Division of Agricultural and Food Chemistry of the ACS **Spring 2024**

CORNUCOPIA

including the AGFD program and abstracts for the

267th American Chemical Society (virtual & live) National Meeting on

March 17 - 21, 2024

in

NEW ORLEANS

Jason Soares & Liz Kreger
Program Chairs

Going to New Orleans? Join the AGFD Chair's Reception at the
Palace Café 605 Canal Street (between Chartres and Exchange)
Tuesday, March 19, 6:00 - 8:00 pm

20 minute walking directions from the Convention Center – exit the Center onto Convention Center Blvd. Turn right. Continue on Convention Center Blvd. to Poydras Street. Turn left on Poydras and continue to S. Peters St. Turn right on St. Peters to Canal St. Cross Canal (watch out for streetcars!). Once across Canal turn left on continue a few blocks to 605 Canal. Palace Café will be 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!

MESSAGE FROM THE CHAIR

It is with great pleasure that I transitioned to the AGFD Division Chair role in January 2024 with gratitude for all the guidance and direction from my predecessor, Dr. Jonathan Beauchamp. Dr. Beauchamp and other key AGFD leaders, including the Executive Committee, have been integral to a smooth transition and I express my sincere gratitude and appreciation for all their support. Special thanks to Mike Appell, Elyse Doria, Carl Frey, Alyson Mitchell, Mike Morello, Steve Toth, LinShu Lui and Mike Tunick for guiding and supporting me as Chair-Elect in 2023 and continuing to point me in the right direction as Chair in 2024. I am humbled by this great opportunity and will strive to keep pushing AGFD forward both technically and programmatically.

Firstly, I want to thank all AGFD members who continue to support the Division by attending and participating in our national meeting programming. Special appreciation and thanks to all the symposium organizers and presiders who continue to go above and beyond to provide the AGFD community programming in relevant and emerging research topics highlighting the latest state-of-the-art research and capabilities in the field of agriculture and food chemistry and more specifically, specific programming aligned with our sub-divisions: Food Bioengineering, Flavor, Food Safety, Functional Foods & Natural Products, Nutrition and Gut Microbiome, Sustainability & Green Technology, and Agriceuticals. Additionally, special thanks to all the presenters. We cannot continue to succeed without your valued contributions and your willingness to share your astounding research with your AGFD community members.
Before I highlight the remarkable AGFD Spring 2024 program, I want to reach back to the 2023 briefly where, although hybrid and virtual options were still available, we saw increasing in-person attendance to AGFD programming at the national meetings, especially at the fall 2023 national meeting in San Francisco. It was great to return to in-person attendance as a Division and once again connect and network with AGFD peers face-to-face. The AGFD program at the Fall 2023 was incredible with over 20 technical symposia comprised of 39 total sessions (13 in-person, 18 hybrid and 8 virtual) with over 300 oral presentations and 100 posters. Technical topics ranged from Forever Chemicals to Sustainable Agriculture to Artificial Intelligence to the Chemistry of Wine Making, amongst others. Also included was the inaugural technical programming for the two recently funded ACS Convergent Chemistry Community grants entitled "Food Security: Tackling Hunger" and ACS Microbiome Research Consortium while the Virtual Graduate Students Symposium in Asia-Pacific Region on Agricultural and Food Chemistry was selected as an ACS President recommendation. Lastly, I want to once again congratulate Liangli (Lucy) Yu, Ph.D., University of Maryland, who won the prestigious 2023 Award for the Advancement of Application of Agricultural and Food Chemistry as well as Xiaonan Sui, Ph.D., Northeast Agricultural University, Harbin, China, who received the 2023 AGFD Young Scientist Award and Zhuohong (Kenny) Xie, Ph.D., US Pharmacopeia, Rockville, MD, who was the inaugural recipient of the AGFD Young Industrial Scientist Award.

The spring 2024 national meeting in New Orleans is especially exciting because of the alignment to the ACS theme "Many Flavors in Chemistry". Special thanks to Dr. Neil Da Costa, thematic chair, for his support of the AGFD programming and organizing an amazing plenary session as well as the Kavli Lectures Series that I encourage all of you to attend. The AGFD Spring 2024 program has 13 technical symposia, 6 specifically aligned with the theme, with 20 sessions (14 in-person, 5 hybrid, 1 virtual) with 145 oral presentations and over 95 posters. Special events include an Urban South Brewery tour and the C4 Communicating Chemistry Culinary Competition at Dickie Brennan's Steakhouse on Tuesday as well as the Withycombe-Charalambous Graduate Student Award Symposium and the AGFD Undergraduate Poster Competition. Technical topics include Paring Flavors with Health and Wellness Food Products, Chemistry of Alcoholic Beverages, A Natural and Sustainable Future for Flavors, Food Allergen Characterization, Modification, and Detection, Toward Precision Nutrition, Sensory beyond Earth: The relevance of flavor chemistry in space exploration, Mycotoxins: Challenges and Future Perspectives, and Food Security: Tackling World Hunger, amongst others. Lastly, I want to highlight the two memorial symposia for key members of the AGFD community – Michael Granvogl Memorial Symposium and Agnes Rimando Memorial International Student Symposium that I encourage you to attend. I want to thank all of the symposium organizers for their outstanding efforts in collectively bringing together a fantastic program that I know the AGFD community will deeply value.

I close with gratitude for being involved in AGFD, not only as Chair in 2024 but also as an AGFD member, and the opportunity to connect and network with all that support our Division. I wish you an enjoyable meeting and for those

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of you coming in-person to New Orleans, I hope to see you at the symposia and perhaps at the Chair's Reception on Tuesday where we can enjoy the company of our peers and perhaps share a drink in appreciation of all the hard work each of us does each day. I am looking forward to seeing you in NOLA!

Jason Soares
AGFD Chair 2024

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FUTURE PROGRAMS

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

Advancement of Application of Agricultural and Food Chemistry Award Symposium Michael Morello mjmorello226@gmail.com Jason Soares Jason.w.soares.civ@army.mil

Young Scientist Award Youngmok Kim youngmok.kim@finlays.net Bhimu Patil b-patil@tamu.edu

Bioproducts from Biomass: Renewable Chemicals and Polymers Helen Ngo Majher Sarker Brajendra Sharma Madhav Yadav Jinwen Zhang jwzhang@wsu.edu

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

Chemistry of Alcoholic Beverages Nick Flynn nflynn@wtamu.edu

Elevating Sustainability and Greentech in Agriculture and Plant-based Foods Michael Appell michael.appell@gmail.com Lingyun Chen lingyun.chen@ualberta.ca Omowunmi Sadik sadik@njit.edu Y. Jane Tseng yjtseng@csie.ntu.edu.tw Liangli (Lucy) Yu lyu5@umd.edu

Extraction, Recombinant Production and Function of Protiens of Food Safety & Food Manufacturing Importance Yuzhu Zhang yuzhu.zhang@usda.gov

General Papers Elizabeth Kreger Elizabeth.Kreger@sensient.com Jason Soares Jason.w.soares.civ@army.mil

General Posters Elizabeth Kreger Elizabeth.Kreger@sensient.com Jason Soares Jason.w.soares.civ@army.mil

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

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

Precision Fermentation and Cellular Agriculture Majher Sarker Jianping Wu jwu3@ualberta.ca

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

Sterling B. Hendricks Memorial Lectureship Award Sarah Leibowitz Michael Morello mjmorello226@gmail.com

Sustainable Agriceuticals Hyunsook Kim Bailiang Li LinShu Liu linshu.liu@usda.gov Wally Yokoyama

Role of Chemistry in Indoor Agriculture Xiaofen Du xdu@twu.edu Yun Yin yunyin2@vt.edu

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Virtual Graduate Student Symposium in Asia-Pacific Region on Agricultural and Food Chemistry Chunxiao Zheng czheng@acs-i.org

Waste Upcycling and Natural Flavor Ingredients Keith Caldwallader Xiaofen Du xdu@twu.edu

Whole Grain Bioactives & Human Health Shengmin Sang ssang@ncat.edu Dmitriy Smolensky Chris Zhu

SAN DIEGO March 23 – 27, 2025

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

James Seiber Memorial Symposium Alyson Mitchell aemitchell@ucdavis.edu

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

Celebrating Citrus Research with Russell Rouseff on his 80th Birthday Xiaofen Du xdu@twu.edu

Forever Chemicals in the Environment - Distribution & Risk Christine Sayes christie_sayes@baylor.edu

Microbial-Based Green Chemistry to Carbon-Neutral/Negative organizers?

