells expressing recombinant CYP3A4 and CYP2C9. The amount of a substrate and the expected target compounds are monitored using LC-MS and GC-MS, after extraction of the analytes from the cell culture's medium. In vivo. Suitable substrates for investigating metabolic processes can be medication or treatments, such as inhalation anaesthetics. The washout study of anaesthetics from the body form a major clinical study we have been undertaking for several years. This study provides useful information that can be used to determine what influences the rate of elimination of the inhalation anaesthetics from the human body. Results from the above research programmes will be discussed in detail, with additional considerations taking into account substrate eligibility (volatility, solubility, take-up by the cells, metabolic rate and overall usability for future enzyme activity tests).

11:00 Washout of terpenes in breath following ingestion of a peppermint oil supplement Y Lan Pham1,2, y.lan.pham@ivv.fraunhofer.de, Ruyi Yu1,3, Jonathan Beauchamp1. (1) Sensory Analytics and Technologies, Fraunhofer-Institut fur Verfahrenstechnik und Verpackung IVV, Freising, Bayern, Germany (2) Chair of Aroma and Smell Research, Friedrich-Alexander-Univ. Erlangen-Nurnberg, Bavaria, Germany (3) Chair of Food Chemistry and Molecular Sensor Technology, Technische Univ. Munchen Fakultat Wissenschaftszentrum Weihenstephan fur Ernahrung Landnutzung und Umwelt, Freising, Bavaria, Germany Trace chemicals in exhaled breath can convey information about the physiological state of the donor. Besides markers of biochemical metabolism or disease-related imbalances, breath can contain volatile components and/or metabolites from dietary and/or pharmaceutical intake. The sequence of absorption, distribution, metabolism and excretion (ADME), commonly exploited in pharmacokinetics studies focusing on serum or urine, can be similarly assessed via breath analysis. This phenomenon has recently been put forward in the field of breath research as an approach for quality assurance/control, through its use as benchmark to compare for sampling protocols and analytical platforms. Known as the Peppermint Experiment, the procedure involves performing regular breath analyses of a small healthy cohort after supplement intervention. Specifically, study participants are required to ingest an encapsulated, over-the-counter capsule containing peppermint oil and provide breath samples at specified intervals over a 6 h period. Over the course of time, the terpenoid constituents of the oil are absorbed in the gut, then transported via the bloodstream to the lungs, where they enter the gas-phase and are excreted via exhalation. Quantitation of these terpenes in breath over time provide data for washout curves, which can subsequently be compared to benchmark values to ascertain alignment with other methods. In the present work, the washout curves of peppermint-derived terpenes were determined across a cohort of ten volunteers through use of three analytical platforms, namely comprehensive gas chromatography time-of-flight mass spectrometry (GCxGC-TOFMS), proton transfer reaction time-of-flight mass spectrometry (PTR-TOFMS) and gas chromatography ion mobility spectrometry (GC-IMS). This talk will introduce the concept of the Peppermint Experiment, discuss the experimental design and report on the outcomes between the analytical platforms (inter-instrumental) and different participants (inter-individual). The strengths and shortcomings of this benchmarking approach will be addressed, as will its implications for other pharmacokinetic studies in relation to food and drug intake.

11:20 Using exhaled nitric oxide to evaluate and quantify regional airway response to inhaled medications Jessica Saunders1, Charles Clem1, Yi Zhao2, Benjamin Gaston1, Michael Davis1, mdd1@iu.edu. (1) Pediatrics, Indiana Univ. School of Medicine, Indianapolis (2) Biostatistics and Health Data Science, Indiana Univ. Purdue Univ. Indianapolis Introduction: Measuring airway pH is challenging and can be done directly or indirectly. Direct measurement requires bronchoscopy and is only reflective of the pH of the areas reachable by bronchoscopy. Indirect measurement can be done using exhaled breath condensate (EBC) pH or acute changes in exhaled nitric oxide (eNO). Both of these indirect methods are sensitive for detecting changes in airway pH but nonspecific with regards to the location within the airways they represent. Moreover, these indirect methods, while representative of airway pH, do not provide an exact measurement of airway pH. A non-invasive method for precisely measuring airway pH compartmentally would allow for detection of local airway pH imbalances and quantification of response to inhaled alkaline therapies. We hypothesized that inhalation of Optate, a safe aerosolized alkaline medication that increases airway pH, would result in compartmental changes in eNO representative of areas of deposition of inhaled Optate. We further hypothesized that we could use these compartmental changes in eNO in conjunction with a modified version of the Henderson-Hasselbalch equation to calculate the pH in each compartment. Methods: Compartmental eNO was measured in healthy human subjects and subjects with asthma before and immediately after inhalation of Optate. Compartmental eNO measurement consists of three exhalations at different flow rates: 30 mL/sec (representing tracheal eNO), 100 mL/sec (representing eNO from the middle airways), and 300 mL/sec (representing acinar eNO). % change was compared in each compartment of each subject after inhalation of Optate. Basline airway pH was directly measured during research bronchoscopy. These values were used in a modified Henderson-Hasselbalch equation to calculate compartmental airway pH. Results: eNO decreased significantly in all compartments ($n = 10$, $p < 0.001$), but not equally. These values were succesfully entered into the modified Henderson-Hasselbalch equation to estimate regional airway pH. Conclusion: Compartmental eNO can be measured by collection of eNO at different expiratory flow rates, and changes differentially between compartments in which aerosol deposition differs. This may allow for the evaluation of compartmental airway

General Papers

8:05 Rapid identification of foodborne bacteria using single-cell Raman spectroscopic analysis combined with a conditional generative adversarial network Kaidi Wang1, kaidi.wang@mail.mcgill.ca, Xiangyun Ma2, Xiaonan Lu1. (1) Food Science and Agricultural Chemistry, McGill Univ. Faculty of Agriculture and Environment, Sainte-Anne-de-Bellevue, Quebec, Canada (2) School of Precision Instrument and Optoelectronics Engineering, Tianjin Univ., China Rapid detection of bacteria at an early stage is crucial to ensure food safety. Raman spectroscopy has been widely used in the detection and identification of foodborne bacteria as it is reliable, label-free, and easy to perform. However, Raman spectra for single-cell analysis are hindered by relatively low signal-to-noise ratio (SNR) and analytical speed. This study aimed to identify different foodborne bacteria using Raman spectroscopy at single-cell level and accelerate the detection using a conditional generative adversarial network (CGAN). Five major foodborne bacteria were investigated, including Campylobacter jejuni, Escherichia coli, Listeria monocytogenes, Staphylococcus aureus, and Salmonella enterica. A total of 1000 single-cell Raman spectra of these bacteria were collected using a homebuilt confocal Raman spectroscopic system with a 671-nm laser. A CGAN was developed to improve the SNR of single-cell Raman spectra and reduce the spectral collection time. Bacterial classification was performed using a convolutional neural network. SNR of single-cell Raman spectra increased from 3.35 to 20.27 after spectral recovery using CGAN and the processed Raman spectra recovered most spectral features. An identification accuracy of 94.9% was achieved for the classification of bacteria using CGAN-recovered single-cell Raman spectra, compared to 60.5% using unprocessed spectra. CGAN can accelerate data acquisition time by one order of magnitude (i.e., 30 s versus 3 s) by improving the SNR by a factor of ~ 6. To conclude, we proposed a rapid and reliable approach to identify foodborne bacteria using single-cell Raman spectroscopy combined with CGAN, providing a powerful tool for epidemiological surveillance of foodborne pathogens in the agri-food chain.

8:25 Natural colorants in plant-based foods: Impact of colorant and droplet characteristics on optical properties of oil-in-water emulsions Donpon Wannasin, dwannasin@umass.edu, David Julian McClements. Food Science, Univ. of Massachusetts Amherst Appearance is the first sensory attribute consumers experience of foods, which therefore has a great influence on consumers choice and liking. For plant-based foods, like meat, fish, egg, or milk analogs, it is important to use pigments that have been derived from natural botanical sources. In general, the appearance of plant-based foods is a result of light absorption by chromophores and light scattering by particles. The objective of this study was to examine the impact of food composition and structure on the appearance of plant-based foods. Oil-in-water emulsions were used as model systems because their composition and structure can easily be controlled and measured. Three plant-based pigments were selected to represent the three primary colors: red beet (red), turmeric (yellow), and butterfly pea flower (blue). Colorant (colorant type and concentration) and oil droplet (size and concentration) characteristics had a significant impact on the chromaticness and lightness of the emulsion. The color intensity of the emulsions increased with increasing colorant concentration, decreasing droplet concentration, and increasing droplet size, which was attributed to greater light absorption by the chromophores. The lightness of the emulsions increased with decreasing colorant concentration, increasing droplet concentration, and decreasing droplet size, which was attributed to greater light scattering effects. We hypothesized that plant-based foods with similar appearances to animal-based ones could be created by blending emulsions with different primary colors. In future studies, the optical properties of various animal-based products (meat, fish, eggs, and milk) will be characterized, and then their colors will be matched by blending different ratios of the three primary-colored emulsions (red, blue, yellow). The results from this project will help to formulate plant-based foods with more similar appearances to the animal-based ones they are designed to replace, which will help attract more consumers and expand the plant-based food market.

8:45 Detoxification of lipid peroxidation aldehyde, 4- hydroxynonenal, by flavonoids in apple and grapefruit Richmond Djorgbenoo1,2, rdjorgbenoo@aggies.ncat.edu, Yingdong Zhu2, Weixin Wang2, Shengmin Sang2. (1) Applied Sci. & Tech., North Carolina Agricultural and Technical State Univ., Greensboro (2) Center for Excellence in Post-Harvest Technology, North Carolina Agricultural and Technical State Univ., Kannapolis Reactive carbonyl species (RCS) are generated as secondary cytotoxic products when polyunsaturated fatty acids (PUFAs) undergo lipid peroxidation. Among the most studied RCS, 4-hydroxy-2-nonenal (4-HNE) is considered as one of the lipid peroxidation biomarkers. The accumulation of this lipid-derived unsaturated reactive aldehyde can covalently modify biomolecules such as DNA, proteins, and phospholipids, leading to various pathological

conditions such as cancers, diabetes mellitus, cardiovascular diseases, chronic kidney disease and other age-related diseases. Dietary polyphenols are believed to scavenge these RCS, but very few studies have been conducted to understand the trapping effects of 4-HNE by dietary polyphenols. This study investigates the interactions between cytotoxic 4-HNE and two important dietary flavonoids, phloretin (Ph) in apple and naringenin in grapefruit, respectively. The study results establish that both flavonoids effectively trap 4-HNE by forming covalent adducts. The major conjugates were purified, and LC-MS and NMR spectroscopy techniques were used to elucidate their structures as different isomeric forms of mono-4-HNE-conjugated phloretin or naringenin via a nucleophilic attack of the flavonoid to the C=O of the 4-HNE and the Michael addition reaction of the flavonoid to the C=C double bond of 4-HNE. To demonstrate their in vivo trapping efficacy, we searched these conjugated in urine and stool samples collected from phloretin or naringenin treated mice and in plasma and urine samples collected from volunteers after eating apples using high resolution LC-MS (QE+/MS) and confirmed their presence in mice and humans. Findings from this study pave the way to understand how dietary flavonoids could act as effective scavengers of 4-HNE by working as a sacrificial nucleophile in-vivo and preventing or reducing the risk of chronic diseases

9:05 Phytochemical characterization of aronia, elderberries, hascaps, and mulberries: New generation of super fruits Andrew G. Ristvey1, Victoria Volkis2, chvolkis2013@gmail.com. (1) Wye Research & Education Center, Univ. of Maryland Extension, Queenstown (2) Natural Sciences, Univ. of Maryland Eastern Shore, Princess Anne Aronia (Aronia mitchurinii), commonly known as the Black Chokeberry, is a fruiting bush native to the East Coast of the US and cultivated as a specialty food crop in Eastern Europe. Our previous research has shown that the content of phenolic antioxidants, including anthocyanins, polyphenols, and flavonoids in aronia juice is one of highest known for fruits, and much higher than for currently trended super-fruit acai berries. In addition, unlike assai berries, aronia can be grown widely in America from north Canada to the north part of Georgia, from coast to coast, and does not require tropical climate. Here we present the phytochemical characterization, cultural management study, ripening study, and food processing applications for this fruit in comparison with a group of super-fruits with similar content of anthocyanins – hascaps, elderberries, and mulberries. For each type of berries, antioxidant content determined by UV/Vis and LCMS methods, mineral content by ICP/MS, developing the antioxidants and soluble sugars over the ripening period, best processing practices preserving antioxidants, and examples of applications are presented.

9:25 Anti-proliferative properties of biologically active compounds extracted from bio-waste materials Magdalena Olkiewicz1, Anna Bajek2, Malgorzata Maj2, Josep M. Montornes1, Bartosz Tylkowski1, bartosz.tylkowski@eurecat.org. (1) Technology Centre of Catalonia Eurecat, Tarragona, Catalunya, Spain (2) Uni. Mikolaja Kopernika w Toruniu Collegium Medicum im Ludwika Rydygiera w Bydgoszczy, Bydgoszcz, Poland Biologically active compounds (BACs), such as polyphenols, have become an intense focus of research interest because of their perceived health-beneficial effects. They occur in a variety of fruits, vegetables, nuts, seeds, flowers, bark, beverages, and even some manufactured food, as a component of the natural ingredients used. They have been reported to exhibit anti-carcinogenic, anti-atherogenic, anti-ulcer, anti-thrombotic, anti-inflammatory, immunomodulating, anti- microbial, vasodilatory, and analgesic effects. Natural deep eutectic solvents (NADES) were first described by in 2011 and they are able to fully address the requirements of "ideal solvents" such as: non-volatile (reduced air pollution), non-flammable (process safety), stable (easier recycling and reuse), biodegradable, non-toxic, inexpensive and based on renewable sources. NADES fully represent green chemistry principles. Thus, they have been considerate as a new generation of chemicals with potential uses in various industrial fields. Indeed, as environmentally friendly solvents, they have been allowed by US Food and Drug Administration to be used in food, cosmetic and pharmaceutical formulations. In this paper we present anti-proliferative and physico-chemical properties of BAC extracted by NADES.

10:00 Influence of chemical structure on the color, molar absorptivity, and stability of naturally derived pyranoanthocyanin pigments Danielle M. Voss, voss.129@buckeyemail.osu.edu, Gonzalo Miyagusuku-Cruzado, Lu Xun, Monica Giusti. Food Sci. and Tech., Ohio State Univ., Columbus Pyranoanthocyanins are naturally derived pigments formed by the reaction of anthocyanins with cofactors like hydroxycinnamic acids, a process occurring as wine ages. Generally, pyranoanthocyanins have vivid colors and impressive heat and bleaching stability, giving them strong potential as food colorants. Their chemical structure is defined by the reactants and influences these characteristics, with hundreds of possible pyranoanthocyanins with unique properties. Our objective was to evaluate the influence of pyranoanthocyanin hydroxyl and methoxy substitutions on color, molar absorptivity, and stability. Eight pyranoanthocyanins were synthesized by reacting anthocyanins with hydroxycinnamic acid cofactors as shown below. Compound identity was confirmed with uHPLC-PDA-ESI-MS/MS. Pigments were isolated with semi-preparatory HPLC, dried, weighed, and dissolved in pH 1 and pH 3 KCl buffers and acidified MeOH at 40 µM. Spectra (260–700 nm) was monitored and used to calculate color data and molar absorptivity coefficients. Pyranoanthocyanins produced colors from yellow (10-phenyl-pyranocyanidin-3-glucoside) to red (10-syringyl-pyranomalvidin-3-glucoside) with an increasing number of substitutions producing a bathochromic shift in λvis-max and a lower hue angle. A substitution's location (-B or -E ring) had minimal influence on color yet affected the solubility in buffers with cyanidin pyranoanthocyanins more prone to precipitate. Pyranoanthocyanins' molar absorptivity coefficients were 3.6 to 7.5 times greater at pH 3 than their anthocyanin precursors. Pyranoanthocyanins' versatile and intense colors contribute to their promising future as colorants, with small changes in structure influencing the hue and stability.