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

WASHINGTON DC August 17 – 21, 2025

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

Application of Renewable Chemicals and Polymers in Agriculture Jinwen Zhang jwzhang@wsu.edu Long Jiang long.jiang@ndsu.edu

CCC Food Security Reducing Food Waste Michael Tunick mht39@drexel.edu

Food Fraud: Chemistry Strategies for Detecting and Reducing Food Crimes Neil Da Costa neil.dacosta@iff.com

OTHER SYMPOSIA OF INTEREST November 4-7, 2024, Auckland, New Zealand
4th International Flavor and Fragrance Conference Michael Qian michael.qian@oregonstate.edu

Urban South Brewery Tour & Tasting

At 6:30 PM on March 18th you can (if 21 & over) learn more about how a brewery is set up and sample some fine beers at the Urban South Brewery, 1645 Tchoupitoulas Street in the Lower Garden District of New Orleans. (504) 267-4852. Participants need to register ($25) through the link Urban South Brewery Tour & Tasting. Note that YCC is sponsoring a separately ticketed Homebrew Workshop immediately following the Brewery Tour. Procure tickets for the Homebrew Workshop through ACS registration. For more information contact Dr. Nick Flynn (806-651-2542) or nflynn@wtamu.edu

********** CORRECTION **********

The AGFD Officer and Committee Leadership Roster appearing in the Spring and Fall 2023 *Cornucopia* issues was incomplete. The correct roster should have listed both Karley Mahalak and Hye-Seon Kim as co-chairs for the Nutrition and Gut Microbiome Subdivision. Thx to Youngmok Kim for pointing out this oversight.

Executive Committee Meeting Minutes

Monday August 14, 2023 5:00-8:00 PM Moscone Center, San Francisco

Attendance: Alyson Mitchell, Jonathan Beauchamp, Jason Soares, Elyse Doria, Tom Wang, Karley Mahalak, Lauren Jackson, Stephen Toth, Kathryn Deibler, Gal Kreitman, Jianping Wu, Liz Kreger, Mike Tunick, LinShu Liu, Lucy Yu, Roberta Tardugno, James Lee, Bhimu Patil, Jinwen Zhang, Yun Yin, Michael Appell, Keith Cadwallader, Michael Morello

Jonathan Beauchamp called the meeting to order at 5:10 PM.

The minutes of the previous Executive Committee Meeting were approved with no changes and are published in the Fall 2023 Cornucopia.

Stephen Toth gave the Treasurer's Report. Councilor reimbursements from the Spring 2023 meeting in Indianapolis have not yet been received by the Division. Revenue for the year was $52,193 and expenditures were $42,620. The Division has $1,041,279 in total assets and is financially healthy. A standing budget for swag was proposed at $2,500 for each meeting and approved by the Executive Committee. A budget of $50,000 was set and approved by the Committee for the Spring 2024 meeting in New Orleans.

Jonathan Beauchamp summarized the Awards Committee Report for Michael Morello (who was unable to attend at the start of the meeting). The IFF Award for the Advancement of Application of Agricultural and Food Chemistry was conferred to Liangli (Lucy) Yu from the University of Maryland. The Young Scientist Award was given to Xiaonan Sui from the Northeast Agricultural University, China. The Young Industrial Scientist Award was awarded to Zhuohong (Kenny) Xie, from US Pharmacopeia, Rockville, MD. The AGFD Fellow Award was awarded to Shiming Li from Huanggang Normal University, China and Rickey Y. Yada from the University of British Columbia, Canada. The Teranishi Fellowship was awarded to Kaidi Wang from McGill University, Canada. The Graduate Student Symposium was cancelled due to a lack of submissions. Two students, Celina Paoletta, Newport University and Christopher Prajogo, UC Davis, California tied for first place in the Undergraduate Poster Competition. Second place was shared by Bret Watson and Jordon Scalia, Shippensburg University, Pennsylvania for their joint contribution and Kourtney Collier, Purdue, Indianapolis received third place in the competition. Michael Morello obtained a list of our 25 and 50 year members and pins will be mailed out by Stephen Toth. Bhimu Patil volunteered to assist Michael Morello with the Young Industrial Scientist Award. The JAFC-AGFD Division Best Research Article of year award went to Shari Dhaene as lead author of an article titled "Sweet Biotechnology: Enzymatic Production and Digestibility Screening of Novel Kojibiose and Nigerose Analogues". The Sterling B. Hendricks Memorial Lectureship was awarded to Gary List from the University of Illinois, Urbana-Champaign and the Kenneth A Spencer Award for Food and Agricultural Chemistry was awarded to Dr. Joel Coats, from Iowa State University.

The Student Committee Report was given by Elyse Doria who indicated that she had organized a student social at the Fall 2023 meeting, which was well attended. She continues to collect student emails during the poster session and is growing the student email list-serve. Several new student members were recruited during the San Francisco meeting.

In the Program Report, Jason Soares indicated that there are about 40 sessions, more than 20 symposia, 116 posters in addition to 20 virtual sessions being presented in San Francisco. Overall, the Division did a great job at programming. The two virtual sessions promoted by ACS for the China Chapter had about 20 sessions. Jason indicated that the new changes in ACS programming have resulted in the Division being allotted a limited number of 4-hour (half-day) sessions. Allotment is based upon average attendance from the previous meetings. As AGFD had light programming in Indianapolis, space was somewhat restricted for San Francisco. This change makes larger programs more challenging for the Program Chair as AGFD historically has fewer symposia in the Spring and therefore receive fewer allotments for Fall programming. Jonathan Beauchamp indicated that Elyse Doria made a spreadsheet for volunteering to help manage the conference information table. The sign-up sheet was sent out to the Executive Committee prior to the meeting. This practice will be continued for the New Orleans meeting. Jonathan also indicated that the ACS Proud to be a Chemist campaign is doing a video series and is interviewing several people from the Division to give short one-on-one interviews. Jonathan will ask if the Division can have video cuts for posting on the Division website. The Spring 2024 National Meeting will be held in New Orleans March 17-21, 2024. The theme of the meeting is the Many Flavors

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of Chemistry. To date we have 14 symposia planned and 7 are in alignment with the thematic programming. The Division has been allotted 16 sessions. ACS funding is now prioritized for joint programming. The abstract call will close Oct 2, 2023. Program workbooks are due mid-October and the final program due in mid-November. Kathryn Deibler asked that we try and make ACS aware that the graduate award deadline of Sept. 29th is unreasonable as students are just returning to campuses at this time. Liz Kreger asked if we could hand out "food gifts" at the New Orleans meeting. All agreed this would be in alignment with what the Division has done at previous ACS meetings. A budget of $11,000 was set and approved in support of the AGFD Communicating Culinary Chemistry Competition: Coastal Cuisine, which will take place during the 267th ACS National Meeting in New Orleans. Liz Kreger indicated that there are already 16 symposia planned for the Fall 2024 National Meeting. Some of the award symposia are going to be combined. AGRO will host the Spencer Award. The 4th International Flavor and Fragrance Conference will be held in New Zealand in 2024.

In Subdivision Reports, LinShu Liu indicated that the Agricuetical Subdivision programmed three sessions in San Francisco and that Bailiang Li, Northeast Agricultural University, China will be the Division secretary for 2024. Gal Kreitman indicated that the Flavor Subdivision held two symposia in San Francisco that were well attended (~75 people). For New Orleans, the Flavor Subdivision has six sessions planned. Yun Yin, Vermont University will be will be the Subdivision secretary for 2024. James Lee indicated that the Food Bioengineering Subdivision has one session in San Francisco and one planned for New Orleans. Jinwen Zhang, Washington State University will be the Subdivision secretary for 2024. A report for the Food Safety Division was not given and a secretary for this Subdivision still needs to be identified. Jianping Wu gave the report for the Functional Foods & Natural Products Subdivision. Jianping indicated that one symposium was given in the San Francisco and that there are two symposia planned for next year. Xiaohong Sun, Dalhouse University will be the Subdivision secretary for 2024. Karley Mahalak indicated that the Nutrition & Gut Microbiome Subdivision was very busy and held an ACS microbiome kick-off with four sessions and 30 speakers in Fall 2023. Jenny Firrman, Eastern Regional Research Center, USDA, will be the Subdivision secretary for 2024. The Sustainable & Green Technology Subdivision has four sessions planned for next year. A secretary for this Subdivision still needs to be identified.

The Councilors Report was given by Lauren Jackson, Michael Tunick and Alyson Mitchell. Several petitions are before the council, amending the rules in case a council member is inactive. There is also a petition to amend the council executive function; removing the oral reporting requirement for non-elected society committees and a petition to add an international representation to the Board of Directors, decreasing the total number of Directors at Large from six to five and creating an International District Director. Michael Tunick gave an update on DAC activities and indicated that the Division of Biological Chemistry is petitioning to change their name to Biochemistry and Chemical Biology. He also indicated that there were only six Innovative Project Grants (IPG) and two strategic planning retreat grants submitted. ACS will spend $67,000 but budgeted $100,000 and will therefore distribute the excess funds to the Divisions.