10:20 Structural and compositional changes in the cell walls of cool-season pasture grasses for two growing seasons Sophia Newhuis1, sdnewhuis@gmail.com, Miranda Kunes-Agbana1, Brynn Angeletti1, Hanna Buecker1, Brittany Harlow2, Isabelle Kagan2, Michael Flythe2, Rachel R. Schendel1. (1) Animal & Food Sciences, Univ. of Kentucky, Lexington (2) Forage-Animal Production Research Unit, USDA Agricultural Research Service, Lexington, Kentucky Grass cell walls are rich in cellulose and arabinoxylan (AX) polysaccharide as well as lignin. Ester-linked phenolic acids such as ferulic and coumaric acids have the potential to cross-link the arabinoxylan polymer both to itself and lignin. These compositional differences in the cell wall of AX affect plants' digestibility for livestock, but there is limited information on how these structural elements of cool-season grasses change over multiple growing seasons. The primary goal of this project is to investigate changes in the monosaccharide profile, arabinose/xylose ratio (A/X), esterified phenolic acid contents, and lignin contents in five cool-season pasture grasses harvested over a four month period across two growing seasons. 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 and 2021; lyophilized; milled (< 0.5mm); defatted; and destarched to isolate insoluble cell wall material. The monosaccharide profile was determined via Saeman hydrolysis followed by high-performance anion-exchange chromatography with pulsed amperometric detection (HPAEC-PAD). Ester-linked phenolic acids were released via alkaline hydrolysis, extracted with diethyl ether following acidification, and separated, detected, and quantified using high-performance liquid chromatography (HPLC). Lignin content was determined using Acetyl Bromide Soluble Lignin (ABSL) analysis. All statistical analyses were done using SAS 9.4. Statistical significance was analyzed via one-way ANOVA, and Tukey-Kramer post-hoc testing was used to reveal significant pairwise differences. A Pearson correlation coefficient was computed to assess the linear relationship between lignin and total coumarates. The percent of glucose remained constant over time, indicating that the proportions of cellulose in the plant cell wall remain the same throughout the growing season. The A/X ratio was higher for all species in 2021 compared to 2020. Lignin contents tended to increase in the hotter months for some species. An increase in total coumarates from 2020 to 2021 occurred for a few species. In contrast, the concentration of total ferulates was statistically unchanged for both years. For 2020, lignin and total coumarates were found to be moderately positively correlated, $r(65) = .30$, $p < .01$.

10:40 Look at the residues not the emissions to understand chemical changes in waterpipe tobaccos during heating John H. Lauterbach, john@lauterbachandassociates.net. Chemistry & Toxicology, Lauterbach & Associates LLC, Macon, Georgia The major ingredients in contemporary waterpipe tobaccos (also known as shisha or hookah tobacco) are products derived from agriculture such as vegetable glycerol, and sugar syrups such as high fructose corn syrup with the tobacco content ranging only from 10 to 30%. Waterpipe tobaccos are used by less than 2% of US users of tobacco products; but use among 18–24-year-olds was recently reported to be 9.2%, so there is continued focus on reducing both the initiation and continued use of such products. However, main toxicants in emissions from waterpipe tobaccos come from the charcoal briquets used to heat the tobacco, not from the waterpipe tobacco as the latter is only heated, but not combusted. With the increasing commercial availability of electric heaters that replace charcoal heating, there will be an emphasis on thermolysis products from the waterpipe tobaccos. Weight loss on heating under conditions specified in ISO 22486:2019, Water pipe tobacco smoking machine — Definitions and standard conditions (electric heating instead of charcoal heating), has been reported to be 30 to 40% of a 10 g portion of waterpipe tobacco, and the weight loss is mainly glycerol, water, and propylene glycol, if used. Sugar thermolysis products, particularly those that lead to furanic compounds in the emissions will receive increased attention. However, determination of such toxicants in the emissions is difficult, but they and their precursors can be determined in the residue after heating with simple LC techniques. Major components in the residue can be determined with columns such as the Phenomenex Luna Omega Sugar column using both refractive index and UV detectors. Minor components are best chromatographed on a Cogent Phenyl Hydride column (250 x 4.6 mm) under aqueous normal phase (ANP) conditions such as 50/50 acetonitrile/water at 1.4 mL/minute with UV detection at multiple wavelengths beginning at 195 nm with confirmatory LC determinations performed on Cogent Amide and Diol columns. Such techniques will be presented for thermolysis of commercial waterpipe tobaccos based on flue-cured tobaccos as well as those based on dark air-cured and burley tobaccos.

11:00 Synthesis and characterization of 2-D Molybdenum-MOF/MXenes composite and their applications in sensing food contaminants Gurjeet Kaur, gurjeetkaurhera@gmail.com, Saloni Sharma, Akash Deep. CSIO, Academy of Scientific and Innovative Research, Ghaziabad, Uttar Pradesh, India This study describes the synthesis of a functional nanocomposite containing Molybdenum-metal organic framework (NH2-Mo- MOF) and transition metal carbides (MXenes). This composite has been explored for the development of an electrochemical immunosensor for Aflatoxin. The synthesis method involved the refluxing and self-assembly methods. For synthesis of Mo-MOF, refluxing of reaction mixture was carried out at 110 C for 12 hrs. The composite (MXenes/ NH2-Mo-MOF) was synthesized via a self-assembly of NH2-Mo-MOF over MXenes at room temperature for 3 h. The synthesized MXenes/ NH2-Mo-MOF nanocomposite was characterized by different techniques such as High-Resolution Transmission Electron Microscopy (HR-TEM), Field-Emission Scanning Electron Microscopy (FE-SEM), X-ray diffraction spectrometry (XRD), Fourier transform infrared spectroscopy (FTIR), and UV-VIS spectroscopy. The nanocomposite was deposited over a screen printed electrode followed by the immobilization of anti-AFB1 antibodies. The sensor has been utilized to detect Aflatoxin (AFB1) with good sensitivity and specificity.

11:20 Colorimetric assay of bacterial pathogens based on Co3O4 magnetic nanozymes conjugated with specific fusion phage proteins and magnetophoretic chromatography Liu Pei1, liupeiouc@126.com, Liu Aihua2. (1) ; Faculty of Life Science and Food Engineering, Huaiyin Institute of Technology, Huaian, Jiangsu, China (2) College of Life Sciences and School of Pharmacy, Medical College, Qingdao Univ., − Institute for Chemical Biology & Biosensing, Qingdao, China It is important to detect pathogens rapidly, sensitively, and selectively for clinical medicine, homeland security, food safety, and environmental control. We report here a specific and sensitive colorimetric assay that incorporated a bovine serum albumin-templated Co3O4 magnetic nanozyme (Co3O4 MNE) with a novel specific fusion phage protein and magnetophoretic chromatography to detect Staphylococcus aureus. The Co3O4 MNE was conjugated to S. aureus-specific fusion-pVIII (Co3O4 MNE@ fusion-pVIII), screened from the S. aureus-specific phage AQTFLGEQD (the phage monoclone is denoted by the peptide sequence). The as-prepared triple-functional Co3O4 MNE@fusion-pVIII particles were capable of capturing S. aureus in sterile milk, which were then isolated from milk magnetically. Assisted by polyethylene glycol, the Co3O4 MNE@fusion-pVIII@S. aureus complex was separated from the free Co3O4 MNE@fusion-pVIII by magnetophoretic chromatography in an external magnetic field. After transferring the isolated Co3O4 MNE@fusion-pVIII@S. aureus complexes into a 96-well plate, diammonium salt of 2,2′-azino-bis(3-ethylbenzo-thiazoline-6-sulfonic acid) and H2O2 were added to develop color because of the peroxidase mimetics activity of the Co3O4 MNE. A S. aureus concentration within 10−10,000 cfu/mL in milk can be detected (detection limit: 8 cfu/mL). The as-developed method is simple, cost-efficient, and sensitive, which is useful for rapidly diagnosing pathogenic bacteria and helpful to prevent disease outbreaks induced by pathogens in developing countries.

Virtual Session Agri-Food Sustainability at a Crossroads: Challenges of the Food, Energy, and Water Nexus

10:05 Microwave-induced specific aggregation behavior myofibrillar proteins Xidong Jiao, jiangnan_jxdong@163.com, Daming Fan. Jiangnan Univ., Wuxi, Jiangsu, China Microwave heating (MW), as a sustainable food processing approach, has advantages in reducing surimi wastewater, saving energy, and

enhancing the gelling properties of surimi gels. However, the molecular forces involved in microwave-induced gels and promotion mechanism are not well understood. In this study, an equivalent energy input model between MW and conventional water bath heating (WB) was established, aggregation behavior and changes in redox proteomics were investigated during MW treatment. The morphology of myofibrillar proteins (MPs) studied by transmission electron microscopy and atomic force microscopy showed that the proteins in WB group is more inclined to irregular cluster aggregation, while microwaves make the molecules tend to be homogeneous, dispersive, and small-scale aggregation, which has been proved to be related to the electrostatic distribution on the protein surface. Moreover, MW could significantly facilitate disulfide bonds formation, resulting a strengthening covalent bonds crosslinking. Further analysis of redox proteomics revealed that a larger number of MPs were found to be highly susceptible to oxidation under microwave irradiation. Notably, MW caused oxidative modifications of cysteine residue at the head of myosin, revealing the enhancement mechanism of MP gelation by excess cysteine cross-linking. Overall, these results clearly indicated that the disulfide bond and electrostatic interaction play an indispensable role in the aggregation process of myofibrillar proteins, and providing a further understanding of the microwave-induced gelling mechanism, which could be meaningful for the green surimi-based products fabrication.

10:35 Plant nutrient delivery system for the enhancement of plant growth using an advanced coating on Zea mays seeds using modified hydroxyapatite nanoparticles Latheesha Abeywardana1, lsa.a@live.com, Chanaka Sandaruwan1, Surani Chathurika2, Veranja Karunaratne3, Nilwala Kottegoda2. (1) Sri Lanka Institute of Nanotechnology Pvt Ltd, Homagama, Western (2) Univ. of Sri Jayewardenepura, Nugegoda, Sri Lanka (3) Univ. of Peradeniya, Central, Sri Lanka Plant development is stunted due to the early growth phase deficiency of plant nutrients resulting curtail of the crop yield. In this study, an advanced seed coating was developed utilizing nanotechnology to achieve the effective delivery of plant supplements accomplishing sustainable and precise release characteristics. Zinc-doped hydroxyapatite/urea nanohybrid was synthesized employing a simple one-pot in situ sol-gel method. Characterization studies manifested a transformation of the lattice environment illustrating the successful doping of zinc into the hydroxyapatite matrix along with the fruitful incorporation of urea. Then, a seed coating was developed incorporating this nanohybrid, spread on maize seeds, and a pot experiment was performed to observe the growth parameters and nutrient availability. The triple nutrient system was responsible for escalating the germination percentage while enhancing plant development indexes such as plant height, plant girth, the number of leaves, root length, root weight, and shoot weight on Zea mays seeds. Moreover, enhancement of cob length, cob diameter, thousand-grain weight, and root-shoot nutrient contents have resulted in the presence of nitrogen, phosphorus, and zinc in the early growth phase. The creation of a unique seed-coating based on modified hydroxyapatite nanoparticles as an efficient triple nutrient delivery system to improve plant growth and development is described in this context. As a macro-micro plant nutrient delivery agent, the nanohybrid is futuristic, and it offers up new avenues for researchers to investigate the appropriateness of metal-doped hydroxyapatite nanoparticles in agriculture.

11:05 Using protein microgels as emulsion stabilizer, texture modifier, and bio-lubricant for designing fat-reduced food products Yifu Chu, yifu4@ualberta.ca, Lingyun Chen. Dept. of Agricultural, Food and Nutritional Science, Univ. of Alberta, Edmonton, Canada Protein-based microgels are soft colloidal particles that show strong potential to act as future fat replacers to develop novel low-calorie food as a strategy against obesity prevalent. Microgels have attracted interest as functional hydrocolloids, which can be applied to improve emulsion stability and texture, and have the potential to mimic the oral lubrication properties of fat droplets at the fat-oral surface. In our lab, we developed a facile method to fabricate uniform whey protein microgel with controllable size by modulating the protein-polysaccharide interactions. The microgel system can stabilize oil-in-water emulsion with long-term stability and strong texture. The individual contributions of microgel, protein and polysaccharide will be discussed, and the microgels can work both at the interface and in the bulk phase to improve the emulsion properties. The protein microgels present in the emulsion system can make 30% oil emulsions that show similar textural properties to emulsions containing 50% oil. Also, protein microgels in the bulk phase can work as an efficient bio-lubricant to provide "soft ball-bearing" lubrication performance in the contacting surfaces. These results demonstrate that the protein microgel system has the potential for food applications in preparing fat-reduced emulsion-based food formulations with a comparable texture to that of full-fat counterparts.

11:35 Impact of environmental change on the food water energy nexus: Can altering our diets help protect the global environment? John W. Finley, Jfinle5@lsu.edu. School of Nutrition and Food Science, Louisiana State Univ. System, Baton Rouge, Louisiana, US The desire for animal-based protein in our current standard American diet continues to grow as world population approaches 9 billion people by 2050. In addition to the demands made by increasing populations for animal protein foods, as standards of living increases, there will be more demand for animal-based protein foods. The animal production milk and meat have been established as significant contributors of greenhouse gas (GHG). Animals, mostly beef, clearly are contributors to GHG production. Also, of equal or greater concern, is the decimation of tropical rainforest to produce feed and grazing land for animal production. One of the obvious solutions is to reduce animal consumption and strive toward consumers embracing plant-based diets. It is not as easy as it appears! Plant-based diets offer a major potential for reduced GHG production. This raises questions about the nutritional comparison between animal-based and plant-based diets. This presentation will discuss the differences in health and nutritional impact of these dietary shifts. Such a shift in diet may help reduce the growing total GHG production impacting global temperature change. Converting to plant-based diets will require re-education of the consumer and an understanding of the health benefits gained by the shift. Historically, convincing consumers to change diets based on health benefits has not been highly successful. This raises the concerns of how to make plant-based foods economical, appealing and nutritious choices.

TUESDAY AFTERNOON

Advances in Food Packaging and Preservation

2:05 PHB/PLA/modified cellulose films, as packaging for chocolate and tropical fruits Cesar A. Sierra1, casierraa@unal.edu.co, Lady Bello-Rocha1, Vanesa Perez-Martinez1, Diego Castellanos2, Carlos Zuluaga3, Oscar Rodriguez1, Paola Yustres4. (1) Chemistry, Univ. Nacional de Colombia, Bogota (2) Institute of Food Sci. and Tech., Univ. Nacional de Colombia, Bogota (3) Dept. of Rural and Agrifood Development, Univ. Nacional de Colombia, Bogota (4) Chemical Engineering, Lakehead Univ., Thunder Bay, Ontario, Canada Considering the increasingly noticeable environmental implications caused by plastic waste, as well as the recent restrictions on single-use packaging, and the significance that all this has in agro-industrial countries such as Colombia, in this work, polylactic acid

(PLA), polyhydroxy butyrate (PHB) and cellulose (Cel) mixtures were studied as possible packaging for the commercialization of chocolate and tropical fruits. This mixture seeks to take advantage of the crystallinity, barrier properties, and biodegradability of PHB, together with the plasticity and thermal resistance of PLA, but modifying the hydrophilicity of the PHB/PLA film through the incorporation of hydrophobic cellulose (chemically modified cellulose through esterification, amidation, and etherification reactions). The latter, to improve packaging stability against humidity and increases their lifetime and that of the packaged products. Therefore, various PHB/PLA/Cel formulations were obtained by solvent casting and extrusion. Characterizing the films by infrared spectroscopy, contact angle, water absorption, oxygen, and water vapor permeability, and stress and strain tests. The results show that the cellulose modification type affects its dispersion and distribution in the PHB/PLA matrix. And that extruded PHA/PLA/Cell films in a 50/49/1 ratio have physicochemical and mechanical properties close to those of polypropylene. Finally, storage trials on tropical fruits and chocolate show that PHA/PLA/Cell packages can maintain the organoleptic properties of the packaged products in excellent condition for up to 8 weeks.

2:40 Development of bacteriophage added coating material to reduce Escherichia coli O157:H7 contamination in mushroom Eylul Evran, sefikaevran@hacettepe.edu.tr, Emine Kübra K. Tayyarcan, Ismail Hakki Boyaci. Dept. of Food Engineering, Hacettepe Universitesi, Ankara, Turkey Escherichia coli O157:H7 (E. coli O157:H7) is a serious foodborne pathogen for human. With the presence of inadequate hygiene conditions during product collection, packaging, or handling, it can contaminate food and cause food-borne diseases. Edible mushrooms can cause some diseases in humans. If the fertilizer used during production is not well sterilized or appropriate conditions are not provided during collection and packaging, pathogenic bacteria like E. coli can transmit to mushroom and can cause food poisoning in human. For this reason, different methods should be developed to prevent pathogenic bacterial contaminations in mushroom. Today, phage therapy is an alternative method to antibiotics for bacterial infections. Bacteriophages, called phages, are viruses that only infect bacteria. Today, lytic phages can be used against pathogenic bacteria that develop antibiotic resistance. In recent years, investigating the use of phages in food packaging materials is among the most popular topics. The release, stability, and effectiveness of phages on pathogenic bacteria in food packaging material are frequently studied. In this study, we performed the isolation and characterization of phages that are effective against E. coli O157:H7 bacteria that can be found in mushroom. We determined the growth parameters during the characterization stages and investigated whether they could maintain their stability with the change of physical parameters such as temperature and pH. We then coated the mushroom by mixing phage with different coating materials (sodium alginate and whey protein concentrate) and investigated the behavior of the phage during storage at 4 and 15°C and its effect on the pathogen. Efficiency of plating (EOP) and one step growth size experiments showed that phages are highly effective against E. coli O157:H7. According to results, phage coated material reduced the bacterial count compared to control group. Thus, it will be shown that phages are bioprotective agents that can be used safely as food packaging material and can be a solution for safer food production.

3:15 Sustainable ultra-high performance liquid chromatography method for analysis of carotenoids using GRAS solvents Jashbir Singh, Bhimanagouda S. Patil, Bhimanagouda.Patil@ag.tamu.edu. VFIC, Horticultural Sciences, Texas A&M Univ. System, College Station Carotenoids are natural pigments and antioxidants that are composed of a poly-isoprenoid skeleton of 8 isoprene units with alternating double and single bonds that form the central part of the molecule. Due to the high hydrophobicity of carotenoids, their extraction and analysis generally involve hexane, ethyl acetate, dichloromethane, chloroform, methyl chloride, and other harsh solvents. Recently, the use of safer, environmentally friendly solvents emerged as a sustainable alternative to conventional organic solvents. Therefore, here we focus on optimizing an ultra-high performance liquid chromatography (UPLC) method to facilitate rapid analysis of carotenoids using Generally Recognized as Safe (GRAS) solvents. The proposed UPLC method involved acidified water (solvent A) and ethanol (solvent B) as a mobile phase. Different stationary phases, temperatures, and flow rate were used to optimize the resolution of the analytes. The method was validated by measuring its linearity, precision, limits of detection, and quantification. The developed method was applied to profile carotenoids from different plant-derived foods such as melons, spinach, and kale. The present method is compatible with liquid chromatography-mass spectrometry and uses GRAS solvents instead of harsh organic solvents. Furthermore, this method can be used for the analysis of carotenoids from different matrixes.

4:10 Photoactive films made from curcumin dopped ZnO nanoparticles and alginate Cristian C. Villa1, ccvilla@uniquindio.edu.co, Leidy T. Sanchez2, Andres F. Cañon-Ibarra1,2, Jhon A. Arboleda-Murillo2. (1) Chemistry, Univ. del Quindio, Armenia, Colombia (2) Food Engineering, Univ. del Quindio, Armenia, Colombia Used in order to extend shelf-life of food products by either controlling microbial growth or by reducing ethylene production, thus, slowing the ripening process on climacteric fruits. Over the last decade, several studies have shown that combinations of metal oxide nanoparticles and UV light act as ethylene scavengers in fruits and vegetables conservation. Likewise, a process called photoinactivation (PDI) in which a molecule is used as photosensitizer is irradiated using visible light, once in the excited state the photosensitizer reacts with oxygen molecules generating radical oxygen specimens (ROS) that are toxic to microorganism. In this work we developed a combination of ZnO Nps as ethylene scavengers and curcumin as photosensitizer. Mechanical, thermal and optical properties of the films were evaluated as curcumin modified ZnO Nps were incorporated

4:45 Effect of gamma irradiation on vitamin D content in high fat finfish Jessica S. Brown, jbrown3@nova.edu, Patricia Calvo, Pujita Julakanti, Abdullah Khan, Fatima Mohiuddin. Nova Southeastern Univ., Fort Lauderdale, Florida Foodborne illness is a major health concern for consumers. Food distributors take a variety of precautions to ensure the safety of our food, such as storing food in refrigerated or frozen conditions or by using modified packaging. However, the application of low dose ionizing radiation (gamma radiation) has been used more frequently to prevent microbial spoilage of various foods. Currently, the FDA has approved the use of gamma irradiation for beef, pork, chicken, shellfish, and crustaceans, to name a few. Another food group that could benefit from the use of this treatment is fish. Fish contain an assortment of microbes in their gills, skin, and gut that work to metabolize the fish after it's been caught which quickly leads to spoilage. The use of ionizing radiation can prolong the shelf life of fish by killing these microbes. Before this type of treatment can be applied, it is important to assess its impact on the nutritional components in this food source, namely Vitamin D. Fish are one of the few natural sources of Vitamin D in food, supplying nearly the recommended daily amount in a single serving. In this study

varying doses of gamma radiation (0-4 kGy) were applied to filets of high fat finfish (salmon and trout) in chilled and frozen conditions. The fish samples were then saponified overnight and the Vitamin D was extracted using liquid-liquid extraction and analyzed by LC-MS. The amount of vitamin D3 and 25-hydroxy-vitamin D3 in irradiated samples was compared to controls to assess whether low dose gamma radiation caused a significant change in concentration.

5:20 Microbial valorization of industrial organic waste to biodegradable smart food packaging materials Lahiru Jayakody, lahiru.jayakody@siu.edu, Lakshika Dissanayake, Sandipty Kayastha, Sandhya Jayasekara, Bhagya Kolitha. School of Biological Sciences, Southern Illinois Univ. Carbondale Industrial waste contains a substantial amount of heterogeneous organic carbon that can be valorized into high-value chemicals and biomaterials. Generally, those waste is used to produce heat, fertilizer, or fuel (i.e., ethanol). Substantial opportunities are available to valorize the carbon into high-value chemicals via synthetic microbes that can be used to produce advanced materials. We will present the latest progress of engineering microbial metabolic pathways to enable valorization of waste organic substances through the biofunneling approach to performance-advantaged chemicals. For instance, the microbial pathways and metabolic engineering strategies can be leveraged to biofunnel the waste carbon efficiently into the targeted platform chemicals such as lactic, succinate, muconate, and biopolymers, including polyhydroxyalketone, and bacterial cellulose. The obtained platform chemicals can be used to produce biodegradable polymers such as polybutylene adipate terephthalate (PBAT) that could replace incumbent polyethylene and polypropylene food packaging materials. Further, nanomaterial and active molecules can be added to the PBAT and other biodegradable polymers to make the active/smart food packaging materials. The green process can remarkably lower the greenhouse gas emission and energy use to produce food-packaging material via industrial waste carbon relative to the petroleum-based production.

Chemistry of Alcoholic Beverages

2:00 Introduction: Chemistry of alcoholic beverages Nick O. Flynn, nflynn@wtamu.edu. Chemistry/Physics, West Texas A&M Univ., Canyon The global alcoholic beverage market share is valued at over 1.5 trillion dollars presenting many opportunities for research and development. This symposium will present the latest research on the chemistry of alcoholic beverages. Prior symposia in this field have covered the chemistry and history of many alcoholic beverages including wine, tequila, whiskey, beer and sake. This presentation will serve as an introduction to the Chemistry of Alcoholic Beverages symposium and will primarily focus on the alcoholic beverage topics that are being presented.

2:10 Effect of filtration and inclusion methods on rapid rapid wort analysis of malts Nick O. Flynn, nflynn@wtamu.edu. Chemistry/Physics, West Texas A&M Univ., Canyon Studies in our lab have explored modifications to the American Society of Brewing Chemists (ASBC) Rapid Malt Color provisional method used to determine the color of beer measured as the Standard Reference Method (SRM). Malt SRM is a vital statistic in the manufacture of beer as it helps to predict the contribution of malt to final product color which is one of the parameters by which beers are evaluated. 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. Earlier studies have suggested that the method, as written, needs to be modified in order to assure accurate analysis of darker malts. In this study, filtration methods and the inclusion of lighter base malts in the grain sample of darker malts were analyzed. This presentation will summarize current findings and present suggested modifications to the method as written.

2:20 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, Kevin Kingsbury2, Abbie Brehm2, Ronald A. Quinlan1, ronald.quinlan@cnu.edu. (1) Molecular Biology and Chemistry, Christopher Newport Univ., Newport News, Virginia (2) Tradition Brewing, 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 efficiencies of extraction from the grains. Here we present our preliminary findings on the taste and aroma profiles of small batch beers made using a Pilsen malt from different growth locations in collaboration with a local craft brewery using high performance liquid chromatography (HPLC) and gas chromatography-mass spectrometry (GC-MS). Non-metric multidimensional scaling (NMDS) ordination and analysis of variance (ANOVA) were conducted on the data to demonstrate the degree of uniqueness. These metabolites not only affect flavor and aroma, but color and foam stability as well. Our findings suggest that the terroir of grains, not just the malting process, play a role in the phytochemical output.

2:50 Dry hopping protocol has a limited influence on the chemical and sensory properties of India pale ale (IPA) beers Bethany Lam1, bethany.j.hausch@gmail.com, Samuel G. Ziegler1, Andrew J. Ledley1, Sudathip San-tan2, Helene Hopfer1, Joshua Lambert1. (1) Food Science, Pennsylvania State Univ., Univ. Park (2) Food Sci. and Tech., Kasetsart Univ. Faculty of Agriculture, Bangkok, Thailand Dry hopping is the process of adding hops to beer at any point after the boiling step. This late hop addition contributes to beer flavor with minor changes to the bitterness. The current market trend is towards hop-forward beers. There is a lack of systematic data on how the hopping protocol influences the final product. In this research, IPA-style beers were brewed with three different alcohol levels (4, 8, 12%) using three post-fermentation hopping protocols. The following hopping protocols were used: single hop addition at a rate of 3.5 g/L with a 10-day hop extraction period, five additions of hops, spaced every 2 days over a 10-day period, with a cumulative hop addition equaling 3.5/L, and a single hop addition at a rate of 3.5 g/L after filtration of the beer, followed by a 10-day extraction. All beers were filtered and carbonated after dry hopping. International bitterness units, total phenolics, and total protein content were measured, and no differences were observed between hopping protocols within an alcohol level. Total phenolics increased with alcohol level, with 12% ABV beer containing approximately double the phenolic content of 4% ABV beers. Preliminary flavor analysis indicates high levels of isoamyl acetate, as well as many other esters. A consumer panel was used to determine the overall liking of the samples and descriptive terms using check-all-that-apply. Banana was more frequently selected as an attribute as the alcohol content increased. As with the chemical analysis, alcohol level was found to be a bigger driver of differences than dry hopping protocol. This initial study indicates that dry hopping protocol has a limited impact on final IPA flavor, although future work should explore dry hopping at a higher rate and using different hop varieties.

3:10 Developing and analyzing the chemical fingerprint for popular whiskeys sold in the US Melissa Hernandez, Jeremy Nevins, jnevins@nextcenturyspirits.com. Next Century Spirits, Raleigh, North Carolina Each whiskey manufacturer seeks to make their whiskey unique and hit on a sensory profile that that their customers will enjoy and differentiate them self from the other competitors. This study is to determine the different "chemical fingerprints" of a group of top selling whiskeys in the US by comparing their chemical profiles. The chemical profiles were analyzed by in house developed GC-FID and GC-MS recipes analyzing compounds like esters, fatty acids, and Cresols composition. This allowed us to compare products across the various whiskey types to compare and contrast their attributes. Interestingly some classifications groups had very similar fingerprints while others had very large differences. We explored these differences and theorize some possibilities for these similarities and differences within and between these classification groups. This information is useful for large and small distillers alike in that these large selling whiskeys set the benchmarks for the customers on their particular genera of whiskey.

3:30 Required education and understanding in chemical kinetics, thermodynamics and sensory evaluation for distillers Gary Spedding, Gspedding@alcbevtesting.com. Brewing and Distilling Analytical Services, LLC, Lexington, Kentucky Distillers and alcohol beverage researchers are not well funded or educated when it comes to better understanding quality control aspects of the business. The processes of fermentation, distillation and spirit-in-wood maturation are extraordinarily complex chemical engines. Final spirits being complex chemical matrices presenting rich volatile aroma and flavor profiles. Brewers and winemakers have a better handle on their products than do distillers, and with a richer history of research and published data. The presentation will cover details of the distilled spirits production processes, introduce the "spirit metabolome" system, the reactions, including Maillard chemistry, involved in the processing of raw material-derived musts/worts through distillation, and the complex chemical kinetic engine model, proposed by the author, that accounts for spirit in wood maturation. The need to better understand the thermodynamic driving forces and chemical kinetics and equilibria behind the myriad of chemical/biochemical/and microbiological reactions required to appreciate distilled spirits production more fully. This overall topic a rich field for chemical research, requiring more input, funding and activity by and for researchers.

4:00 Investigation of the volatile composition of apple ciders from dessert apple cultivars with and without skin contact during fermentation using a metabolomics-based approach Yanxin Lin1, yfl5629@psu.edu, Michele Warmund2, Misha Kwasniewski1. (1) Food Science, Pennsylvania State Univ., Univ. Park (2) Plant Sciences, Univ. of Missouri, Columbia Culinary dessert apples, generally thought of as less desirable for cider production than heirloom cider varieties are still used due to their high yield, low cost, etc. However, little is known about the aromatic profile of ciders produced from these cultivars, and if their flavor can be adjusted with alternate processing such as allowing extended skin contact (i.e., processing as one would a red wine). To better understand the aroma profile, five (the year 2018) and eleven (the year 2019) cultivars of common dessert apples were ground and divided into treatments i) a “non-skin” trial with pressing prior to fermentation like normal cider production, or ii) an “on-skin” trial with fermentation prior to pressing. Volatiles were characterized by HS-SPME-GC-MS/MS based on the integrated metabolomic approach. Principal component analysis visualized only significant features in 2019 and 2018 (1159 and 1340), respectively. Feature detection was followed by compound identification and semi-quantification using authentic standards. Compounds identified in the various samples are known to illicit responses described as sweet, fruity, and floral with classes of compounds contributed by both apple- and yeast-derived volatiles. The partial least squares-discriminant analysis further demonstrated clear separations in cultivars and treatments. The ‘Gala’ and ‘Jona Gold’ samples all generally had the highest overall intensities with ‘Gala’ positively correlated with eugenol and 1-butanol. The skin treatment increases the content of the detected compounds, especially in the cultivars that tended to have low intensity in traditionally produced ciders, although the impact in some cases was highly cultivar dependent (e.g., the content of ethyl 2-methylbutyrate in 'Fuji' sample increased 14-fold after skin treatment, but much less in other cultivars). This work demonstrates that there is a huge aroma difference in ciders produced by dessert apples that can be utilized by producers and that revisiting common processing practices may allow further expansion of potential flavors from common cultivars.

4:20 Chemical characterization and sensory evaluation of wine formulated with African black olive (Canarium schweinfurthii Engl) fruits Omujal Francis1, fomujal@gmail.com, John Bosco Lamoris Okullo2, Sheila Natukunda4, Richard Komakech5, Jacob Godfrey Agea3. (1) Chemistry, Natural Chemotherapeutics Research Institute, Kampala, Uganda (2) Forestry and Biodiversity, Makerere Univ. College of Agricultural and Envir. Sci., Kampala, Uganda (3) Agricultural Sciences, Makerere Univ. College of Agricultural and Envir. Sci., Kampala, Uganda (4) Food Technology, Nutrition and Bio Engineering, Makerere Univ. College of Agricultural and Envir. Sci., Kampala, Uganda (5) Botany, Natural Chemotherapeutics Research Institute, Kampala, Uganda African black olive (Canarium schweinfurthii Engl , Family, Burseraceae),a neglected indigenous wild fruit tree growing in Sub Saharan Africa, produces purplish to blackish coloured fruits. These fleshy nutritious fruits, rich in phenolic compounds including anthocyanins, have been eaten as a snack with no value addition. This study evaluated the chemical and sensory attributes of wine formulated with C. schweinfurthii fruits. The formulation of the wine was conducted using standard methods for wine production using pulp concentrations of 20oB, 22oB, 24oB, 26oB. Chemical characteristics of the wine were determine using analytical standard methods while sensory evaluations were conducted using a trained panel of tasters based on hedonic scale assessment (1- dislike extremely - 9 like extremely). The pH, titratable acidity, total dissolved solids and alcohol content of the wine formulations ranged from 4.103 - 4.187, 0.253±0.004 - 0.279±0. 005, 7.0 ±0.0 - 10.5±0.0 and 13.2 ±1.0 -16.0±0.0% respectively. The bioactive components i.e., total phenols, total tannins and total flavonoids ranged from 26.96 ±0.82-29.25±0.78mg/100ml Garlic Acid Equivalent (GAE), 14.90 ±0.71-24.96±0.78mg/100ml GAE and 2.56±0.50-14.51±0.99 mg/100ml Quercetin Equivalent (QE) respectively. Sensory evaluation showed scores in ranges for appearance (6.4±1.43-7.1±1.35), colour (6.3±1.32-7.1±1.23), flavor (5.9±1.53-7.1±1.48), clarity (7.0±1.62- 7.2±0.98), aroma (7.0±1.62-7.2±0.98), taste (5.4±1.75-7.6±1.07), mouth feel (5.8±1.75-7.7±1.05) and general appearance (6.0±1.61- .5±1.20). The formulation that was reported to be the most preferred was 26oB, and the reason considered to buy it was mostly taste (82.9%), flavor (72.7%) and aroma (60.0%). Further sensory evaluation of the preferred formulation with another wine product in the market with similar colour attributes showed no significant differences ($p \leq 0.05$) in their flavour, aroma, taste, mouth feel and general acceptance, and reason the tasting panel would consider to buy it over the market product was its taste. Generally, there were significant differences ($P \leq 0.05$) in the

chemical characteristics and sensory scores of the different formulations. Canarium schweinfurthii wine has high alcohol content, bioactive compounds and unique taste that is acceptable to consumers. There is need to characterize the bioactive and sensory compounds that contribute to C schweinfurthii wine unique taste and flavour.