The Nominations Report was given by LinShu Liu. The nomination of Professor Coralia Osario Roa, University of Columbia as the 2024 Vice-Chair was approved. Alyson Mitchell and Stephen Toth were both approved to continue in their roles as Division Secretary and Division Treasurer, respectively, for 2024. The Division approved the nomination of Alyson Mitchell and Lauren Jackson to serve as Councilors for the Division (2024-26) and the nomination of Brian Guthrie as an Alternate Councilor (2024-26) for the Division. The Division bylaws allows for electronic balloting. The deadline for the voting is November. Alyson asked that another Executive Committee member run the balloting to avoid any potential conflict of interest. Michael Appell will run the balloting.

The Cornucopia Report was given by Alyson Mitchell on behalf of Carl Frey. An electronic version of the Cornucopia was sent out to members via email and 100 hard copies of the short (no abstracts) version were printed for distribution at the San Francisco meeting. The Fall 2023 Cornucopia without abstracts (28 pages) and with abstracts (136 pages) were both record page counts for our Division. A few minor edits received after the document went to the printer appear in the version posted on the AGFD site. Jonathan suggested having an earlier deadline for Carl so that edits can be corrected prior to printing.

The Hospitality/Public Relations Report was given by Alyson Mitchell who indicated that 80 tickets were made available for the Division Awards Dinner being held Tuesday, August 15 from 6:00-8:00 PM at Fogo De Chao. A dinner for the Executive Committee was organized for after the Executive Committee meeting.

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Jonathan Beauchamp gave the Membership Report on behalf of Michael Qian. Current Division membership is lower than pre-COVID and is about ~1800, however several new members were recruited during the SF meeting.

The Journal Report was given by Michael Tunick on behalf of Lucy Yu. The Journal of Agricultural and Food Chemistry expects 10,000 submissions in 2023. The impact factor of the Journal is now 6.1. Lucy Yu and Veronika Somoza are now executive editors. The impact factor of ACS Food Science and Technology and ACS Agricultural Science and Technology are 2.3 and 2.5, respectively. Fall symposia organizers will be asked to solicit their speakers for interest in putting together a special issue for these journals.

Mike Appell gave the Communications Report and indicated that he has successfully sent out emails from the WIX website server. Alyson will be working with Michael to migrate the AGFD Listserv to the WIX website server. There was discussion regarding the best way to achieve a seamless transition. Alyson will send out two notifications to the old Listserv letting recipients know that the Listserv will be discontinued and ask members to update their email addresses in the ACS membership profiles. A change will be made from monthly newsletters to quarterly newsletters.

An update on the upcoming Strategic Planning Retreat was given by Lauren Jackson. The retreat is planned for Oct 7-8th in Washington D.C. A survey was sent out to members, however to date the response level has been low (~55 responses out of ~1800 members). The survey will be held open for another week and Michael Appell will send out a survey reminder email via the WIX website server.

Michael Morello gave the report for the Senior Program Guidance Committee. The committee met twice since the Spring 2023 Executive Committee Meeting. The committee addressed promotion for the Fall 2023 meeting and the space limitations imposed by ACS related to previous in-person programming. Moving forward, ACS will be using an algorithm to assign space and ACS will be trying different programming models for the Spring and Fall Meetings, with greater emphasis on in-person attendance at the spring meeting. AGFD has always had larger programs in the Fall so the new ACS model will present on-going challenges for AGFD. The committee discussed ways to either limit symposia or incorporate more time for discussion and networking. The committee proposed having a subcommittee to create webinars for the Division, identify speakers, work on registration and operations and on promoting the webinars. The idea of having AGFD Subdivisions rotate annually to give a webinar was presented. It was noted that other ACS Divisions are giving high level training classes (short courses) as Webinars (3-4 lectures) and that this may be a good option for our Division. SPGC now has access to Subdivision member lists and will work with Subdivision leaders on how best to engage members.

In New Business, Jason Soares gave an ACS slide presentation on reimaging the ACS meetings through 2030 to better meet the needs of key stakeholders. The new ACS program will be rolled out 2025-2027. The impact of these changes on the Division was discussed and will be addressed during the Strategic Planning Retreat. The impact of the new limits in allotted symposia/sessions at National Meetings was discussed. The strategy of joint programming to share sessions, was recognized, however concern was voiced that joint programming across divisions will become a tall task for volunteer organizers. The pros and cons of limiting the number of sessions in each symposium to two was discussed.

Fereidoon Shahidi discussed a resolution to have AGFD serve as the official scientific body of the International Union/Academy of Food Science and Technology (IUFoST/IAFoST) representing USA. This topic will be discussed during the Business Meeting as Fereidoon was not present to discuss this resolution.

Michael Morello has the new pins for our 25-year members and has ordered past-chair pins which will be given out at the next meeting. The Membership Chair is responsible for identifying 25 and 50 year members. Michael Qian will be reminded of this obligation. Michael Tunick indicated that he is not getting any nominations for the Division Service Award and asked for folks to make more nominations. Kathryn Deibler indicated that it would be helpful to have a redacted paper copy of names of our members for the meetings. This would help in identifying members when giving out swag and tickets for the awards reception.

Michael Morello is timing out of the term-limited ComSci committee and a position for 2024-27 will be open. The various committees of ComSci were discussed. Nominations for the ComSci will be open until Oct 6th. The Division makes the nominations. AGFD members will be notified of this opportunity via email.

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Johnathan Beauchamp recapped the objectives of the Past-Chairs Club which were clarified during the Strategic Planning Committee meeting. The Executive Committee approved the formation of this new committee, which will have no authority or over-sight and agreed that it will provide the Division with critical institutional knowledge and support. Participation on the committee is voluntary.

The meeting adjourned at 7:32 PM. *Minutes submitted by Alyson Mitchell*

Business Meeting Minutes

Wednesday August 15, 2023 12:00-1:00 PM Moscone Center, San Francisco

Attendance: Alyson Mitchell, Jonathan Beauchamp, Jason Soares, Elyse Doria, Lucy Yu, Roberta Tardugno, Michael Morello, Michael Appell, Tom Wang, Xuetong Fan, Fereidoon Shahidi, Mathias, Michael Tunick, Robert McGorrin

Jonathan Beauchamp called the meeting to order at 12:07 PM

Alyson Mitchell summarized the minutes of the Executive Committee meeting. A motion was approved to create a *Past-Chairs Club* as an advisory council for the Division.

The slate of candidates proposed for two Councillors and one Alternative Councillor positions, presented during the *Executive Committee* meeting, was approved and passed unanimously. Councillors nominated include: Alyson Mitchell and Lauren Jackson (Councillors 2024-2026) and Brian Guthrie (Alternative Councillor 2024-2026). Michael Appell will conduct an electronic vote to fill these positions prior to November.

Fereidoon Shahidi discussed a resolution to have AGFD serve as the official scientific body of the International Union/Academy of Food Science and Technology (IUFoST/IAFoST) representing USA. The 22nd IUFoST World Congress 2024 will be held in Italy. IUFoST membership is composed of multiple organizations. To be a part of IUFoST there is a nominal fee (~$500). Members can vote and be involved in programming and leadership. Fereidoon requests an AGFD affiliation for co-programming. It was noted that all affiliations need to go through ACS for approval. Michael Appell put forward a motion to proceed with exploring this affiliation, with a limit of $1,000 in financial membership commitment, and that Jonathan Beauchamp act as AGFD liaison in this process. The motion was approved.

The meeting adjourned at 1:00 PM. *Minutes submitted by Alyson Mitchell*

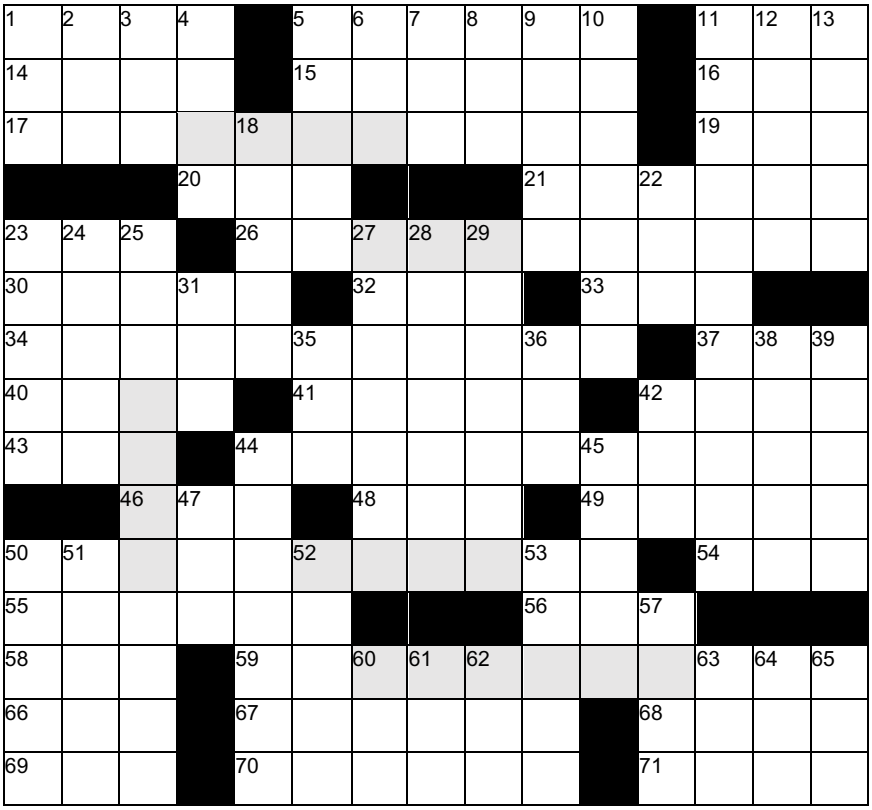
AWARD NEWS

IUFoST Lifetime Achievement Award

The International Union of Food Science and Technology announced **Fereidoon Shahidi**, University Research Professor and Distinguished Scholar in the Department of Biochemistry at Memorial University of Newfoundland, as the winner of its prestigious Lifetime Achievement Award, recognizing his pre-eminence in and contributions to the field of Food Science and Technology, especially in the field of nutraceuticals and functional foods. Dr. Shahidi's nominating peers highlighted his Food Science research contributions and education efforts. He has >1,000 publications (books, chapters, reviewed journal articles). His research and publications have contributed profoundly to understanding the composition and properties of many raw materials and processed foods. In 2023 Prof. Shahidi received the IFT Chicago section Lifetime Achievement Award in honor of Nicolas Appert. Fereidoon served in the AGFD leadership rotation culminating in AGFD Chair, as Alternate Councilor, leads the AGFD Fellows Selection Committee and helped originate the Functional Foods and Natural Products subdivision. He is an AGFD and ACS Fellow.

AGFD congratulates Fereidoon and looks forward to his continued success and contributions.

SECRET FLAVORS OF NEW ORLEANS



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

Congratulations to Veronica Mall of Leibniz Institute for Food Systems Biology for submitting a correct solution to the Fall '23 Cornucopia puzzle

ACROSS

1 Woodworker's tool
5 Email addy component
11 Usual T-shirt size options
14 Film unit or fishing need
15 Bryce Canyon formation
16 N.C. river (w/2 DOWN)
17 *Member of a clever elite
19 Enough! Give __ rest!
20 Chimpanzee or bonobo
21 Fancy glass-stoppered perfume bottle
23 Thief's flight: 'on the __'
26 *Cue to C & W singer McEntire
30 Tijuana bud
32 Tijuana year
33 *O Sole* __
34 A nod and a wink
37 WED, THU, __, SAT
40 'Inside' prefix
41 Woe is me.
42 Actor Hale, Alda or Ladd
43 Big outdoor gear retailer
44 Guitar lick played by actor Crothers
46 Ignited, illuminated
48 Keats' *Ode__Nightingale*
49 Proposal, suggestion
50 *The skinny on the baby powder biz
54 Notable time period
55 Sandwich from Viet Nam
56 Ford sedan of the 70's
58 Miner's quest
59 *Hey, I'm looking for Bert's roomie.
66 Some characters other than LTRS
67 'And others' in ancient Rome
68 Pleasant town on the French Riviera
69 Short typed dashes
70 Like stronger coffee, usually
71 A pair of plow pullers on a farm

DOWN

1 __ chair or __ candy
2 See 16 ACROSS
3 A school of Buddhism
4 *Frozen* queen
5 Oh, man! Do I have to?
6 Ballet dancer support, often
7 He can be 'II', sometimes
8 Despot Amin
9 Cheer for a flying saucer
10 One urban renewal aim
11 Variety, or a hint to * clues
12 Anti-sexual abuse movement
13 Singer/songwriter Rimes
18 Lab/kitchen splash guard
22 Jackie's #2
23 Point of amusement for a cat
24 Many a molecule with N
25 *It's often just the sniffles or a tummy ache
27 Rice that smells nice
28 Jennifer of *Friends*
29 Roll you bring to the gym
31 __-cache or __metric
35 Spasm that sounds like a clock
36 Document signed to protect IP
38 US decathlete gold medalist: __ Johnson
39 Spectroscopic structure determination method: __-red
42 'Who's a good dog?' response
44 Unable to solve a puzzle
45 Nick of 1982 flick *48 Hrs.*
47 Line from 1963 JFK speech: "__ bin ein Berliner."
50 Singer/songwriter Burnett
51 Hammerin' Hank __
52 Sporty Mazda 2 seater
53 *Pomp and Circumstance* composer
57 Bond nemesis with a mechanical 1 DOWN
60 Long, narrow fish
61 Sort, type, kind
62 'Never' in Nuremberg
63 Put the kibosh on
64 Sometimes cubical cooler
65 Poetic late day

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 ~1800 AGFD members via the application form (below) or on-line at www.agfoodchem.org or www.acs.org (click on Communities, Technical Divisions, Technical Division List) or call ACS (800)333-9511 (in US) or 616-447-3776 (outside US). Payment by Visa/MasterCard or AmEx.

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

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

ROSTER OF AGFD OFFICERS & COMMITTEE LEADERSHIP

Chair - Serves 1 year. Presides over Division meetings/appoints committees
Jason W. Soares US Army DEVCOM Soldier Ctr Jason.w.soares.civ@army.mil

Chair-Elect - Serves 1 year. Substitutes for Chair as needed. Organizes technical programs at national meetings.
Liz Kreger Sensient Flavors & Extracts
Elizabeth.Kreger@sensient.com

Vice-Chair - Serves 1 year. Assists Chair-elect. Develops future technical programs.
Coralia Osorio Roa UNAL
cosorior@unal.edu.co

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 - Edits newsletter.
Carl Frey cfreyenterprise@gmail.com

Councilors - Represent Division for 3 years on ACS council.
Alyson Mitchell (thru '26)
aemitchell@ucdavis.edu
Lauren Jackson (thru '26)
lauren.jackson@fda.hhs.gov
Michael Tunick (thru '24)
mht39@drexel.edu

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

Student Activities - Attracts and retains graduate/undergraduate student members. 2 year term.
Elyse Lauren Doria, eldoria@ucdavis.edu

Nominations - Develops officer slate. Served by immediate past chair.
Jonathan Beauchamp
jonathan.beauchamp@ivv.fraunhofer.de

Finance - Monitors Div. finances. 1 year term. Served by immediate past chair.
Jonathan Beauchamp
jonathan.beauchamp@ivv.fraunhofer.de

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

Alternate Councilors - Substitute for Councilors. Serve 3 years.
Kathryn Deibler (thru '24)
kdd3@cornell.edu
Michael Qian (thru '24)
Michael.qian@oregonstate.edu
Brian Guthrie (thru '26)
Brian_Guthrie@cargill.com

At-Large Executive Committee Members - Assist in Div. management. Serve 3 years.
Jane Leland (thru '26)
JLelandEnterprises@gmail.com
Robert McGorrin (thru '26)
robert.mcgorrin@oregonstate.edu
Bosoon Park (thru '24)
bosoon.park@usda.gov
One vacancy

Awards – Oversee awards process.
Chair Michael Morello
mjmorello226@gmail.com
AGFD Fellow Awards
Fereidoon Shahidi fshahidi@mun.ca
Young Scientist Award
Youngmok Kim
youngmok.kim@finlays.net
Young Industrial Scientist Award
Bhimanagouda (Bhimu) Patil
b-patil@tamu.edu
AGFD Distinguished Service Award
Michael Tunick mht39@drexel.edu
Roy Teranishi Graduate Fellowship
Liangli (Lucy) Yu lyu5@umd.edu
Student Awards
Kathryn Deibler kdd3@cornell.edu

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

Public Relations – Publicizes Div.
Alyson Mitchell
aemitchell@ucdavis.edu

Membership - Recruits and retains Division members. Michael Qian
michael.qian@oregonstate.edu

Agriceutical Sub.Div.
Chair Hyunsook Kim
Hyunsk15@henyang.ac.kr
Chair-elect, Yuzhu Zhang
yuzhu.zhang@usda.gov
V-chair Ying Wu ywu@Tnstate.edu
Secretary Bailiang Li
15846092362@163.com

Food Bioengineering Sub.Div.
Chair Kwang-Guen Lee
kwglee@dongguk.edu
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Vice-chair Changqing Wu,
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Secretary Jinwen Zhang
jwzhang@wsu.edu

Flavor Sub.Div.
Chair Xiaofen Du xdu@twu.edu
Chair-elect Joonhyuk Suh J.Suh@uga.edu
Vice-chair Yun Yin yunyin2@vt.edu
Secretary Yu Fang yufang@coca-cola.com

Food Safety Sub.Div.
Chair Xiaonan Lu xiaonan.lu@mcgill.ca
Chair-elect Boyan Gao
gaoboyan@sjtu.edu.cn
V-chair Vivian Wu vivian.wu@usda.gov
Secretary Yanhong Liu
Yanhong.liu@usda.gov

Functional Food/Nat. Product SubDiv
Chair Kenny Xie KYX@usp.org
Chair-elect Yingdong Zhu
yzhu1@ncat.edu
Vice-chair Khizar Hayat
khizaraura@gmail.com
Secretary Xiaohong Sun
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Nutrition & Gut Microbiome Sub.Div.
Chair Laurel Doherty
Laurel.a.doherty.civ@mail.mil
Chair-elect Ida Pantoja-Feliciano
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Vice-chair Tom Wang
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Secretary Jenni Firrman
Jenni.firrman@usda.gov

Sustainability/Green Tech. Sub.Div.
Chair Yufeng Jane Tseng
yjtseng@csie.ntu.edu.tw
Chair-elect Lingyun Chen
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Vice-chair Omowunmi "Wunmi" Sadik
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Secretary Yi-Shu Tu
georgetu@gmail.com

Food Security: Tackling World Hunger CCC – March 17–20, 2024

CCC will emphasize the role of chemistry in addressing world hunger through food security via 3 blocks of activities:
1) Flagship symposium: crop production nanotechnology, sustainable food packaging & advanced food safety solutions.
2) Student Posters: novel food ingredients and technologies for improving food security.
3) Co-sponsored symposia: challenges and advancements in food allergen detection, sustainable flavor extraction, mycotoxin management and research aimed at enhancing global food security and safety.