4:40 Application of spectroscopy for quality screening in the production of pisco distillate Yalan Wu, wu.5671@buckeyemail.osu.edu, Luis Rodriguez-Saona. Food Sci. & Tech., The Ohio State Univ., Columbus Pisco is a Peruvian spirit drink produced by distilling fresh must of fermented grapes in accordance with traditional methods established in the normative rules contained in the Peruvian Technical Standard. The distillation aims to recover the maximum amount of ethanol and positive characteristic aromas while minimizing the undesirable (methanol, copper, furfural and acetaldehyde) compounds in the distillate. Analytical methods for monitoring quality in spirits are highly time-consuming and labor-intensive. We aimed to provide the Pisco industry with predictive algorithms interfaced with field-deployable portable spectroscopy (UV/FT-IR) sensors for predicting multiple quality traits in their distillate products. A total of 153 Pisco samples were obtained from the Peruvian market or donated by Bodega San Nicolas (Ica, Peru). Samples included 75 samples collected at different distillation stages. Ethanol, methanol, acetaldehyde, ethyl carbamate and furfural content were analyzed by Gas Chromatography-Mass Spectrometry(GC-MS), and copper levels were assessed by Inductively Coupled Plasma Optical Emission Spectrometry(ICP-OES). For modeling, partial least squares regression combined with variable selection techniques were investigated. Our data showed that 17 of 153 samples' ethanol levels were below the legal limit (38%), showing possible dilution with water. We also successfully predicted the ethanol (RP 1.0 and SEP 0.59 mg/100 mL), methanol (RP 0.92 and SEP 0.07 mg/100 mL) and acetaldehyde (RP 0.90 and SEP 0.23 mg/100 mL) contents in Pisco samples. The results showed that ethyl carbamate and furfural concentrations in Pisco were not a safety concern. ICP-OES analysis showed that 53% of the analyzed Pisco samples had higher levels of copper than the allowed level (5 mg/L). UV-Vis spectrometer predicted copper levels with excellent precision (RP >0.95). Portable FT-IR and UV-Vis spectroscopies are promising tools to predict quality parameters in Pisco samples. These methods could provide reliable and rapid assessments for alcoholic beverage quality control purposes with less sample preparation and personnel training.

5:00 Determination of key odorants in Chardonnay marc skins Sarah Warner, swarne12@vols.utk.edu, John P. Munafo. Food Science, UT AgResearch, Knoxville, Tennessee Chardonnay marc, a coproduct of the winemaking industry, is a combination of skins, seeds and stems that is left behind after the juice pressed from the grape. This coproduct amounts to over half a million tons a year and was previously composted, turned into animal feed, or thrown out. Recently, it has been dried, milled, and used as a healthy and flavorful food ingredient. Some investigations have suggested that grape marc, including Chardonnay marc, has the potential to benefit human health, including possible improvements in cardiovascular health, gastrointestinal health, and modulation of inflammatory response. Previous research has been conducted characterizing odorants present in Chardonnay marc skins; however, omission studies have not been performed, thus, the key odorants contributing to the pleasant aroma of the skins remained unknown. In the present study, omission tests were performed by comparing aroma simulation models with one odorant omitted to determine the significance of the omitted odorant. The key odorants in Chardonnay marc skins were determined to be 3-methylnonane-2,4-dione (hay), ethyl octanoate (fruity), oct-1-en-3-one (mushroom), hexanal (green), (2E,4E)-deca-2,4-dienal (fatty), (2E,4E)-nona-2,4-dienal (fatty), and β-ionone, (floral, violet), linalool (floral, citrus), HDMF (caramel), and 3-(methylsulfanyl) propanal (potato). This study established a foundation for future studies focusing on the key odorants driving Chardonnay marc aroma and to aid in delivering optimal and consistent aroma profiles for this emerging food ingredient.

5:20 Quantitative errors and analytical method improvement of volatile sulfur-containing compounds in Chinese Baijiu Zhanglan He1, hezhanglan@wuliangye.com.cn, Dong Zhao1, Jia Zheng1, Michael C. Qian2. (1) Wuliangye Yibin Co Ltd, Yibin, Sichuan, China (2) Oregon State Univ., Corvallis Sulfur-containing compounds (VSCs) are a very important class of aroma compounds in alcoholic beverages, including Chinese baijiu. Headspace solid-phase microextraction (HS-SPME) coupled with gas chromatography-pulsed flame photometric detection (GC-PFPD) or chemiluminescence detection (GC-SCD) is a used approach in the quantitation of VSCs due to its high selectivity and sensitivity. However, the competitive adsorption of volatile compounds on the SPME fiber is an unavoidable drawback. The volatile composition varies widely in different styles of baijiu, but the effects of volatile matrix on the analytical accuracy of VSC in baijiu has never been reported. This study investigated the analytical error of 18 VSCs in Chinese baijiu, using six internal standards commonly used in literature. The quantitation errors of VSCs were evaluated both on CAR/PDMS and DVB/CAR/PDMS fibers under different concentrations of the major volatile compounds in Chinese baijiu. The results showed that ethyl hexanoate and ethyl butanoate had the most influential impact on the quantification of VSCs in Chinese baijiu. It was essential to match the right internal standard-VSC pair to improve the quantification accuracy. In addition, it was found that baijiu's aroma types (strong, light, and soy sauce aroma) affected quantification accuracy regardless of the internal standard used for analysis. The larger the difference in the matrix composition, the more significant the quantitative deviation would be. The study proposed a new approach of employing an internal standard system and corresponding matrix for the quantification of VSCs in baijiu using HS-SPME-GC-SCD to achieve acceptable accuracy. This new approach could be adopted by the industry for quality control and new product development across different aroma types of baijiu and brands.

5:40 Sensitive volatile phenol analysis in Chinese Baijiu using direct injection-on-line trapping coupled with gas chromatography-tandem mass spectrometry (LVI-Ttrap-GC-MS/MS) Kangzhuo Yang1, yangkangzhuo@wuliangye.com.cn, Zhanglan He1, Jia Zheng1, Zhipeng Liu1, Dong Zhao1, Michael C. Qian2. (1) Wuliangye Yibin Co Ltd, Yibin, Sichuan, China (2) Oregon State Univ., Corvallis Volatile phenols, including guaiacol, 4-methyguaiacol, 4-ethylguaiacol, eugenol, phenol, o-cresol, p-cresol, m-cresol, 4-ethylphenol and 2,6-dimethylphenol , are important aroma compounds in Chinese Baijiu. A fast and sensitive quantitation method of volatile phenols in Baijiu was developed using direct large-volume injection-on-line trapping coupled with - gas chromatography - triple quadrupole mass spectrometry (LVI-Ttrap-GC-MS/MS). Stable isotope phenolic compounds were mixed with the Baijiu, and the sample (20 µL) was directly injected into a MMI injector without any further sample preparation and concentration. The removal of ethanol and enrichment of volatile phenols were achieved with on-line Tenax resins packed in the split/splitless liner under solvent-vent mode. The initial trapping temperature, vent flow, vent time, final temperature, vent pressure, desorption time, desorption flow, and other parameters were optimized. The developed method had excellent correlation

coefficients with R2 in the range of 0.9994-0.9999 for all volatile phenols ranging from 0.7 to 530 μg/L. Recoveries under three concentrations (10, 50, and 100 μg/L) were from 87-115% in strong, light, and sauce aroma-type baijiu matrix. The method represented a standard deviation in three concentrations (10, 50, and 100 μg/L) less than 4% for all volatile phenols. The limit of quantification (LOQs) in baijiu samples was lower than 0.7 μg/L. The method was further applied to analyze the distribution of volatile phenols in various Chinese baijiu samples.. The results showed that nongxiangxing baijiu had high concentrations of p-cresol and phenol, followed by sauce aroma-type baijiu and others. p-Cresol, 4-ethylguaiacol, and 4-ethylphenol, were important volatile phenolic compounds in Chinese baijiu according to their detected sensory threshold and calculated OAVs.

WEDNESDAY MORNING March 29
Advances in Food Packaging and Preservation
8:05 Effectiveness of bacteriophage-loaded edible coatings to control foodborne pathogens on fresh-cut apples Emine Kübra K. Tayyarcan, kubratayyarcan@gmail.com, Eylul Evran, Ismail Hakki Boyaci. Food Engineering, Hacettepe Universitesi, Ankara, Turkey Foodborne infections and intoxications are still among the most critical health concerns worldwide. Escherichia coli, Salmonella enterica subsp. enterica serovar Enteritidis (S. Enteritidis) and Typhimurium (S. Typhimurium) are among the foodborne pathogens causing problems in both raw and processed foods. Since fresh-cut fruits are consumed without any pre-processing, they have a high risk of causing foodborne illness in the case of contamination. In recent years, researchers have sought more effective and environmentally friendly alternatives in the fight against pathogens. Phage therapy using bacteriophages has become an extremely prominent alternative. Edible coatings have also been one of the innovative approaches to limit contamination and expand the shelf life of fruits. Within the scope of this study, it is aimed to combine these two alternatives, form bacteriophage-loaded edible coatings using biopolymers and apply them to fresh-cut apples. To this end, Salmonella and E. coli phages were used to form edible coatings prepared with sodium alginate and whey protein concentrate. After preparation and characterization, the bacteriophage-loaded edible coatings were applied to fresh-cut apples which were artificially contaminated with a bacterial mixture including Salmonella spp. and E. coli. The efficacy of the edible coatings was screened during the storage at 4 °C for 7 days. The impact of the coatings on the survival of bacteria in the simulated gastric fluid was also determined. As a result, it was determined that coatings containing phage decreased the number of bacteria compared to the control group, both during storage and in simulated stomach conditions. The bacteriophage-loaded edible coating was found to be a promising candidate for reducing bacterial load in apples and contributing to the safer consumption of fresh-cut fruits.

8:40 Reusable and daylight induced antibacterial ethylene-vinyl acetate copolymer films Shahid U. Islam, Gang Sun, gysun@ucdavis.edu, Zheng Zhang. Biological and Agricultural Engineering, Univ. of California Davis Ethylene-vinyl acetate (EVA) polymer with daylight-induced antibacterial and antiviral functions was prepared by incorporating vitamin K3 into EVA during a blending process. Vitamin K3 was recently investigated and identified as a photo-sensitizer theoretically and experimentally, which can effectively generate hydroxyl radicals, singlet oxygen and hydrogen peroxide, representative reactive oxygen species (ROS) under daylight exposure. The generated ROS agents are biocides that can quickly and complete kill a broad spectrum of microorganisms and safe to human, environment, and potentially applicable in food packaging materials. EVA polymer is a common material employed in food packages for prevention of oxygen penetration through the films. The EVA and VK 3 blends (EVA/VK3 polymers) were processed into films with desired mechanical and optical properties, as well as with desired antibacterial and antiviral functions. The photo-active functions and antimicrobial performances were quantified by using analytical chemical and microbiological methods. Reusability of the photo-active functions were demonstrated. The results revealed that the EVA/VK3 could be a potential food packaging material to produce reduced biological contamination and transmission.

9:35 Anthocyanin-based food packaging for monitoring the freshness of fresh cut fruits and vegetables Partha Pratim Das, das1.parthapratim@gmail.com, Peddapapannagari Kalyani, Mudrika Khandelwal. Materials Science and Metallurgical Engineering, Indian Institute of Technology Hyderabad, Telangana The losses of fresh farm produce can be reduced by applying proper packaging approaches and thereby helping to increase the shelf life. To date, various packaging approaches (Active food packaging, Modified atmospheric packaging, edible coating and films, etc.) are utilized to increase the shelf life of fresh farm produce. With the advancement in technology, intelligent/smart food packaging comes into existence and tries to utilize natural resources to develop smart food packaging. Anthocyanin is one of the natural pigments which is extracted from berries which generate a wide range of colours, thereby can be used as a pH sensitive indicator in food packaging. Red-Cabbage extracted anthocyanin (RCA) is loaded on freeze dried bacterial cellulose (FD-BC) to make the pH-sensitive indicator and is used in the form of pads (2x2 cm) in the packaging. This study will help to monitor the packed cut fruits and vegetables using a low cost anthocyanin loaded BC-pads in real time application. This can help predict the shelf life left as well. Bacterial cellulose advantage of high surface area hence producing a sensitive colour changing material.

10:10 Structure and properties of flexible starch-based double network composite films induced by dopamine self-polymerization Hao Xu1, harry_xuhao@163.com, Long Chen1, Zhengyu Jin1,2. (1) school of Food Sci. and Tech., Jiangnan Univ., Wuxi, Jiangsu, China (2) Collaborative Innovation Center of Food Safety and Quality Control, Jiangnan Univ., Wuxi, Jiangsu, China Star-based packaging materials are being developed to alleviate environmental pollution and greenhouse gas emissions associated with plastic-based ones. However, the high hydrophilicity and poor mechanical properties of pure-starch films limit their widespread application. In this study, dopamine self-polymerization was used as a strategy to improve the performance of starch-based films. Spectroscopy analysis showed that strong hydrogen bonding occurred between polydopamine (PDA) and starch molecules within the composite films, which significantly altered their internal and surface microstructures. The composite films had a greater water contact angle that was more than 90 degrees, which indicated that the incorporation of PDA reduced their hydrophilicity. Additionally, the elongation at break of the composite films was 11-fold higher than pure-starch films, indicating that PDA improved film flexibility, while the tensile strength decreased to some extent. The composite films also exhibited excellent UV-shielding performance. These high-performance may have practical applications in food and other industries as biodegradable packaging materials.

General Papers
8:05 Non-targeted identification of botanical origin markers for honeys Lei Tian1, lei.tian@mail.mcgill.ca, 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 Honey has been reported as one of the most common food ingredient that is affected by food fraud worldwide. Many honey fraud cases were identified as mislabeling of botanical origin as the botanical origin can impact the market price of honey. Currently available methods for the identification of botanical origin of honey either are time-consuming (e.g., pollen analysis) or only target a few "known" types of markers (e.g., phenolic compounds). A quick and effective method is therefore needed for the identification of honey origin. Non-targeted analysis, using high-resolution mass spectrometry (HRMS) and advanced data processing tools, is able to investigate a broad range of fingerprints in honey, and the unique features can be served as chemical markers for the identification of botanical origin. In this study, a non-targeted method based on liquid chromatography (LC) coupled to HRMS was applied to explore the non-saccharide fingerprints of honeys of different floral origins (incl. buckwheat, blueberry and clover) collected from markets in Canada. Honey samples were analyzed using a "dilute and injection" method followed by a LC-quadrupole time-of-flight (QTOF)-MS analysis. Fold change and ANOVA analysis was conducted, and several features were identified as botanical markers. For example, a feature m/z 121.0300 [M-H]- was identified as a botanical marker for buckwheat honeys, and its structure was later confirmed by MS/MS and chemical standard as 4-hydroxybenzaldehyde. The present results demonstrate that LC-HRMS-based non-targeted workflow can be used to identify novel molecular markers for honey botanical classification. This workflow relies on a rapid (<20 min per sample incl. sample preparation) and simple (no extraction step) analytical method, which can be easily translated to study the authenticity of other liquid/semi-liquid food (eg. alcoholic beverages or maple syrup).