CCC Flagship Symposium (March 17) at Morial Conv. Ctr.

Food Security: Tackling World Hunger CCC: Highlighting Chemistry from Multiple Divisions 8:30am - 11:45am rm 336
Michael Morello, Zhuohong Xie organizers/presiders, Christy Haynes, Slawo Lomnicki, Sherine Obare, presiders

Graphene synthesized from a microbial culture as a nanocarrier for plants Nandini Bhattacharya, presenter; Mandira Kochar, Himadri Bohidar, Wenrong Yang, David Cahill

Silica nanomaterials to improve crop production
Christy Haynes, presenter

Assessment of the antioxidant potential of Indian spice extracts for enhancing the oxidative stability of salmon fish oil Nutan Kaushik, presenter, Asha Kumari, Rasa Slizyte, Revilija Mozuraityte, Hedi Johnsen

Incorporation of dairy by-products into hydrogel structures for cultivated meat production Patrick Charron, Christopher Foley, Irfan Tahir, Rachael Floreani, presenter

Pioneering sustainable food packaging: Biodegradable anti-bacterial silk coating for enhanced food safety and waste reduction Yagmur Yegin, presenter, Benedetto Marelli

Food Security: Tackling World Hunger CCC: Highlighting Chemistry from Multiple Divisions: 2:00pm - 06:00pm rm 336
Michael Morello, Zhuohong Xie, organizers/presiders, Christy Haynes, Slawo Lomnicki, Sherine Obare, presiders

Iron-based amendments decrease bioaccumulation of arsenic in lettuce grown in a contaminated soil Adeyemi Adeleye, presenter, Ziwei Han

Blighia sapida, a versatile fruit, alleviating hunger and promoting good health Andrea M. Goldson-Barnaby, presenter, Debbie Phillips

Flavors of specialty crops from controlled environment agriculture
Yun Yin, presenter, Jingsi Liu, Isabel Gutierrez, Michael Evans

Novel nanoparticle platforms for improved plant genetic engineering Gozde Demirer, presenter

Development of phage-CRISPR nexus for microbial food safety
Juhong Chen, presenter

Sustainable technologies for protein ingredient production from alternate crops: A path forward for zero hunger Nandika Bandara, presenter, Thilini Dissanayake, Anuruddika Hetti Hewage

Functional foods in the daily diet: The potential of plants and fruits traditionally consumed in the Yucatan peninsula Luis Pena-Rodriguez, presenter

CCC Student posters (March 17) at Morial Conv. Ctr. Hall C
AGFD General Poster Session and Undergraduate Poster Competition 7:00pm - 9:00pm
Kathryn Deibler, Elizabeth Kreger, Jason Soares, organizers

Variation in the β-carotene content of Blighia sapida under various processing methods Debbie Ann Phillips, presenter, Andrea M. Goldson-Barnaby

Narrow-wavelength red LED lighting on quality and aroma expression of hydroponic fennel (Foeniculum vulgare Mill.)
Jingsi Liu, presenter, Adam Sumner, Alex Harris, Song Li, Bastiaan Bargmann, David Haak, Yun Yin

On-site fluorescent detection of microbial contamination using a graphene oxide CRISPR-Cas12a (GO-CRISPR) sensor
Tom Kasputis, presenter, Qiaoqiao Ci, Juhong Chen

Sustainable plant protein ingredient production from fava bean using choline chloride and glycerol deep eutectic solvent system
Anuruddika Hetti Hewage, presenter

Mung bean protein isolate: A novel food ingredient with enhanced functional properties extracted by a deep eutectic solvent Thilini Dissanayake, presenter

Characterization of purple star apple (Chrysophyllum cainito L.) as a promising functional food Gabriela Rubi Tapia-Alvarez, presenter, Elida Gastelum-Martinez, Karlina Garcia-Sosa, Lia Valencia-Chan, Rosa Moo-Puc, Inocencio Higuera-Ciapara, Luis Pena-Rodriguez

Carbon nanodots for the delivery of biomolecules in N. benthamiana Jesus Galeana, presenter

Mechanisms of arsenic immobilization by iron nanoparticles in a cultivated soil: Arsenic speciation and the role of iron sulfidation
Ziwei Han, presenter, Adeyemi Adeleye

Co-Sponsoring symposia (all in Morial Conv. Ctr.)
Food Allergen Characterization, Modification, and Detection
8:00am - 11:45am March 17 rm 357
Christopher P. Mattison, Qinchun Rao organizers/presiders

Extraction & Biotechnology: A Natural and Sustainable Future for Flavors: 8:00am - 11:50am March 18 rm 337
Xiaofen Du, organizer, Lewis Jones, Elizabeth Kreger organizers/presiders

Mycotoxins: Challenges and Future Perspectives:
8:00am - 12:00pm March 19 rm 357
Hans-Ulrich Humpf, Lauren Jackson organizers/presiders, Benedikt Cramer, presider

Mycotoxins: Challenges and Future Perspectives
2:00pm - 06:00pm March 19 rm 357
Hans-Ulrich Humpf, Lauren Jackson organizers/presiders, Hamed Abbas, presider

Paring Flavors with Health and Wellness Food Products
2:00pm - 05:30pm March 19 rm 336
Xiaofen Du, Danhui Wang organizers/presiders,

Mycotoxins: Challenges and Future Perspectives
8:00am - 12:00pm March 20 rm 340 Hans-Ulrich Humpf, Lauren Jackson organizers/presiders, Chris Maragos, presider

AGFD TECHNICAL PROGRAM

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

SUNDAY MORNING March 17
Morial Conv. Ctr. rm 357
Food Allergen Characterization, Modification, and Detection Financially supported by CCC Food Security: Tackling Hunger C. P. Mattison, Q. Rao, *Organizers, Presiding*
8:00 Introductory remarks.
8:05 Natural/artificial mutations and nitrogen/sulfur metabolism control for hypoallergenic buckwheat production. **T. Katsube-Tanaka**, Y. Yasui
8:30 Gluten in fermented or hydrolyzed foods: Challenges and opportunities for quantitative analysis. **R. Panda**, C. Galanis
8:55 Chemical and molecular analysis of heated pecan nuts. **C. Brown**, **R.A. Adams Dupre**, **P. Anne Zito**, **B. Smith**, C.P. Mattison
9:20 Transfer of shrimp proteins in shared batch fryers. **X. Jiang**, R. Beverly, J. Kidd, J. Cluster, K. Swajian, L. Jackson
9:45 Intermission.
10:00 Effectiveness of cleaning treatments for removing nut butter residue from shared processing equipment. **H. Green**, J. Kidd, J. Warren, L. Jackson
10:25 Investigation of in silico allergen identification methods based on nano-UHPLC-ESI MS/MS characterization data. **N. Diaz-Fortier**, **D. Mucs**, T. Hirata, A. Daikoku, I. Baskerville-Abraham
10:50 Biosimilar protein immunotherapy: Tolerance inducing immune response in patients with cow milk anaphylaxis. **N. Marsteller**, I. Randhawa
11:15 FDA regulatory update on food allergens. **L. Jackson**
11:40 Concluding Remarks.