8:25 Water soluble vitamin analysis in feed using mass spectroscopy detection Darrell E. Clinton, dclinto@purdue.edu, Halina D. Inerowicz. Office of Indiana State Chemist, Purdue Univ., West Lafayette Determination of water-soluble vitamins in animal feed can be a challenging analytical procedure with most current methods using high performance liquid chromatography (HPLC) with ultraviolet (UV) or fluorescence detection. In this study, the analysis of several B vitamins; thiamine (B1), riboflavin (B2), niacin (B3), pantothenic acid (B5) and biotin (B7), in different feed matrices using ultraperformance liquid chromatography (UPLC) with QDa single quadrupole mass detector. The application of mass spectroscopy reduces preparation and analysis time and does not involve derivatization agents which may be used in HPLC with other types of detectors. The results of the proposed method met the criteria for a single laboratory validation and could be used as a routine method for analysis of water-soluble vitamins in animal feed as well as expanding the analysis to include pyridoxine (B6) and cyanocobalamin (B12).

8:45 Inhibiting ice recrystallization with corn cob hemicelluloses Matthew W. Reeder, mreeder1@vols.utk.edu, Tao Wu. Food Science, The Univ. of Tennessee Knoxville Herbert College of Agriculture, Knoxville, Tennessee One of the main defects of frozen food products is ice recrystallization—the growth of larger ice crystals at the expense of smaller ones. Ice recrystallization causes the loss of flavor, color, moisture, and overall sensory acceptance. This can be even more detrimental to foods designed to be served frozen, such as ice cream. Many frozen and unfrozen food products currently contain food stabilizers to improve their texture, stability, and other physical properties. Stabilizers mainly come in the form of polysaccharide gums such as locust bean gum, guar gum, etc. Considering the current stabilizers' decent performance and recent price increase, new and more sustainable stabilizers have become necessary. Our lab has completed much research on various polysaccharides' ice recrystallization inhibition activity and most recently has found good activity in hemicelluloses originating from corn cobs. Over a 7-day incubation period, 0.5% corn cob hemicelluloses were able to reduce the average ice crystal size by 32.31% in a model ice cream system of 25% sucrose. This activity was similar for concentrations as low as 0.2%, as well. Further tests will include viscosity influences of hemicelluloses compared to commercial stabilizers, monosaccharide characterization, activity in a commercial ice cream mix, and other physical influences of the hemicelluloses on a commercial mix.

9:05 Proteolytic treatment of waste dairy ice cream to accelerate butterfat separation Chen Liang1, qwfylc@gmail.com, Rafael Garcia1, Benjamin Plumier1, Changhoon Lee1, Farah Huynh1, Joseph Uknalis2. (1) Dairy and Functional Foods Research Unit, USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania (2) USDA-ARS Eastern Regional Research Center, Wyndmoor, Pennsylvania Ice cream manufacturers generate large amounts of products that will not be sent to retailer for a variety of reasons. Being abundant in ice cream, butterfat may potentially be recovered as a nutritionally valuable ingredient to be reapplied in human food processing. Creaming of butterfat could happen spontaneously but very slowly in the ice cream emulsion. Milk proteins adsorbed on fat globule membranes inhibit the separation caused by fat globule aggregation and coalescence. In this study, industrial proteases were chosen as treatments to disrupt the stabilization of milk proteins on fat globules. Flavourzyme and Formea CTL (chymotrypsin-like protease) were selected and tested on a variety of ice creams. The proteolytic treatments with 1% w/w enzyme/protein dose and an hour reaction duration at 50 °C promoted 20-60% of original emulsion weight segregated as serum under mild centrifugation (2,000 ×g, 20 °C, 10 min), compared to control without segregation. Studies on the stability of treated ice cream emulsions revealed that faster creaming rate, larger migrating particle size, and decreased continuous phase viscosity were associated with the accelerated separation. Investigation into the destabilization mechanisms suggested the two enzymes might work differently; Flavourzyme may primarily promote the formation of fat aggregates by coagulating the adsorbed milk proteins, and chymotrypsin predominantly encouraged fat coalescence by removal of proteins from the fat globule membranes. The protein-fat complex formed by Flavourzyme treatment was more susceptible to centrifugal separation compared to fat globules. Coagulation of milk proteins is likely to be more efficient in fat and emulsion destabilization. Common practices to coagulate milk proteins such as pH adjustment, and rennet used in cheesemaking will be compared with Flavourzyme. These results provide an effective first-step for ice cream manufacturers to separate butterfat from waste ice cream and shed light on how proteolytic treatments aid in the demulsification of protein-stabilized oil-in-water emulsion.

9:25 Profiling the non-starch polysaccharides of hempseed cell walls Miranda K. Agbana1, m_kunes@yahoo.com, Brittany Harlow2, Mirko Bunzel3, Michael Flythe2, Rachel R. Schendel1. (1) Dept. of Animal & Food Sciences, Univ. of Kentucky, Lexington (2) USDA Agricultural Research Service, Washington, DC (3) Dept. of Food Chemistry and Phytochemistry, Karlsruher Institut fur Technologie, Karlsruhe, Baden-Württemberg, Germany Interest in hempseed as a dietary fiber source for humans and a feed component for ruminant animal diets has risen in recent years. While basic macronutrient assessments of various hempseed varieties have been conducted, detailed information about the cell

wall components of hempseed is lacking. Feeding a selection of oilseeds (including hempseed) to cattle resulted in different ruminal fermentation traits and it is known that microbes vary in their ability to target specific cell wall substrates, necessitating a precise characterization of the polysaccharides in hempseed cell wall fiber. Hemicellulose, cellulose, and lignin are the typical components of plant cell walls. Since hemp (Cannabis sativa) is a dicotyledonous plant, it is expected that xyloglucans will be present as the main hemicellulose. High amounts of pectins are also often found in the primary cell walls of dicot plants, but the arabinan and galactan side chain configurations of rhamnogalacturonan I can vary drastically from species to species. To elucidate the cell wall profile of hempseed, we performed a Total Dietary Fiber analysis (AOAC 2011.25), two monosaccharide composition analyses, arabinan and galactan screening, xyloglucan profiling, Acetyl Bromide Soluble Lignin analysis, and methylation analysis. The hempseeds were found to contain approximately 59% dietary fiber (prior to protein or ash correction). Saeman (sulfuric acid) hydrolysis resulted in a monosaccharide profile for the insoluble fiber fraction that consisted mainly of glucose (67.3%) and xylose (27.2%) with small amounts of arabinose, galactose, and galacturonic acid; the water-soluble fraction contained arabinose (9.5%), galactose (18.7%), glucose (34.8%), mannose (15.6%), and galacturonic acid (21.5%). Methanolysis produced monosaccharide profiles with less glucose for both fractions and more xylose (88.8% for the insoluble fraction and 20.7% for the soluble fraction). Acetyl Bromide Soluble Lignin was quantified as 20.4%. Methylation analysis revealed an abundance of 1,4-linked xylopyranoses, indicative of large amounts of xylans, and 1,3,5-linked arabinofuranose was present, suggesting the presence of branched arabinans. These data suggest that hempseed could be a good source of dietary fiber and has differential effects on microbial fermentation.

9:45 Thermo-chemical decarboxylation kinetics study for cannabinoid acids in hemp (Cannabis sativa L.) by pressurized liquid system Urvashi Urvashi1, urvashi398@gmail.com, John Hatfield1, SangHyuck Park2, Chad A. Kinney1, Joon-Hee Han3, Kenneth J. Olejar1. (1) Chemistry, Colorado State Univ. - Pueblo (2) Institute of Cannabis Research, Colorado State Univ. – Pueblo (3) Chuncheon Bioindustry Foundation, Chuncheon-si, Korea (the Republic of) Cannabis is increasingly becoming a hot topic among the scientific community after Epidiolex® approval by FDA in June 2018. In December 2018, hemp (≤ 0.3% THC) was a permitted crop under US Farm Bill, adding to the resource's availability. Cannabis only produces acidic cannabinoids and to access the neutral form the -COOH moiety must be removed. Heating the plant material/extract results in decarboxylation; but cannabinoid thermolability can result in degradation, evaporation, or conversion to undesired metabolites. To avoid these, a thermo-chemical conversion of acidic cannabinoids during pressurized liquid extraction (PLE) was reported by our group.1,2 PLE operates using a pseudo-closed system under elevated pressure and temperature. Pressure is maintained (11 MPa) while temperature can be varied from 40-200 °C. Extraction combined with purification yielded cannabidiol (CBD) crystals of > 90% purity.2 We therefore, examined thermo-chemical decarboxylation kinetics of hemp in the PLE system. Triplicates at five temperatures, each at ten different time points were monitored to find the optimum temperature and time. Data showed agreement with literature3, revealing a pseudo-first order reaction. Increased temperature with shorter reaction time resulted in maximum neutral cannabinoid content at a faster rate. Higher temperatures were determined to result in a low reaction rate compared to lower temperatures This indicated at high temperature first order kinetics do not fit, as reactions occur almost spontaneously. Moreover, after 60 mins there is no change in the molar concentration of acidic cannabinoids. The activation energies and Arrhenius constants were established for cannabinoids of interest. Present study will allow researchers to establish the optimum thermo-chemical decarboxylation conditions for maximum cannabinoid conversion.

10:00 Thermo-chemical decarboxylation kinetics study for cannabinoid acids in hemp (Cannabis sativa L.) by pressurized liquid system Urvashi Urvashi1, urvashi398@gmail.com, John Hatfield1, SangHyuck Park2, Chad A. Kinney1, Joon-Hee Han3, Kenneth J. Olejar1. (1) Chemistry, Colorado State Univ. - Pueblo, Pueblo, Colorado, US (2) institute of cannabis research, Colorado State Univ. - Pueblo, Pueblo, Colorado, US (3) Chuncheon Bioindustry Foundation, Chuncheon-si, Korea (the Republic of) Cannabis is increasingly becoming a hot topic among the scientific community after Epidiolex® approval by FDA in June 2018. In December 2018, hemp (≤ 0.3% THC) was a permitted crop under US Farm Bill, adding to the resource's availability. Cannabis only produces acidic cannabinoids and to access the neutral form the -COOH moiety must be removed. Heating the plant material/extract results in decarboxylation; but cannabinoid thermolability can result in degradation, evaporation, or conversion to undesired metabolites. To avoid these, a thermo-chemical conversion of acidic cannabinoids during pressurized liquid extraction (PLE) was reported by our group.1,2 PLE operates using a pseudo-closed system under elevated pressure and temperature. Pressure is maintained (11 MPa) while temperature can be varied from 40-200 °C. Extraction combined with purification yielded cannabidiol (CBD) crystals of > 90% purity.2 We therefore, examined thermo-chemical decarboxylation kinetics of hemp in the PLE system. Triplicates at five temperatures, each at ten different time points were monitored to find the optimum temperature and time. Data showed agreement with literature3, revealing a pseudo-first order reaction. Increased temperature with shorter reaction time resulted in maximum neutral cannabinoid content at a faster rate. Higher temperatures were determined to result in a low reaction rate compared to lower temperatures This indicated at high temperature first order kinetics do not fit, as reactions occur almost spontaneously. Moreover, after 60 mins there is no change in the molar concentration of acidic cannabinoids. The activation energies and Arrhenius constants were established for cannabinoids of interest. Present study will allow researchers to establish the optimum thermo-chemical decarboxylation conditions for maximum cannabinoid conversion.

10:20 Bioprocess development to produce xylitol by Escherichia coli K12 from hemicellulosic hydrolysates Robert Turner1,2, rturner@mwbioprocessing.com, Mike Racine1,2, David Demirjian1,2. (1) Midwest Bioprocessing Center, Peoria, Illinois (2) zuChem Inc, Peoria, Illinois Xylitol is a 5-carbon sugar alcohol naturally found in fruits and vegetables. It is approximately as sweet as sucrose but has 40% fewer calories. It has no unpleasant after-taste and has a pleasant cooling effect in the mouth. It is anti-cariogenic and does not cause a significant insulin response. As a result, it has gained use in foods for special dietary uses, sugar-free confectionaries, mouthwashes, toothpastes and chewing gum. It can be produced chemically by catalytic hydrogenation but requires pure D-xylose. We have developed a scalable, economical process, producing it biologically from hemicellulosic hydrolysates of agricultural byproducts. One of the greatest problems with such biological approaches is the production of arabitol from L-arabinose present in the hydrolysate. We have developed a commercial process that reduces arabitol production. Our second-generation strain reduces arabitol production even further.

10:40 Novel drug-delivery approach against infectious disease by using ovotransferrin nanoparticles Hisham Radwan Ibrahim, k2504042@kadai.jp. Food Science and Biotechnolgy, Kagoshima Univ., Graduate School of Agriculture, Kagoshima, Kagoshima, Japan Infectious diseases are stressing clinical problems that continue to challenge the healthcare sectors. Development of carriers to allow targeted therapeutics that are more specific in their activity could provide advances in treatment of infectious diseases. Gold nanoparticles (GNPs) have the possibility of providing endless opportunities in drug delivery due to their less toxicity, ease of functionalization, and show improved permeability and accumulation of therapeutics at the target site. GNPs are functionalized by conjugation with proteins to introduce a platform for targeting when protein is recognized by cellular receptors. Ovotransferrin (OTf) of egg albumen is recognized by transferrin receptor (TfR) in cellular iron-uptake event. Many of infected human cells and pathogens seem to overexpress TfR, hence OTf could display unique features worth using as drug-targeting molecules in GNPs therapy. Here, we introduce a new approach in which OTf was used as a capping ligand for GNPs in which hydrophobic antibiotics were loaded. The OTf-capped GNPs rendered antibiotics water soluble, exhibited potent antibacterial action and specific drug targeting to intracellular infections.

11:00 Longan pulp polysaccharides regulate gut microbiota and metabolites to protect intestinal epithelial barrier Yajuan Bai2,1, xbaizxyq@sina.com. (1) Hainan Academy of Agricultural Sciences Institute of Agricultural Products Processing Design, Haikou, Hainan , China (2) Chinese Academy of Agricultural Sciences Institute of Food Sci. and Tech., Haidian District, Beijing, China This study aimed to evaluate the effects of digestion and fermentation behavior on the bioavailability and intestinal barrier protection of LPIIa. The results showed that the molecular weight of LPIIa had no significant changes after gastrointestinal digestion in vitro. After fecal fermentation, more than half of LPIIa was utilized by gut microbiota in a continuous depletion pattern. Compared with LPIIa, fermented LPIIa protected intestinal epithelial barrier better by increasing tight junction and mucin expression. Short chain fatty acid yield was increased by LPIIa both in vitro and in vivo. LPIIa improved the relative abundances of Lactobacillus, Bifidobacterium, Sutterella, Collinsella, Pediococcus, and Dorea, decreased the relative abundances of Acidaminococcus, Clostridium_sensu_stricto_1, and Desulfovibrio in the colon. The obtained results reveal that the role of LPIIa in promoting gut health is closely related to the interactions between LPIIa and gut microbes, and LPIIa has potential as an adjuvant for intestinal epithelial protection.

Virtual Session Before the Coffee Break: The Rich and Complex Chemistry of Coffee

10:05 The physical chemistry of coffee brewing John Melrose, jrmelrose@gmail.com. Consultant, Banbury, United Kingdom Coffee brewing involves the release of molecules from grains into coffee beds. Physical chemistry inside grains modulates the release. Multi-scale modelling quantifies effects by solving for hindered diffusion within grains and the surface flux. Source and sink terms model partitioning to phases within grains. Results are compared with measured kinetics during brewing and gas stripping: data for total yield, Caffeine, Acetaldehyde, Acetic acid and others. Key parameters are those of hindered diffusion, grain size and porosity, oil-water partition coefficients and acid dissociation levels. The relative roles of hindered diffusion due to structure and co-solutes are estimated - the latter has a strong effect in the case of gas stripping. For organic acids, the level of neutralisation is key; but this opens new questions on the role of bases within the coffee grains. The release of non-polar molecules is controlled by partitioning between water and oil phases internal to coffee grounds. The grain modelling can be combined with hydrodynamic models of the coffee bed, flow through the bed into the cup, and crucially the pressure-flow characteristics of different coffee brewers; examples will be shown.

10:25 Proton transfer reaction mass spectrometry analysis of coffee flavour compounds: A long story open to innovation Franco Biasioli, franco.biasioli@fmach.it. Sensory Quality Unit, Fondazione Edmund Mach Istituto Agrario di San Michele all'Adige, San Michele all'Adige, Trentino-Alto Adige, Italy Proton Transfer Reaction Mass Spectrometry (PTR-MS) is an example of Direct Injection Mass Spectrometry (DIMS) or of Chemical Ionisation Mass Spectrometry methods. The key features of these methods are the directs analysis of volatile compounds with high time resolution and sensitivity. Food Sci. and Tech. was one of the first fields, along with environmental and health sciences, where the potential of PTR-MS was investigated and coffee was the benchmark product used to identify strengths and weaknesses in comparison with established approaches, mostly by the work of Chahan Yeretzian at the Nestlè Research Laboratory in Lousanne, Switzerland. Most of the subsequent research lines were proposed and tested in those days, yet new technical developments, such as the introduction of time-of-flight mass analysers and the possibility of rapid switching among different ions, and more interdisciplinary approaches make PTR-MS the basis for innovation and further exploitation still today. While PTR-MS and other similar techniques are limited to volatile compounds and lack in specificity as compared with gas chromatography, still, they outperform other approaches where sensitivity and fast analysis are the key issues. Here we present a short review of coffee related PTR-MS applications with emphasis on recent technical developments and on our research. Following the fate of a coffee bean from roasting to the drinking of a cup of coffee gives hints on coffee roasting, coffee origin traceability and nose-space coffee analysis.

10:45 It's all in the brew: How extraction parameters influence the aroma composition during espresso coffee brewing Nina Buck1,2, nina.buck@ivv.fraunhofer.de, Andreas Stenzel1,3, Jonathan Beauchamp1. (1) Dept. of Sensory Analytics and Techologies, Fraunhofer-Institut fur Verfahrenstechnik und Verpackung IVV, Freising, Bayern, Germany (2) Dept. of Chemistry and Pharmacy, Friedrich-Alexander-Universitat Erlangen-Nurnberg, Bayern, Germany (3) Dept. of Nutritional Science, Justus Liebig Univ. Giessen, Hessen, Germany The sensory attributes of coffee as a beverage are driven by the composition of its constituent aroma compounds and non-volatile compounds. Coffee flavor is influenced throughout the entire production chain, but the final coffee extraction process itself allows the consumer to modulate the aroma to their personal preferences, to some degree. In this work, we investigated how the main extraction parameters of espresso coffee, namely grind coarseness, temperature and flow, affected the aroma composition in the final brew. To this end, we utilized proton transfer reaction time-of-flight mass spectrometry (PTR-TOFMS), which allows for direct analysis in real time, with high sample throughput. The PTR-TOFMS instrument was coupled to a liquid calibration unit (LCU), which was supplied with filtered, aqueous aliquot samples of coffee brewed from an espresso machine using different extraction parameters. The LCU acted to vaporize the individual coffee samples, thereby allowing constituent volatiles to be analyzed directly by PTR-TOFMS in the gas phase. This approach was used to explore qualitative and quantitative changes in the aroma composition of coffee in relation to brewing parameters. Sensory evaluations by a trained panel provided further insights to link

changes in aroma composition to perceptual differences. This talk will present the novel analytical configuration and report on observed changes in coffee aroma influenced by individual extraction parameters in coffee brewing.

11:05 Exploring unique coffee flavours of fermented high-end specialty coffee: Towards the fourth wave coffee Aviel El Khouri, Samo Smrke, smrk@zhaw.ch, Sebastian Opitz, Alexander Mistretta, Chahan Yeretzian. Coffee Excellence Center, Zurich Univ. of Applied Sciences, Switzerland Third wave coffee has its origin in the 1970s when coffee businesses started sourcing high-quality specialty coffee and delivering it freshly roasted to consumers. Over the past decade specialty coffee has become ubiquitous, and its market share has continuously grown. Presently, there is no consensus about what the fourth wave could be like. One of the developments has been the emergence of heavily fermented coffees. These exhibit very characteristic, clearly defined, and intense aromas and command a price up to 100-times higher than the commodity market price. Arabica coffee from the farm Iris Estate, Geisha variety, has been post-harvest processed by three methods: washed (W), pulped natural (PN), and fermented by so-called 'carbonic maceration' (CM). The aim was to elucidate the impact of CM on the flavour profile, as compared to the W and PN process. Sensory evaluation had revealed that CM creates characteristic flavour notes that were described as raspberry with hint of rose water. The aroma compounds of the roasted and ground coffee were analysed using solid-phase micro extraction gas chromatography (SPME-GC) and detected by both sniffing (GC-O) and mass spectrometry (GC-MS).
The study found six compounds that are considered contributing to the characteristic raspberry flavour of the CM coffee. These compounds were consistently identified as intense with raspberry notes when sniffing CM coffee, but not in W coffee. Three out of the six were identified and characterized by means of MS, whereas the other three were detected only by GC-O and could not be characterised by MS. The link of an experimental fermentation post-harvest processing technique to characteristic flavour compounds and sensory notes in the cup could be established. Such studies may ultimately allow such coffees to become scalable and more readily available for everyone to experience and enjoy.

11:25 Sensory impact and changes in the volatile profiles of special coffees obtained by dry and wet processes Wellington da Silva Oliveira1,2, wellingtonoliveira1408@gmail.com, Nina Buck1,3, Jonathan Beauchamp1, Camila Arcanjo4, Aline de Oliveira Garcia2. (1) Dept. of Sensory Analytics and Technologies, Fraunhofer Institute for Process Engineering and Packaging IVV, Freisin, Germany (2) Food Science and Quality Center, Instituto de Tecnologia de Alimentos, Campinas, São Paulo, Brazil (3) Dept. of Chemistry and Pharmacy, Friedrich-Alexander-Univ. Erlangen-Nurnberg, Bayern, Germany (4) School of Food Engineering, Univ. of Campinas, Sao Paolo, Brazil The flavor and aroma of coffee are affected by different factors, including the processing method. The processing is carried out before roasting to separate the coffee bean from the pulp and husk. Wet and dry methods have been used for this purpose, which impacts the chemical composition of the bean, and consequently, the volatile profile and final quality of the coffee beverage. This study aimed to evaluate the impact of different processing techniques on the final quality and volatile profile of coffees. For this, 20 samples were subject to dry (n=10) and wet processing (honey process, n=10). The samples were subjected to a sensory evaluation by trained assessors (n = 10). The fragrance of the powder, aroma, defect, acidity, bitterness, flavor, aftertaste, body, astringency and overall quality of the beverage was evaluated. Furthermore, the volatile profiles of all coffees were evaluated using gas chromatography-mass spectrometry/olfactometry (GC-MS/O). The volatile profiles of coffees processed by the honey method shower a slight lower number of volatile compounds than the coffee obtained by the dry process. However, the honey method showed a predominance of compounds responsible for sweet notes, such as furaneol. Moreover, a higher incidence of pyrazines, such as 2-ethyl-6-methyl pyrazine, responsible for nutty and roasty notes, were observed in coffees obtained by natural processes. Finally, the coffees showed global quality higher than 8.3 with different notes regarding the sensory attributes evaluated. The impacts of the processes on the sensory attributes of the beverage will be discussed.

12:00 Chemistry and analysis of chlorogenic acids from coffee Nikolai Kuhnert, N.Kuhnert@jacobs-Univ..de. Jacobs Univ. Bremen gGmbH, Bremen, Germany Chlorogenic acids (GGAs) are ubiquitous phenolic plant secondary metabolites, abundant in coffee. By definition CGAs are hydroxycinnamoyl esters of quinic acid thus existing in nature as sets of regioisomeric compounds. Most plants including coffee produce sets of multiple isomers, eg. all six isomers if dicaffeoyl quinic acid. Using a variety of isomer sensitive mass spectrometry methods including tandem mass spectrometry, ion mobility mass spectrometry or energy resolved mass spectrometry we could introduce methods that not only distinguish CGA isomers, but also provide methods for unambiguous structure elucidation. In coffee roasting the 45 CGA derivatives in a green arabica coffee bean are converted to an estimated 200 new CGA derivatives. Again, these can be identified using tandem mass spectrometry approaches. Finally, I complement my presentation by sharing some interesting findings on general CGA profiles from the world of coffee, including some latest findings on CGA biological activity, including promise to reduce Covid-19 infections.

12:20 Neglected coffee chlorogenic acids: p-coumaroyl-, sinapoyl- and di-acyl-quinic acid isomers in different coffee botanical species Luciano Navarini, luciano.navarini@illy.com, Silvia Colomban. Research, illycaffe SpA, Trieste, Friuli Venezia Giulia, Italy Coffee beans are a well-known source of chlorogenic acids (CGAs), a large class of esters formed between (-)-quinic acid and trans-hydroxycinnamic acids (caffeic, ferulic but also p-coumaric and sinapic acids). These compounds are important for their influence on the beverage sensorial properties, being aroma precursors of key volatile compounds, for product authenticity and traceability and for their biological activity with potential benefits on human health. This class of compounds counts several positional isomers which cannot be easily distinguished without adequate standards and reliable methods of analysis. Recently, thanks to studies of MS fragmentation pattern, identification of many isomers has been achieved by proper LC-MS protocols and many structures of new CGA isomers have been disclosed. From a quantitative point of view, CQAs monoester isomers are by far the most abundant, reaching together more than 80% of total chlorogenic acids. In these compounds the hydroxyl groups at C-3, C-4 and C-5 of the (-)-quinic acid ring are esterified with a single caffeic acid moiety. In addition to CQAs isomers, green coffee beans are particularly rich of two other classes of chlorogenic acid compounds: di-caffeoylquinic acid (diCQAs) and mono-feruloylquinic acid (FQAs) isomers. Much less abundant chlorogenic acids, and for this reason known as "minor", are mono-p-coumaroylquinic acids (pCoQAs), mono-sinapoylquinic acids (SiQAs), homo di-acylquinic acid isomers such as diferuloylquinic acids (diFQAs) and dimethoxycinnamoylquinic acids (DQAs), and hetero di-acylquinic acid isomers such as caffeoylferuloylquinic acids (CFQAs), caffeoyl-dimethoxycinnamoylquinic acids, feruloyl-dimethoxycinnamoylquinic acids. Minor chlorogenic acids

have not been the subject of detailed investigations and their qualitative and quantitative profile are scarcely reported in the literature and mostly focused on the two commercially exploited coffee botanical species: Coffea arabica and c. canephora. The aim of this work is to offer an overview of minor CGAs profile in different green Coffea species. Qualitative and quantitative robust data are the prerequisite to select best sources for isolation and then to have the chance to investigate bioavailability and biological activity of these neglected chlorogenic acids. Finally, minor chlorogenic acids profile may play an important role in disclosing the biosynthetic pathway of chlorogenic acids in coffee which is not yet fully clarified.

12:40 Anti-obesity and anti-aging effects of coffee components
Yeonhwa Park, ypark@foodsci.umass.edu, Renalison Farias-Pereira, Junhyo Cho. Univ. of Massachusetts Amherst Coffee is one of most consumed beverages with many health benefits. To determine the roles of coffee bioactives in obesity, we used the Caenorhabditis elegans as a model, which is a eukaryotic, multi-organ nematode. The energy homeostasis and lipid metabolism of C. elegans are well-conserved compared to the mammals, which makes this as a useful model in life science research, along with advantages of small body size, large brood size, short lifespan, easy maintenance, completely sequenced genome, and many available mutants. First, we found that treatments of green coffee bean extract and 3-O-caffeoylquinic acid (a major chlorogenic acid in green coffee bean extract) significantly reduced fat accumulation over the control in wild-type C. elegans. This was dependent to sbp-1 (an ortholog of the mammalian sterol regulatory-element binding protein involved in lipogenesis) and daf-16 (an ortholog of the mammalian Forkhead box O transcription factor, involved in the insulin/insulin-like growth factor receptor pathway). Next, we found that cafestol, a coffee diterpene and an agonist of Farnesoid X receptors (a functional homolog of the human FXR), significantly reduced fat accumulation by increasing fat oxidation and energy expenditure via DAF-12-dependent pathway. Thirdly, kahweol, a diterpene found in coffee, significantly reduced fat accumulation by reducing food intake in C. elegans. Based on this observation, we further tested the role of kahweol in aging as reduced food intake is one of well-known factors for extending lifespan. Treatment of kahweol significantly increased lifespan; 22% increase in average lifespan and 30% increase in median lifespan. Kahweol extended lifespan via daf-16-dependently, but not due to reduced food intake, in C. elegans. Taken together, these finding suggest the health benefits of coffee bioactives, particularly associated with anti-obesity and anti-aging.

1:00 NMR-spectroscopic applications to control coffee
authenticity Vera Gottstein1,2, Vera.Gottstein@cvuaka.bwl.de, Dirk W. Lachenmeier1, Thomas Kuballa1, Mirko Bunzel2. (1) NMR, Chemisches und Veterinaruntersuchungsamt Karlsruhe, Baden-Württemberg, Germany (2) Dept. of Food Chemistry and Phytochemistry, Karlsruher Institut fur Technologie, Karlsruhe, Baden-Württemberg, Germany Authenticity of coffee is an increasingly important issue in food control. A food is considered authentic if its characteristics match the declaration. For coffee, these can be characteristics such as the species, the geographical origin or the cultivation method used. Verification of coffee authenticity can be performed with proton nuclear magnetic resonance (1H-NMR) spectroscopy with targeted or non-targeted approaches. In targeted methods, the identification and quantification of specific compounds is carried out. In contrast, the non-targeted method focuses on detecting as many constituents as possible without identifying or quantifying them. This allows a specific pattern to be detected, which is also known as a chemical fingerprint. These patterns can then be used to distinguish two classes of samples. An example of the application of 1H-NMR spectroscopy in a targeted approach is the differentiation of the species Coffea arabica and Coffea canephora. The distinction is achieved by quantifying the compound 16-O-methylcafestol, which is only present in Coffea canephora. Moreover, the coffee constituents 5-hydroxymethylfurfural, trigonelline, N-methylpyridinium, formic acid, chlorogenic acid, caffeine, acetic acid, and lactic acid can be quantified by 1H-NMR spectroscopy in order to verify the coffee quality. The analysis of authentic coffee samples by 1H-NMR spectroscopy in combination with multivariate data analysis allows the detection of differences and specific patterns. Based on this, classification models ban be built. The created classification models can then be used to verify the authenticity of new, unknown coffee samples. This methodology was used to investigate the authenticity of coffee in terms of the geographical origin, the type of cultivation as well as the roasting process and the degree of roast. The geographical origin was considered first at continent by continent and then at the level of countries, with Ethiopia, Brazil, and Colombia being studied in more detail. The cultivation method was considered in relation to organic and conventionally produced coffee. The results of the non-targeted approach showed that it is possible to verify the authenticity of coffee with respect to both the continents and the countries Ethiopia and Brazil. A distinction between organically and conventionally produced coffees was not achieved. In contrast, it was possible to distinguish coffees according to the roasting process and the degree of roast.

WEDNESDAY AFTERNOON
Before the Coffee Break: The Rich and Complex Chemistry of Coffee
2:05 Chemistry in your cup: Chemical characteristics of cold
brew coffee Niny Z. Rao, niny.rao@jefferson.edu, Evan Schwarzmann, Marlena P. Washington, Meghan D. Grim, Megan Fuller. Biological and Chemical Sciences, Thomas Jefferson Univ. - East Falls Campus, Philadelphia, Pennsylvania Both small and large commercial coffee brewers have recently begun offering cold-brew coffee drinks to customers with claims that these cold-water extracts contain fewer bitter acids, due to brewing conditions, while still retaining the flavor profile. With very little research existing on the chemistry of cold-brew coffee, consumers are left to the marketing strategies of companies regarding the contents of cold-brew coffee. Our goal is to provide some scientific information about this new coffee trend. The present research employs a simple French press-style set-up to brew both cold brew and hot brew coffee. We varied the brewing time, the origin of beans, and the degree of roast to understand how these parameters affect the acidity, antioxidant activity, as well as concentration of caffeine in the coffee brew.

2:25 Espresso bitterness and acidity: Influence of process
parameters temperature, flow and coffee grind on non-volatile components Benedikt Schmieder1, benedikt.schmieder@tum.de, Nina Buck2, Verena Pannusch1, Mirjana Minceva1. (1) Biothermodynamics, Technische Universitat Munchen, Bayern, Germany (2) Sensory Analytics and Technologies, Fraunhofer-Institut fur Verfahrenstechnik und Verpackung IVV,Freising, Bayern, Germany Brewing espresso is considered a craft and even an art by some. Several different rules, recommendations, but also myths exist on influencing espresso bitterness and acidity. An experiment based on the box-behnken design was performed with different temperature (84°C, 89°C, 94°C), flow (1.0 ml/s, 1.5 ml/s, 2.0 ml/s) and coffee grind setting. The extracted espresso was collected in ten fractions and the concentrations of caffeine, trigonelline, chlorogenic acids and chlorogenic acid lactones as well as several organic acids were analysed. Using the resulting

extraction kinetics, the influence of the process parameters on the extracted non-volatiles was analysed for ristretto, espresso and double espresso quantities. For each coffee type guiding principles to influence espresso bitterness and acidity are presented.