Morial Conv. Ctr. rm 336
Food Security: Tackling World Hunger CCC: Highlighting Chemistry from Multiple Divisions Cospons. AGRO, ANYL, ENVR Financially supported by CCC Food Security: Tackling Hunger M. J. Morello, Z. Xie, *Organizers, Presiding* C. L. Haynes, S. M. Lomnicki, S. Obare, *Presiding*
8:00 Withdrawn
8:30 Introductory Remarks.
8:40 Graphene synthesized from a microbial culture as a nanocarrier for plants. **N. Bhattacharya**, M. Kochar, H.B. Bohidar, W. Yang, D. Cahill
9:10 Silica nanomaterials to improve crop production. **C.L. Haynes**
9:40 Intermission.
10:00 Assessment of the antioxidant potential of Indian spice extracts for enhancing the oxidative stability of salmon fish oil. **N. Kaushik**, A. Kumari, R. Slizyte, R. Mozuraityte, H. Johnsen
10:30 Incorporation of dairy by-products into hydrogel structures for cultivated meat production. P. Charron, C. Foley, I. Tahir, **R. Floreani**
11:00 Pioneering sustainable food packaging: Biodegradable anti-bacterial silk coating for enhanced food safety and waste reduction. **Y. Yegin**, B. Marelli
11:30 Discussion.

Aquatic Photochemistry Spons. ENVR, Cospons. AGFD, GEOC

SUNDAY AFTERNOON
Morial Conv. Ctr. rm 335
Withycombe-Charalambous Graduate Student Symposium E. Kreger, J. W. Soares, *Organizers* K. Deibler, *Organizer, Presiding*
2:00 Introductory Remarks.
2:05 3D-printed hydrogel-based nanocomposites for sustainable food packaging. **O. Popoola**, A. Finny, I. Dong, S. Andreescu
2:35 Untargeted flavoromics provides new insight into the impact of high-tunnel and open-field production on the variations of aroma profiles of industrial floral hemp. **Z. Gu**, **B. Chen**
3:05 Development of a microfluidic device to enrich and detect zearalenone in food using quantum dot-embedded molecularly imprinted polymer. **M.Z. Hua**, X. Lu
3:35 Intermission.
3:45 Solubilization of limonene by phospholipid vesicle dispersions. **A. Webley**, S.R. Dungan, S.E. Ebeler
4:15 Developing polymer-based delivery systems to improve bioaccessibility and bioefficacy of procyanidin dimers. **Z. Yin**, Q. Huang

Morial Conv. Ctr. rm 336
Food Security: Tackling World Hunger CCC: Highlighting Chemistry from Multiple Divisions Cospons. AGRO, ANYL, ENVR Financially supported by CCC Food Security: Tackling Hunger M. J. Morello, Z. Xie, *Organizers, Presiding* C. L. Haynes, S. M. Lomnicki, S. Obare, *Presiding*
2:00 Introductory Remarks.
2:10 Iron-based amendments decrease bioaccumulation of arsenic in lettuce grown in a contaminated soil. **A.S. Adeleye**, Z. Han
2:40 *Blighia sapida*, a versatile fruit, alleviating hunger and promoting good health. **A. Goldson-Barnaby**, D.L. Phillips
3:10 Flavors of specialty crops from controlled environment agriculture. **Y. Yin**, J. Liu, I. Gutierrez, M. Evans
3:40 Novel nanoparticle platforms for improved plant genetic engineering. **G.S. Demirer**
4:10 Intermission.
4:30 Development of phage-CRISPR nexus for microbial food safety. **J. Chen**
5:00 Sustainable technologies for protein ingredient production from alternate crops: A path forward for zero hunger. **N. Bandara**, T.N. Dissanayake, A. Hetti Hewage
5:30 Functional foods in the daily diet: The potential of plants and fruits traditionally consumed in the Yucatan peninsula. **L.M. Pena-Rodriguez**

Aquatic Photochemistry Spons. ENVR, Cospons. AGFD, GEOC

SUNDAY EVENING
Morial Conv. Ctr. Hall C
AGFD General Poster Session and Undergraduate Poster Competition K. Deibler, E. Kreger, J. W. Soares, *Organizers*
Note – first 23 posters listed below also presented at Monday Evening Sci-Mix

Poster01 Effects of ethylene exposure on Hass avocados (*Persea americana*) during ripening in the presence of Cavendish bananas (*Musa acuminata*) over a five-day period. **A. Gao**, A. Lee, S. Hsia, L. Qu, R. Choksey, A. Burgos, I. Choksey, L. Jannotti, E. Lopez-Couto, C. Yiyuan, R. Jannotti

Poster02 Genetically-encoded nanoparticles for siRNA-mediated crop genetic engineering. **V.H. Pistilli**, M. Legendre, G. Demirer

Poster03 All-natural healthy power aid drinks from specialty crops rich by antioxidants, essential oils, and terpenes. **L. Osman**, B. Sylla, A.G. Ristvey, V. Volkis

Poster04 Exploring flavors of edible ants: A path to sustainable gastronomy and consumer acceptance. **S. Alvarado Martinez**, A. Raza, D. Lopez, V. Esparza, J. Zhao, **C. Liu**

Poster05 Developing an Ochratoxin A nanoaptasensing screening system with a plasmonic platform. **A. Fabian**, A. Saldana, S. Córdova, Y. Hernandez, B.C. Galarreta

Poster06 Comprehensive comparison of the dynamics of kombucha fermentation in a silicone bag and a glass jar. **K. Chamberlain**, E. Swartz, J.N. Richardson, J. Kegerreis

Poster07 Investigating the impact of sugar source variation on kombucha fermentation. **I. Loscher**, A. Czarnecki, J.N. Richardson, J. Kegerreis

Poster08 Semi critical CO_2-ethanol assisted extraction of photoinduced bioactive pigments from seaweed algae: Advances in renewable dyes production for food supplements and pharmacy applications. **A. Chatmon**, V. Wamiru, T. Chavez-Gil

Poster09 Development of a high-performance thin layer chromatography (HPTLC) method for the qualification and quantification of soya saponin compounds. **G. Chavarria**, A. Sibaja-Salazar, S. Nates, V. Alvarez-Valverde, P. Jimenez-Bonilla

Poster10 Categorization of organic compounds in agricultural soils. **N. Reilly**

Poster11 Unraveling the health implications of modified sucralose. **I. Beasley**, D. Crain, M. Jorgensen, T. Mason, I.N. Nawarathne

Poster12 Comprehensive metabolomic profiling for elderberries (*Sambucus spp.*) in uncovering bioactive compounds. **N. Bostick**, P. Martano, M. Uy, S. Mahdi, X. Jones, Q. Yang, R. Mu

Poster13 Creating a glucometer-based device to observe the ripening of *Aronia mitschurinii*. **R. Buzzetto**, E. Cable, A.G. Ristvey, V. Volkis

Poster14 Effects of betulin derivatives from birch and sycamore bark on *Drosophila melanogaster*. **F. Davies**, M. Gross, L. Speranza, M. Wilklow-Marnell

Poster15 Molecular cloning of bacterial exopolysaccharide forming enzymes in sugarcane processing and biological and agricultural impacts. **J. Fein**, Y. Qi, G.O. Bruni, **E. Terrell**

Poster16 Understanding the flavors and aromas in wine and beer. **B. Bartholomew**, B. Caggiano, M.B. Jacobs

Poster17 Determination of xanthophyll carotenoid content in vegetables recommended for macular degeneration prevention through high performance liquid chromatography and heat exposure. **M. Tarrance**, K.W. Barnes

Poster18 Dr. Pepper Vanillin Flavor Compound determination and analysis using SPME and Headspace Analysis. **M. Tarrance**, K.W. Barnes

Poster19 Analysis of heavy metals in dark chocolate. **V. Pipinich**, **R.C. Dudek**

Poster20 Characterization of purple star apple (*Chrysophyllum cainito L.)* as a promising functional food. **G.R. Tapia-Alvarez**

Poster21 Evaluating chemical catalysts' thermal and kinetic effects on starch gelatinization. **S. Dupree**, T. Nguyen

Poster22 Increasing desirable aroma compounds in Pennsylvania wines by treating post-harvest grapes with elemental sulfur. **J.J. Messner**, M. Vincent, R. Elias, M. Kwasniewski

Poster23 Sustainable formulation solutions for dsRNA-based biopesticides for next-gen agricultural pest control. **S. Malik**, **A. Kumar**, M. Mondal, A. Pereira, F. Moshiri, K. Nawaz, T. Zanker, I. House, D. Gladson, S. Tomaschke, **J. Shoemake**, L. Nitcher

7:00 Publishing trends in journals of the ACS Agricultural and Food Chemistry portfolio. **C. Osorio Roa**, L.L. McConnell, T. Hofmann

7:00 Application of untargeted headspace solid-phase microextraction-gas chromatography-mass spectrometry for volatile metabolomics-based authentication of plant-based milk alternatives. **R. Handoyo**, E. Pagliano, Y. Hu

7:00 Variation in the β-carotene content of Blighia sapida under various processing methods. **D.L. Phillips**, A. Goldson-Barnaby

7:00 Mechanisms of arsenic immobilization by iron nanoparticles in a cultivated soil: Arsenic speciation and the role of iron sulfidation. **Z. Han**, A.S. Adeleye

7:00 On-site fluorescent detection of microbial contamination using a graphene oxide CRISPR-Cas12a (GO-CRISPR) sensor. **T. Kasputis**, Q. Ci, J. Chen