2:45 Multidimensional gas chromatography approach to elicit the odour-structure activity of chiral 2-methyltetrahydrothiophen-3-one in coffee Aileen Pua1, Yunle Huang1, Vivian Goh1, Lingyi Li2, Maurin Cornuz1, maurin.cornuz@mane.com, Benjamin Lassabliere1, Lionel Jublot1, Bin Yu1. (1) Mane SEA Pte Ltd, Singapore (2) National Univ. of Singapore Coffee has attracted significant research interest owing to its complex volatile composition and aroma, which imparts a pleasant sensorial experience that remains challenging to analyse and interpret. Majority of the analytical challenges are associated with coffee's matrix complexity, hence state-of-the-art instrumental techniques are particularly important for the understanding of niche volatile compounds in coffee. In this study, thin-film solid-phase microextraction (TF-SPME) coupled with comprehensive apolar-polar gas chromatography (GCxGC) and a quadrupole time-of-flight mass spectrometer (QTOF/MS) was utilised to fingerprint eight specialty coffees, with the purpose of enriching and resolving trace organosulfur compounds (OSCs) in these samples. A total of 50 OSCs were detected in this manner, of which 2-methyltetrahydrothiophen-3-one (2-MTHT) was of particular interest due to its stereoisomerism, which was hypothesized to result in structure-odour activity. After confirming the differences in odour properties between the 2-MTHT enantiomers (chiral GC-olfactometry) and elucidating their absolute structures (nuclear magnetic resonance, NMR), (R)-2-MTHT was deduced to be the enantiomer possessing a lower odour threshold. The enantiomeric ratios of 2-MTHT in coffee matrices were also elucidated using heartcutting apolar-chiral GC-GC coupled to a MS and flame photoionisation detector (FPD) on solid phase extraction (SPE)-purified coffee. Further sensory analyses also indicate that 2-MTHT may be a potential driver of coffee quality, with (R)-2-MTHT possibly having a greater sensory impact in-matrix. In conclusion, niche solutions for sample preparation, separation, and detection are critical for understanding the contribution of trace and impactful odorants to coffee aroma.

3:05 NMR and sensory studies on interactions between odorants and melanoidins in coffee beverages Michael Gigl, michael.gigl@tum.de, Thomas Hofmann, Oliver Frank. TUM School of Life Sciences, Technische Universitat Munchen, Freising, Bayern, Germany A freshly prepared cup of coffee is cherished by consumers all over the world due to its characteristic and pleasant bitter taste and the alluring "roasty/sulfury" odor notes. The compounds responsible for the unique olfactory sensation of percolated coffee beverages, analyzed by means of the molecular sensory science approach are well understood. Previous studies provided comprehensive aroma reconstitution models consisting of less than 30 odorants using aroma extract dilution analysis, gas chromatography-olfactometry and headspace gas chromatography-mass spectrometry. While the aroma of freshly percolated coffee brew can be reconstituted quite well, the influence of the melanoidin containing high molecular weight (HMW) fractions on the sensory quality of coffee brew during storage in closed vessels, is still largely unknown. Former studies clearly indicated that especially odor active thiols exhibit high binding activity towards coffee melanoidins. However, mostly covalent interactions have been considered so far and the impact of non-covalent π-π interactions on coffee flavor remains unclear. To gain comprehensive knowledge of odorant melanoidin-interactions and their impact on olfactory perception, sensory and quantitative 1H-NMR (qHNMR) experiments were performed to allow the direct and non-invasive analysis of molecular interactions between key coffee odorants and HMW melanoidins. Sensory experiments showed a drastic decrease of "roasty/sulfury", "earthy" and "smoky" aroma notes, as well as an elevated "sweetish/caramel-like" aroma impression. By means of qHNMR, a clear distinction between covalent and non-covalent interactions could be achieved by monitoring time dependency of odorant polymer interactions. As a result, 2-furfurylthiol exhibited π-π interactions as well as covalent interactions, while pyrazines and hydroxyphenols showed only non-covalent π-π stacking. While, aldehydes incubated with HMW material showed only covalent interactions at longer incubation times, whereas furanones, as well as diketones showed no interactions with the HMW. This lack of binding affinity of the "sweetish/caramel-like" smelling 4-hydroxy-2,5-dimethyl-3(2H)furanone in combination with the high binding affinity of coffee thiols consequently provides explanation of the sensory evaluation and strongly contribute to the fast deterioration of "roasty/sulfury" aroma notes of freshly brewed coffee.

3:25 Electrochemical assessment of coffee qualities Christopher H. Hendon, chendon@uoregon.edu, Robin Bumbaugh, rbumbau4@uoregon.edu. Chemistry and Biochemistry, Univ. of Oregon, Eugene It is difficult to assess the qualities of solvated coffee on a timescale comparable to its rate of cooling and volatile loss. This is an important challenge because the coffee industry relies on extractions prepared using seemingly reproducible protocols. Yet, it has been shown that the composition of coffee extracts can vary wildly with minor fluctuations in brew parameters, making it difficult to predict the composition of the beverage without drinking it. This talk details the development of an electrochemical method to assess solvated coffee compounds using a three-electrode electrochemical method, performed using either commercial or home-made potentiostats. We demonstrate that there is a well-defined relationship between total dissolved solids (concentration of coffee material by mass) and current passed at reducing potentials. We also show that our method can discern differences in roast profile, origin, and random variation during preparation.

4:00 Using microwave energy for the rapid hydrolysis of coffee for amino acid profiling Alicia D. Douglas, alicia.stell@cem.com, Benedict Liu, Maria Swasy, Candice Cashman. CEM Corporation, Matthews, North Carolina Coffee is one of the most widely consumed beverages in the world, offering thousands of varieties. These varieties can have different physiochemical characteristics that can be used to assess flavor and quality. One of these characteristics is the amino acid profile. To obtain an amino acid profile an acidic or alkaline hydrolysis step is required to free the individual amino acids from their respective proteins. The traditional approach to amino acid hydrolysis involves heating samples to 110 °C in sealed tubes for extended time periods up to 24 hours. Analysis of the resulting hydrolysate is generally accomplished via LC-UV or LC-MS analysis, with the former requiring a precolumn derivatization step. Often, the amino acid hydrolysis sample preparation step represents a bottleneck for many laboratories. Thus, the CEM Discover Prep microwave system is an attractive alternative for busy laboratories. In addition, decreased reaction times allows for experiments such as this to be studied in undergraduate laboratory settings. In this work, the CEM Discover Prep system was used to rapidly hydrolyze different coffee varieties. The samples were neutralized, derivatized using the Waters AccQ-Tag Ultra reagent kit, and analyzed using a Waters ACQUITY UPLC H-Class system equipped with a PDA detector. The amino acid profiles obtained were compared, showing different profiles for different varieties of coffee. Furthermore, results for one coffee sample were compared to data

established following a traditional amino acid hydrolysis protocol, and it was found that the Discover Prep yielded excellent recoveries with tight standard deviations for triplicate samples. The CEM Discover Prep is an ideal choice for both industry and academic laboratories seeking to reduce sample preparation times, combine instrumentation for acid and base hydrolysis, and obtain cleaner hydrolysates, while maintaining accuracy and precision.

4:20 Green chemical synthesis of various nanoparticle species using spent coffee grounds Brian G. Yust1, bribriwork@gmail.com, Niny Z. Rao2, Evan Schwarzmann2. (1) Physics, Thomas Jefferson Univ. - East Falls Campus, Philadelphia, Pennsylvania (2) Chemistry & Biochemistry, Thomas Jefferson Univ. - East Falls Campus, Philadelphia, Pennsylvania Nanotechnology and nanoparticles (NPs) have become a common part of our modern society with uses ranging from medicine and biotechnology to cosmetics, synthetic lubricants, and food safety products. Among these technologies, one emerging NP synthesis method is to utilize food waste products, such as spent coffee grounds (SCGs), adding value and a secondary use for materials which would otherwise have been discarded. SCG synthesis is considered a green synthesis technique which avoids unnecessary exposure to toxic chemicals and reduces harmful waste by replacing caustic precursors with food-derived active compounds. This is in contrast to the many other bottom-up synthesis methods including traditional wet-chemical synthesis, thermal decomposition, hydrothermal, sol-gel, and microemulsion, that utilize hazardous or toxic chemicals and often also produce hazardous or toxic chemical waste. Further, after these syntheses, chemical residues may remain on the surface of these NPs which can affect their biocompatibility, water solubility, end-use function or other attributes. Thus, in this study, we seek to expand the understanding and applicability of SCG syntheses of various NP species using SCG extract as the reducing, nucleating, or capping agent in a wet-chemical synthesis. We analyze the impacts of SCGs acquired by hot brew, cold brew, and espresso techniques. Of particular interest are the total antioxidant activity and total caffeoylquinic acid of extracts obtained from SCGs as they play a major role in reduction and nucleation of metal ions during synthesis. Potential new avenues for NP synthesis will also be discussed.

4:40 Potential of near infrared spectroscopy and machine learning to predict volatile changes during coffee roasting Biniam Kebede, biniam.kebede@otago.ac.nz, Stella Green, Joy Sim. Univ. of Otago, Dunedin, New Zealand The global coffee industry is a booming one with a rich history that spans the globe. Due to the sheer size of this industry and the multitude of factors affecting growth and processing, there is a high degree of complexity in the resulting coffee quality, which is intrinsically linked to its volatile composition. There is no standardisation of what constitutes light, medium or dark roast in the industry and no rapid, non-destructive methods of predicting the coffee volatiles as an indication of quality. The current study aimed to establish a rapid Near Infrared Spectroscopy (NIR) method of detecting coffee volatiles non-destructively coupled with a machine learning approach to assess the effect of different roasting degrees on coffee bean volatile composition. Washed arabica coffee beans from Ethiopia and Congo were roasted in triplicate roast batches to industry-validated light, medium and dark degrees. These were analysed with HS-SPME-GC/MS and NIR in parallel. The PLS-R model was constructed to predict volatiles from the NIR data, enabling rapid indication of the roast degree. This work successfully predicted 32 compounds (such as furans, ketones, phenols, pyrroles, esters, and pyridines) from the NIR data with R2 values above 0.8 and low error. Ultimately, this approach allowed for the successful rapid, non-destructive prediction of key roast degree discriminatory marker volatiles and paves the way for the development of fast, hand-held NIR equipment methodology to predict coffee volatiles in the industry to discriminate based on roast degree and beyond.

5:00 Investigating the flavor of natural (dry process) coffee Mario R. Fernández-Alduenda2, Patrick Silcock1, pat.silcock@otago.ac.nz. (1) Dept. of Food Science, Univ. of Otago, Dunedin, New Zealand (2) Specialty Coffee Association, Irvine, California Processing of the coffee bean at the origin is increasingly becoming a major tool for specialty coffee producers around the world to differentiate the flavor of coffee beans. The processing method of coffee after harvest influences the final flavor and proceeds predominantly though either a wet (washed) or dry (natural) process. The natural process consists of drying the whole coffee fruit prior to removing the pulp. To understand the flavor of Arabica natural coffee, in particular the 'fruity' or 'winey' character (sometimes called 'Mocha'), three studies were designed. These investigated: 1. the sensory character of washed and natural coffee from 22 farms in Guerrero, Mexico using fast sensory profiling (FSP); 2. flavor of natural and washed coffees from seven countries using FSP, volatile organic compounds (VOCs) of green beans using proton transfer reaction mass spectrometry (PTR-MS) and VOCs of roasted beans using gas chromatography mass spectrometry/olfactometry (GC-MS/O); and 3. manipulation of the coffee cherries drying rates to modify microbial growth and achieve different flavor characters, assessed as above. FSP of natural coffees from Mexico were characterized as tropical, red fruit, dried fruit and fermented, whereas washed coffees were described as floral, spicy and nutty. Geography (including country-specific processing factors) dominated the flavor of the coffee from study 2, though the mocha character of a naturals sub-group was linked to the presence of ethyl 2-methyl-butanoate and ethyl 3-methyl-butanoate. Varying the drying conditions modified the flavor of the resulting coffee and modified the ethanol: methanol ratio, indicating that the microbial composition was altered by drying conditions. Fermentation for two days prior to drying, favored the production of red fruit and fermentation flavors, and induced correspondingly higher abundances of ethyl 2-methyl-butanoate and 3-methyl-butanoate. Fermentation during post-harvest processing appears to create compounds that can be carried over through roasting and directly impact the cup.

THURSDAY MORNING March 30
Virtual Session General Papers
10:00 Bioactive phenolic compounds profiling of prairie berries Chamali Kodikara1,2,3, chamali.kodikara@agr.gc.ca, Nandika Bandara3, Thomas Netticadan1,2, Sura Srinivas1, Champa Wijekoon1,2,3. (1) Morden Research and Development Centre, Agriculture and Agri-Food Canada, Morden, Manitoba (2) Canadian Centre for Agri-Food Research in Health and Medicine, Winnipeg, Manitoba (3) Dept. of Food & Human Nutritional Sciences, Univ. of Manitoba, Winnipeg, Manitoba Traditional berries including Vitis riparia (wild grape), Prunus virginiana L (chokecherry), Ribes hirtellum (gooseberry) and Amelanchier alnifolia L (Saskatoon berry), are cold hardy fruits consumed by prairie Canadians, including the indigenous population and are widely distributed in the prairie provinces. Phenolic compounds are an important group of bioactive molecules present in berries. Due to the presence of high antioxidant activity of polyphenols, there has been an increasing interest in identifying their potential health benefits. Recent findings have shown that diets rich in antioxidants protect humans against degenerative diseases such as diabetes, cancer, and neurogenerative and cardiovascular diseases. This research aimed to examine the phenolic compound compositions of twelve different berries, including wild blueberries (Vaccinium

corymbosum) and wild raspberries (Rubus idaeus), thereby identifying potential bioactive compounds and metabolite markers unique to each crop using HPLC and LC-ESI-MS/MS. We have identified 65 phenolic compounds present in the selected berries. Wild grapes were rich in phenolic compounds such as resveratrol, while gooseberries were rich in isoquercetin and paracoumaric acid. Moreover, saskatoon berries were rich in chlorogenic acid and quercetin. In addition, rutin-trihydrate and chlorogenic acid were identified as the most abundant phenolic compounds in chokecherry. This study will help to utilize indifferent prairie berries, in the food, nutraceutical, and pharmaceutical industries.

10:20 Characterization of Cumberland rosemary, Conradina verticillata, essential oil Claire Gorman, cgorman7@vols.utk.edu, John P. Munafo. Food Science, UT AgResearch, Knoxville, Tennessee Conradina verticillata, also known as Cumberland Rosemary, is a highly aromatic shrub within the Lamiaceae family. This threatened species is common in the Cumberland River watershed in the southeastern portion of the US. Cumberland Rosemary has an odor comparable to culinary Rosemary, but differs in subtle notes such as eucalyptus, earthy-mushroom, and clove. Cumberland Rosemary plants are comprised of two major above-ground plant organs, stems and leaves (needles). When producing essential oil via steam distillation, the whole plant (stems and leaves) is used. The contribution each of these plant organs have to the overall odorant profile of the essential oil remains unknown. Thus, the objective of the present study was to determine the contribution of each of the plant organs to the overall profile of the essential oil and determine the essential oil yield. The odorants were analyzed by gas chromatography-mass spectrometry (GC-MS), and the essential oil yield (1.42%) was determined using a Clevenger apparatus. Key odorants analyzed included 1-octen-3-one (earthy, mushroom), 1,8-cineole (eucalyptus), borneol (earthy), (-)-bornyl acetate (earthy, fruity), eugenol (spicy), menthone (mint), and camphor (herbaceous). This study determined the percent composition of each selected odorant in the stems, the leaves, and the whole plant (stems and leaves) and determined the essential oil yield, establishing a foundation for future studies in Cumberland Rosemary essential oil production.

10:40 Saltiness enhancement through the synergism of pyroglutamyl peptide mixtures Oshin Sahni, foshin@vols.utk.edu, John P. Munafo. Food Science, UT AgResearch, Knoxville, Tennessee Cardiovascular disease, including heart disease and stroke, are two of the biggest killers according to WHO's 2019 report on the most common causes of death worldwide. Accordingly, high blood pressure is one of the most prominent risk factors for cardiovascular disease. The positive relationship between high sodium intake and elevated blood pressure is well known. Thus, the enhancement of salty taste perception with decreased sodium content may be a promising sodium reduction strategy. However, reduction of sodium in food changes the sensory profile of the food, which generally results in lower consumer acceptance. A lack of desirable flavor is one of the major obstacles to overcome to increase acceptability of low sodium foods. Thus, there is a pressing need and opportunity to enhance salty taste, while maintaining low sodium levels. One solution may be the application of naturally derived saltiness enhancing peptides. These peptides have been identified from multiple food sources including arginyl peptides from fish protein hydrolysate, gamma-glutamyl peptides from beans, and pyroglutamyl peptides from mushrooms. In addition, it has been previously shown that mixtures of pyroglutamyl peptides can increase salty taste perception greater than the individual peptides at similar concentrations; however, this synergistic effect is not well understood. The objective of this current study was to determine the detection threshold of select pyroglutamyl peptides in a model broth containing 0.2% sodium chloride (NaCl), 0.003125% monosodium glutamate (MSG), and 0.003125% guanosine 5′-monophosphate (GMP) and compare the individual thresholds of peptides to the thresholds of pyroglutamyl peptide mixtures. The results of these fundamental studies lay the groundwork for future investigations aimed at the commercial application of pyroglutamyl peptide mixtures for enhanced saltiness perception in reduced-sodium foods.

11:00 Investigating the biodegradability of eco-friendly straws in prospective disposal environments Asif Ali, asifbinmunawar@gmail.com, Rafael M. Santos, Emily Yi Wai Chiang. School of Engineering, Univ. of Guelph, Ontario, Canada The present research investigates the biodegradability of straws made from agave waste. The benefit of agave straws are two-folds i.e., utilizing the agave waste resulting from tequila production, and producing biodegradable straws to eliminate a single-use plastic straws. The testing is conducted under possible disposal environments such as ocean water, soil, and compost pile. It aims at developing a novel approach for studying the biodegradability of eco-friendly straws by looking at the leaching of tracer components (incorporated in straws during manufacturing process) while degradation. It is an in-situ organic material-alteration technique, that can aid in studying the biodegradability process. The methodology of the present work includes the manufacturing of straws with tracer materials, setting up and conducting the simulated disposal experiments, analyzing the samples (which includes, ATR-FTIR, ICP-MS, TGA-MS, P-XRD, WDXRF techniques). It also contains comparing the results with standard biodegradability tests such as ASTM D5988/D6954 and the "tea bag index". The development of this method could help in identifying the extent of biodegradability of several eco-friendly products, and complement other biodegradability tests being presently conducted. The novelty of this work would aid in identifying further pathways to improve the biodegradability testing and studying the fate-mechanism of agave-based packaging/utensils materials. The understanding would also help to improve the biodegradability investigation of other waste-based products.

11:20 Myoglobin post-translational modifications in high- and normal-pH beef Ranjith Ramanathan1, ranjith.ramanathan@okstate.edu, Surendranath Suman2, Frank Kiyimba1, Shuting Li2, Jing Chen3, Gretchen Mafi1. (1) Animal and Food Sciences, Oklahoma State Univ., Stillwater (2) Animal and Food Sciences, Univ. of Kentucky, Lexington (3) Proteomics Core Facility, Univ. of Kentucky, Lexington Post-translational modification represents various functional groups that are added to proteins following translation. The addition of functional groups to amino acids influences structure and function of proteins. Although post-translational modification in myoglobin from normal beef is reported, limited knowledge is currently available on myoglobin post-translation modifications in high-pH beef. Therefore, the overall goal of this study was to determine the extent of post-translation modifications in myoglobin from high-pH beef compared with myoglobin from normal-pH beef. Eight (n = 8) normal-pH and high-pH dark-cutting beef carcasses (24 h postmortem) were selected from a commercial beef processor. The normal-pH (pH = 5.4) and high-pH (pH = 6.8) beef loins (longissimus lumborum muscles) were selected based on the pH values to determine post-translational modification in myoglobin. Sodium dodecyl sulfate-polyacrylamide gel electrophoresis was used to separate myoglobin from other sarcoplasmic proteins. The protein band (17 kDa) representing myoglobin in the gels was excised and subjected to in-gel tryptic digestion. The tryptic peptides were extracted, concentrated, and subjected to liquid

chromatography-electrospray ionization-tandem mass spectrometry. Mass spectrometric data were analyzed using Proteome Discoverer for identification of post-translational modifications such as methionine oxidation; lysine acetylation; lysine mono-, di-, and tri-methylation; arginine mono- and dimethylation; lysine carboxymethylation; serine, threonine and tyrosine phosphorylation; 4-hydroxynonenal (HNE) alkylation at histidine, and lysine. Tandem mass spectrometry identified phosphorylation, acetylation, carboxymethylation, and mono-, di-, and tri-methylation in normal-pH and high-pH beef myoglobins. In normal-pH beef myoglobin seven lysines were acetylated, while 11 lysine sites were acetylated in myoglobin from high-pH beef. Similarly, seven sites were phosphorylated in normal-pH myoglobin, while 10 sites were modified in high-pH myoglobin. Carboxymethylation, mono-, di- and tri-methylation also demonstrated differential modifications between normal- and high-pH beef myoglobins. In summary, postmortem muscle pH influences the extent of post-translational modifications in beef myoglobin. The binding of functional groups to myoglobin, in part, can influence oxygen binding and contribute to darker meat color.

11:40 Development and validation of a food frequency questionnaire for adults in Fiji to estimate nitrate and nitrite intake Adrian A. Chetty1,2,3, adrian.chetty@fnu.ac.fj, Joslin J. Lal1, Surendra Prasad1. (1) Chemistry, The Univ. of the South Pacific, Suva, Rewa, Fiji (2) Pure Sciences, Fiji National Univ., Nasinu, Rewa (3) Nutrition and Food Sciences, Univ.e do Porto, Portugal Food frequency questionnaires are frequently used to survey the food consumption patterns in the population. They are a useful epidemiological tool that can assess the link between disease patterns and food consumption. The present study reports the development of a food frequency questionnaire (FFQ) for the purpose of estimating nitrate and nitrite intake for the adult population in Fiji. The developed FFQ is a 162-food item, semi-quantitative, google form-based questionnaire that looks at the commonly consumed foods and beverages in Fiji. The food items have been categorized into 9 groups. The study population (n = 250) comprised Fijian adults between the age range of 18 – 65. The developed FFQ has been validated by a 24-hr diet recall study (n = 70). The estimated, nitrate and nitrite, dietary daily intake (EDI) was compared to existing tolerable daily intakes (PTWI/ADI) for these analytes. The developed and validated FFQ can be used in future epidemiological surveys in Fiji and the pacific.

12:00 In silico, in vitro, and ex vivo assessment to evaluate the antihyperglycemic, antioxidant and cytotoxic activity of Carica papaya L. leaf extract Pawan Prabhakar, pawanprabhakar@iitkgp.ac.in. RMSoEE, Indian Institute of Technology Kharagpur, West Bengal The present research aims to propose and validate the hypothesis that bioactive phytoconstituents of Carica papaya leaf extract also inhibit the activity of alpha-amylase and alpha-glucosidase critical enzymes involved in the pathophysiology of diabetes. In silico study reveals that the reported major compounds have shown an excellent binding affinity for the enzymes in the range -9.3 to 7.7 Kcal /mol, with good pharmacokinetic properties and low to a mild level of toxicities. The total phenol content and flavonoid content were found to be 57.92± 0.75 mg GAE/g of dry plant sample and 25.72±0.18 mg QE/g of dry plant sample. The antioxidant activity was 73.53±0.42% at a higher concentration of 125 µg/mL (IC50, 52.44± 0.07µg/mL) for DPPH assay, while the reducing power assay was determined to be 31.7±2.23 mg TE/g of dry plant sample. The alpha-amylase inhibitory activity was also concentration-dependent, and the most potent activity was observed at 125 µg/mL, with an inhibition percentage of 75.49± 1.41% (IC50, 40.03±2.61 µg/mL). Subsequently, the highest inhibitory potential for the alpha-glucosidase was 67.82±1.45% at 125 µg/mL (IC50, 66.52±1.52µg/mL). The chorioallantoic membrane assay has shown the growth and promotion of blood vessels up to 62.50 µg/mL concentration. Furthermore, the inhibition and attenuation of blood vessels were observed at the 125 µg/mL revealing its toxic effect at higher concentration.

12:20 Organophosphate esters in UK diet: Exposure and risk assessment Gbadamosi R. Muideen1,2, gbadamosimr@tasued.edu.ng, Stuart Harrad1, Abdallah Mohamed1. (1) School of Geography, Earth, and Envir. Sci., Univ. of Birmingham, United Kingdom (2) Chemical Sciences, Tai Solarin Univ. of Education, Ijebu Ode, Ogun, Nigeria Food ingestion has been established as an important human exposure route to many environmental contaminants (brominated flame retardants, dioxins, organochlorine pesticides etc). However, information regarding dietary exposure to organophosphate esters (OPEs) in the UK remains limited. This study provides the first comprehensive dataset on OPEs in the UK diet by measuring concentrations of eight OPEs in 393 food samples, divided into 15 food groups, collected from Birmingham, UK. All target OPEs were measured above the limit of quantification in at least one of the food groups analysed. Concentrations were highest (mean ∑8OPEs = 18.4 ng/g wet weight (ww)) in milk and milk products, followed by those in cereal and cereal products (mean ∑8OPEs = 15.9 ng/g ww), with concentrations lowest in chickens' eggs (mean ∑8OPEs = 1.61 ng/g ww). Interestingly, concentrations in animal-derived foods (mean ∑8OPEs = 44.2 ng/g ww) were statistically indistinguishable (p value less than 0.05) from plant-derived foods (mean ∑8OPEs = 36.8 ng/g ww). Estimated daily dietary intakes (EDIs) of ∑8OPEs under mean and high-end exposure scenarios for the four age groups considered were: toddlers (420 and 1547 ng/kg bw/day) greater than children (155 and 836) greater than elderly (74.3 and 377) greater than adults (62.3 and 278) ng/kg bw/day, respectively. Baby food contributed 39% of ∑8OPEs exposure for toddlers, with non-alcoholic beverages contributing 27% of exposure for children, while cereal and cereal products (25%) and fruits (22%) were the main contributors for adults and the elderly. The concentrations of OPEs in UK foodstuffs were generally of the same order of magnitude as those reported for other countries and our estimates of dietary exposure were well below the corresponding health-based limit values.

12:40 Global GAP and harmonized MRL facilitating international trade study case Denise Cerqueira1, denise.de-cerqueira@corteva.com, Jeremy Barnekow1, Carmen Tiu2. (1) Regulatory Sciences, Corteva Agriscience Indianapolis Global Business Center, Indiana (2) Regulatory, Corteva Agriscience Indianapolis Global Business Center, Indiana The ideal global residue package is characterized by a harmonized Good Agricultural Practice (GAP) in different geographies, number of trials that meets national and global requirements, robust representative data of different climates zones resulting in globally harmonized MRLs. This concept brings benefits for the grower, for the regulators and for the registrants. In different countries, the use of the same global critical GAP in residue studies can be challenging if we consider the efficacy and biology perspectives but can bring the advantage of one MRL for an specific active, facilitating international trade. The present study case demonstrates that residues studies conducted in different geographies under the same critical GAP can derive the same MRL proposal. A total of 22 trials in cucurbits (muskmelon, melon, rockmelon and zucchini) were carried out in the US (8 trials), Brazil (6 trials), Australia (8 trials) in 2020, 2021 and 2017, respectively, under the same critical GAP in a program designed for a CortevaTM active to be registered in its countries and to be used for a JMPR/Codex

assessment. Even though different number of trials were placed to fulfil each local regulation, the residue levels found, that meet the proposed enforcement residue definition, provided the same MRL of 0.3 mg/kg (OECD MRL calculator) for each country. As consequence, globally harmonized MRL values eliminate trade barriers when complying with the GAP, which benefits the whole food chain.

1:00 Role of food science in forensic science Altaf Rajani, altafrajani7575@gmail.com, Pranav Y. Dave, pranav.y.dave@nfsu.ac.in. School of Engineering and Technology, National Forensic Sciences Univ., Gandhinagar, Gujarat, India In early days, it is easy to conduct crimes by giving someone poisonous material in food. Some of the poisonous materials are unable to detect in post-mortem. By forensic science technique, it is easy to find the crime reason by examine the crime scene or the human body, which was murdered. Here food science plays an important role in investigation, by analysis different food items from the crime scene. The science of food is the study of food components, their behaviour under different environmental conditions, process of harvesting, milling, exposure to heat, cold, acid, alkalis etc. Today, the field of food science has progressed from basic physical, chemical and biological reactions that take place during processing to the fields of biotechnology, food engineering, packaging and its effect on the consumer. Here forensic chemistry becomes a small part of food forensic science for examine the food evidences from the crime scene. This review paper explains the relation of food science and forensic science. It also describes the brief introduction of various poisonous materials, their effects and how the crime has been taken place by using various poisonous materials. It explains the brief introduction of forensic science and food science. The paper is also mentioning that, how food science is an important aspect of the forensic science.

1:20 Highly sensitive SERS-based tool made of gold nanosphere coated glass Petri dish for rapid detection of indole in shrimps and determination of freshness Anupam Das, anumaharajbbc@gmail.com, Lynn Terry, Huiyuan Guo. Chemistry, Binghamton Univ., New York Indole level in seafood is a vital parameter to determine whether seafood is fresh or spoiled. To detect and preserve the freshness of seafood, rapid, easy to use, and highly sensitive techniques are needed to identify the presence of indole in food. In this study, we developed a highly sensitive surface-enhanced Raman scattering (SERS) based tool to detect indole in shrimp. The tool relies on an innovative sample container made of a gold nanosphere (AuNS) coated glass Petri dish, glass@AuNS. The glass@AuNS was proven to be an efficient plasmonic SERS substrate having an analytical enhancement factor (AEF) of the order of 106. When the indole-containing shrimp extracts were incubated on the glass@AuNS plasmonic substrate, the Raman signals of indole were significantly enhanced due to the Raman enhancement effects of the glass@AuNS plasmonic substrate. The SERS intensity and concentration of indole helped construct a standard calibration curve leading to a limit of detection (LOD) of 4.97 nM for indole. The standard calibration curve allowed determination of the concentrations of indole from spiked and spoiled shrimp samples as low as 0.0088 μg/100 g of shrimp. Apart from the high sensitivity, the detection technique was rapid (<10 min), and easy to handle and fulfilled requirements for determining the freshness of shrimp. Overall, this is a novel, facile, and sensitive analytical method to detect indole in shrimp with possible future applications in other seafood.

1:40 Classification of seaweeds based on tannin composition using differential sensing Daniela Garcia, danielagarcia@utexas.edu, Ethan Yu, Susanna Kim, Jessica Richardson, Maximiliano Ledesma, Mindy Tran, Diana Zamora-Olivares. Freshman Research Initiative, Univ. of Texas at Austin College of Natural Sciences Ruminants and livestock supply chains account for nearly half of global methane emissions, making reduction of enteric methane a topic of high importance. Methane is produced as a metabolic end-product in fermentation by methanogenic bacteria, and its production has been linked to the quality and composition of feedstock given to the ruminants. Recently, several types of brown seaweed have been identified to reduce enteric methane emissions when added to ruminant animal diets. Tannins are polyphenolic molecules with protein binding properties and play a key role in enteric methane reduction displaying diverse effects on ruminant digestion. Tannins are abundant in brown seaweeds which in turn are specifically utilized for methane mitigation in cattle. Therefore, it is of importance to study seaweeds and their tannin composition to understand the impacts they have on livestock when presented in the feed and forecast their effects on digestion. Herein, we investigated the phenolic fingerprint of four species of brown seaweeds - Ascophyllum nodosum, Fucus serratus, Fucus vesiculosus, and Fucus spiralis. The aim was to detect and classify each seaweed based on its tannin fingerprint by applying differential sensing methods coupled with chemometrics. Lyophilized seaweed samples were obtained by Professor Walsh at Queen's Univ. Belfast. In our lab, the seaweed extracts containing polyphenols and tannins were obtained by applying a two-phase liquid-liquid extraction protocol. The extracts were utilized for differential sensing analysis, in which a peptide-based sensor array was built using different combinations of peptides, metals and indicators, known as sensing ensembles, to detect the tannins present in the seaweed extracts. Upon addition of the seaweed extracts to the peptidic array, the tannins displaced the indicators from the peptidic ensembles via Indicator Displacement Assays, giving as a result measurable absorbance changes. Chemometrics such as Principal Component Analysis and Linear Discriminant Analysis were utilized to analyze the multivariate data set by reducing the dimensionality and allowing to identify and visualize important patterns. The seaweed species were correctly classified with 100% accuracy according to their tannin composition. Interestingly, the seaweeds were classified according to their genus where the Fucus samples were found in closer proximity to each other, while distinctly separated from the Ascophyllum genus

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Schedule of Technical, Business and Social Meetings (all times Central Daylight Time)

Sunday March 26	Noon-1:00pm	Future Programs	via Zoom
Sunday March 26	1:00pm-2:00pm	Special Topics/Business	via Zoom
Sunday March 26	2:30pm-5:00pm	Executive Committee	via Zoom
Tuesday March 28	6:00-8:00pm EDT!	AGFD Chair's Reception	Buca Di Beppo, 35 N. Illinois St.