7:00 Mung bean protein isolate: A novel food ingredient with enhanced functional properties extracted by a deep eutectic solvent. **T.N. Dissanayake**

7:00 Sustainable plant protein ingredient production from fava bean using choline chloride and glycerol deep eutectic solvent system. **A. Hetti Hewage**

7:00 Narrow-wavelength red LED lighting on quality and aroma expression of hydroponic fennel (*Foeniculum vulgare* Mill.). **J. Liu**, A. Sumner, A. Harris, S. Li, B. Bargmann, D. Haak, Y. Yin

7:00 Identification of phytomarkers from *Byrsonima bucidifolia* fruits and their correlation with antioxidant activity: Chemometric approach. **M.G. Poot**

7:00 Carbon nanodots for the delivery of biomolecules in *N. benthamiana*. **J.M. Galeana**
, É. Gastelum-Martínez, K. García-Sosa, L.S. Valencia-Chan, R. Moo-Puc, I. Higuera-Ciapara, L.M. Pena-Rodriguez

7:00 Carcass and meat quality characteristics of pasture-raised lambs as influenced by highly digestible fiber containing agro-byproducts. **J. Lee**, S. Wildeus

7:00 Design of new and environmentally safe fungicides using AI and molecular modeling. **M. Shaver**, J.A. Darsey

7:00 Incorporation of bioactive compounds from *Melaleuca Alternifólia* essential oil in pea, potato and rice starch films. **F. Matta Fakhouri**, J.O. Zoppe, V. Augusto Garcia, J. Velasco

7:00 Mechanical properties of flexible films based on pea starch and cellulose nanocrystals produced by blown film extrusion. A. Dambros, F. Yamashita, **J.O. Zoppe**, J. Velasco, F. Matta Fakhouri

7:00 Research on changes in aroma components derived from citrus essential oils in beverages by time passing. **T. Sugawara**, T. Yoshimoto, K. Fukushima, N. Tanaka, N. Miyazawa, S. Ishizaki

7:00 Characterization of metabolome alterations in barley (*Hordeum vulgare* L.) induced by *Bipolaris sorokiniana*. **L. Kurzweil**

7:00 Biochar-Metal Organic Framework (BC-MOF) composites for the removal of rice fungicide(s) from water: An experimental and molecular simulation-based evaluation. **C. Reddy**, N. Singh, T. Banerjee, A. Mandal

7:00 Aflatoxin mitigation effect of 2,5-Diketopiperazines on *Aspergillus flavus* from Louisiana. M. Kumarihamy, G. Moore, Y. Guo, R. Sweany, C. Carter-Wientjes, **M. Lebar**
7:00 Identifying sensory descriptors and aroma-active compounds in domestic edamame. **R. Miller**, L. Hamilton, S. Duncan, T. Kuhar, R. Boyer, B. Zhang, J. Lahne, Y. Yin
7:00 Does condensed tannin protect zein nanoparticles from digestion?. **J. Jefferson**, S. Mallikarachchi, A.E. Hagerman
7:00 Condensed tannin characterization by modified saw tooth HPLC system. **K. Williams**, A.E. Hagerman
7:00 Evaluation of MIB and GSM reactivity using solid phase microextraction-GCMS. **W. Roussell**, R.A. Adams Dupre, B. Smith
7:00 GC-MS determination of sterols in dried morel mushrooms. **T.W. Nalli**, A. Overgard, S. Quint, N.Y. Walker, C.W. Chu
7:00 Almond shells: A natural bio-absorbent for reducing and recovering the phenolic content of winery wastewaters. **E. Doria**, L.A. Lerno, A.E. Mitchell
7:00 Chemical composition of different extracts of *Conyza bonariensis*. **M. Estrada**, I. Fabing
7:00 Formation mechanisms and potential toxicity of oxidized triacylglycerols in food during thermal processing. H. Zhu, C. Wang, **B. Gao**, L. Yu
7:00 Nano-based modification of phosphorous fertilizers: A path towards sustainable phosphate supply. **S. Mazumdar**, M.A. Quadir, A.N. Bezbaruah
7:00 Cultural management and applications of *Ocimum tenuiflorum (*Holy Basil*)* grown in Maryland. **E. Cable**, H. Den Ouden, V. Volkis
7:00 Protective effects of Citrus depressa peel extract on non-alcoholic fatty liver disease in mice fed a high-fat diet. **Z. Su**, X. Chen, G. Wei
7:00 Plant maturity affects the phenolic composition and antioxidant properties of green basil (*Ocimum basilicum* L.) cultivars. **H.P. Lawson**, E.D. Niemeyer
7:00 Influence of cultivar and seed source on the phenolic composition and antioxidant properties of *Monarda* herbs. H.P. Lawson, **E.D. Niemeyer**
7:00 Comparison of Headspace GC-MS techniques to characterize volatile phenols contributing to smoke taint in Pinot Noir wines. **S.J. Toth**, A. Noble
7:00 Effects of thermal and non-thermal processing on allergen removal from pistachio shell waste. **L. Fereidooni**, A. Morais, M.B. Shiflett
7:00 Assessing the biosynthetic inventory of the biocontrol fungus *Trichoderma afroharzianum* T22. **W. Han**, Z. Wu, Z. Zhong, J. Williams, S. Jacobsen, Z. Sun, Y. Tang
7:00 Investigation of natural polyphenols as potential colorectal cancer (CRC) therapeutics. J. Kardos, **T. Rennie**, J. Porter
7:00 Comparison of Logk', $LogP_{oct}$ and $LogD_{oct}$ values for the catechol flavones. **W.L. Whaley**, M. Gregory, T. Gibbs, S. Tuck
7:00 Beer we go! Analysis of carbonated and nitrogenated beers. **A.S. Frantzen**, S. Atkins, H.S. Gibson
7:00 Analyzing the effects of pulsed electric field in the winemaking process. **M.H. Lorentz**, O.M. McDougal, P. Santiago-Mora
7:00 Analysis of flavor and aromatic compounds in whisky using both gas and liquid chromatography and mass spectrometry. **E. Hendrix**, C.J. Monceaux
7:00 Lipoxygenases in Costa Rican soybean seeds: Influence on oil nutritional profile. **L. Vega Fernandez**, A. Holst, H. Mock, A. Irias-Mata
7:00 Discrimination of the geographical origin of various agricultural products by applying machine learning algorithms on data produced from different spectroscopic techniques. **J. Kapolos**, K. Papadimitriou, K. Dalaklidi, A. Koliadima, M. Papadelli
7:00 Algae as a precursor of seafood flavor in alternative seafood. **A. Raza**, E. Cramton, J. Baker, C. Liu, J. Zhao
7:00 Isomerization of hop alpha acids during wort boiling. **I. Hofland**, M.D. Schuder
7:00 Metabolomic analysis in organic and conventionally grown elderberries. **X. Jones**, S. Mahdi, N. Bostick, S.J. Eber, N. Navarrete-Tindall, R. Mu, Q. Yang
7:00 Essential oils: A natural solution for preserving potato quality in storage. **A. Alzarqaa**, V. Jeliazkov
7:00 Development of zein nanoparticles for encapsulating avocado seed extract as a functional ingredient. **T. Chuacharoen**
7:00 Non-targeted volatile and non-volatile analyses of pectin samples to correlate molecular composition with sensory evaluation. **C. Nauman**, **D. Chambers**, A. Zarth, L. Chan
7:00 Insecticidal potential of leaf extracts of *Heliotropium indicum* Linn (Boraginaceae) for control of insect pests of stored grains. **B.M. Adeniyi**
7:00 HS-SPME-GC-MS/Olfactometry-based sensory-directed flavoromics to uncover aroma boundary compositions of commercial barley malts with a wide Lovibond variation. **Z. Gu**, **B. Chen**
7:00 Toward a comprehensive understanding of ultracentrifugal milling on the processing properties and aroma profiles of yellow pea flour. **Z. Gu**, **B. Chen**
7:00 Acidic degradation and byproduct formation of MIB and GSM in aqueous environments. **R.A. Adams Dupre**, W. Roussell, B. Smith
7:00 Phosphorus reduction opportunities from animal agriculture utilizing a corn ethanol distillers grain feed substitute. **K. Ruffatto**, G. Shurson, R. Muenich, R. Cusick
7:00 The era of chemical spaces: Mining relevant chemistry. C. Lemmen, D. Comer, **J. Holowachuk**, A. Neumann
7:00 Characterizing food profiles and detecting contaminants with hyperspectral imaging. **G.A. Killian**
7:00 Characterization and quanitification of the polyphenols found in differing teas. **M.S. Sykes**, M.J. Crawford
7:00 Non-targeted analysis and standard free screening of PFAS using high-resolution mass spectrometry and ion mobility. **S. Putnam**, A. Kiehne, S. Bodendiek, E. Niehaus, B.K. Teeter
7:00 Food Analysis with Raman Microscopy. **S. Redes**

MONDAY MORNING March 18
Morial Conv. Ctr. rm 357
Agnes Rimando Memorial International Student Symposium M. H. Tunick, *Organizer* R. Tardugno, *Organizer, Presiding*
8:00 Introductory Remarks.
8:05 Influence of complex coacervation on the structure and texture of plant-based protein-polysaccharide composites. **X. Hu**, D.J. McClements
8:25 Phytotoxic activity of grammicin produced by *Xylaria* sp. infecting *Handroanthus serratifolius* (Bignoniaceae). **D. Barreto**, C. Rodrigues de Carvalho, J. Bajsa-Hirschel, S. Queiroz, S.O. Duke, C.L. Cantrell, L. Rosa
8:45 RuBisCo: An edible and functional protein applied in emulsions. **M. Müller**, H. Frielinghaus, O. Holderer, T. Heiden-Hecht
9:05 Metabolomic analysis with machine learning algorithms enables the evaluation of postharvest color stability in different pecan varieties. **M. Kang**, R.B. Pegg, L. Wells, P.J. Conner, J. Suh

9:25 Production and bioactivity of isoflavones from elicited hairy root cultures of pigeon pea. **G. Gajurel**, A.R. Sharma, S. Abdel-Karim, M.A. Alam, F. Medina-Bolivar
9:40 UHPLC-HRMS and GC-MS analyses of bioactive compounds in prairie berries in Canada and their antioxidant potential. **C. Kodikara**, S. Sura, N. Bandara, T. Netticadan, C. Wijekoon
9:55 Intermission.
10:10 Optimization of ultrasound-assisted extraction of xanthophylls from *Tagetes erecta* L. using hydrophobic deep eutectic solvents (HDES). **S. Ghoshal**, A. Dutta, S. Saha, A. Kundu, A. Mandal
10:25 Optimization of gluten-free bread's health benefits with Artichoke Leaf Extract and Sourdough Biotechnology. **A. Annunziato**, **F.M. Calabrese**, **R. Francavilla**, **M. De Angelis**
10:40 Exploring novel magnetite nanoclay: A breakthrough composite for pesticide removal from water. **A. Sil**, N. Narayanan, T. Banerjee, N. Singh, N. Jain, S. Gupta
10:55 Ultrasound-assisted extraction of betalains from dragon fruit (*Hylocereus* sp.) peels: Optimization using response surface methodology-genetic algorithm (RSM-GA) hybrid model and chemo-profiling. **D. Mondal**, A. Dutta, A. KUNDU, S. Saha
11:10 Synthesis and fungicidal activity of novel indazolylchromones. **R. Kundu**, P. Kaushik, N. Shakil, V. Rana
11:25 Bioactive phytochemicals from *Litsea glutinosa* bark for potential antifungal activity against *Penicillim expansum*. **S. suman**, **A. Kindu**, A. Dutta, S. Saha, A. DAS

Morial Conv. Ctr. rm 337
Extraction & Biotechnology: A Natural and Sustainable Future for Flavors Financially supported by CCC Food Security: Tackling Hunger X. Du, *Organizer* L. Jones, E. Kreger, *Organizers, Presiding*
8:00 Introductory Remarks.
8:05 Palm kernel oil: Physicochemical properties and volatile compounds. **V.T. Wyatt**, A. Aryee, P. Asuzu, P.N. Asare-Okai, N.A. Tawiah
8:30 Ionic liquids as green solvents of choice for the extraction of natural bioactive compounds. **M. Uroos**
8:55 From plant to palate: Refining cannabis extraction for flavor and fragrance. **M.E. Sosa**, I.W. Oswald, T. Paryani, T. Martin, K. Koby
9:20 The Aroma of Vanilla Extracts. K. Pechinger, C. Helcke, **L. Jones**
9:45 Intermission.
10:05 Characterization of hybrid Vanilla beans using DTD-GC-MS analysis. **S.J. Toth**, A. Noble
10:30 Unified quantitation method enables the elucidation of cheese flavor. **C.J. Feyerabend**, V.K. Mittermeier, M. Gigl, C. Dawid
10:55 Evaluation of different cell disruption methods to extract nutritional and flavor constituents of yeast biomass. **K.R. Cadwallader**, N. Hwisa, A. Chatha
11:20 Discussion.

Morial Conv. Ctr. rm 335
Chemistry of Alcoholic Beverages Cospons. YCC N. O. Flynn, *Organizer, Presiding*
8:00 Introductory Remarks.
8:05 Introduction: Chemistry of alcoholic beverages. **N.O. Flynn**
8:15 Beer foam: A chemistry wonderland. **C. Bamforth**
8:45 Chemistry underlying hangovers. **A.E. Mitchell**
9:05 Evaluation of rapid wort color method using caramel malt series and inclusion methods. **N.O. Flynn**
9:25 Chemical and sensory evaluation of 40 hop varieties: Insights into the relationship between aroma properties and growing regions using two-dimensional gas chromatography. **M.A. Ojeda**
9:45 Markers on the ageing of hoppy ales and non-alcoholic beers. **C. Schubert**, S. Lafontaine, N. Rettberg
10:05 Intermission.
10:20 Quantifying flavor: Characterization of a craft brewery experience using HS-GC-MS and LC-QTOF. **R.A. Quinlan**, D. Mitchell, B. McBride, D. Liskin, A. Higgs, A. Brehm, K. Kingsbury
10:40 Effect of copper complexation on polyfunctional thiol stability in beer. **M. Vincent**, M. Naziemiec, A. Silakov, R. Elias
11:00 Crafting the future of beer: Rapid and *in-situ* quality monitoring using portable IR spectroscopy. **h. bao**, L. Rodriguez-Saona
11:20 Advancing non-alcoholic beer quality: Examining the impact of NAB chemical profiles on industrial professionals' perceptions and preferences. **S. Lafontaine**, E. Leitner
11:40 Next-generation strategies for non-alcoholic lager beer production: A focus on both ethanol removal and flavor preservation. **Z. Zhou**, Y. Jin, K.R. Cadwallader

Achieving Environmental Justice in the Chemistry Enterprise: Connecting Innovation, Global Impacts and Burden Interdisciplinary Perspectives on Environmental Justice Spons. ENVR, Cospons. AGFD, AGRO, CEI, CHAL, CHED, CPRC, SCHB, SOCED
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MONDAY AFTERNOON
Morial Conv. Ctr. rm 335
Chemistry of Alcoholic Beverages Cospons. YCC N. O. Flynn, *Organizer, Presiding*
2:00 Introductory Remarks.
2:05 Withdrawn
2:25 ^{1}H-NMR-based metabolomics for profiling the chemistry of alcoholic beverages. **N. Kruse**, C. Anklin, T. Spengler
2:45 From the chemistry of raw materials and fermentation on to the shelf-life stability of beer and distilled spirits. **G. Spedding**
3:05 Effect of proof on the headspace concentrations of methoxyphenols found in whiskey. **L. Demoranville**, S.Y. Cabrera, M. Curran, M. Mittal, K. Williams, S. Yusufji
3:25 Application of spectroscopy technology in identification and quality screening of Pisco distillates. **Y. Wu**, L. Rodriguez-Saona
3:45 Evolution of chemical profiles in rice: From milling to malting and its influence on beverage/ beer quality. **B.P. Guimaraes**, R. Sen, S. Lafontaine
4:05 Quality and acceptability of wines processed using underutilized African edible indigenous fruits. **O. Francis**, S. Natukunda, W. Olupot
4:25 Concluding Remarks.

Morial Conv. Ctr. rm 357
Sensory Beyond Earth: The Relevance of Flavor Chemistry in Space Exploration N. C. Da Costa, *Organizer* J. Beauchamp, L. Julia, S. McGrane, *Organizers, Presiding*
2:00 Introductory remarks.
2:05 Consequences of olfactory loss. **T. Hummel**
2:30 The effects of a One-Year Antarctic Sojourn at the Concordia Research Station on olfactory and gustatory

functions. **I. Mack**, B. Klos, S. Wolf, S. Thoolen, H. Hagson, A. Meyer, P. Enck
2:55 HABSIM – Unique R&D Infrastructure for closed-loop food production in space and on Earth. **T. Blomqvist**, D. Schubert
3:20 Microwave processed ready-to-eat meals as a palatable and nutritional option for space missions. **M.L. Montero**, C.F. Ross
3:45 Intermission.
4:05 Development of a virtual reality tool ('food in space') for collecting sensory data during immersion for space ground-based strategy. G. Loke, I. Peake, A. Besnard, K. Kantono, G. Iles, L. Newman, **J. Low**
4:30 Correlations between food odour perception during space simulated analogs and their volatile profiles. **J. Chandrapala**, **G. Loke**, I. Peake, G. Iles, J. Low
4:55 Exploring effective tasting delivery modalities for tasting sensory studies in simulated space analogs. **T. Prabodha**, L. Ong, C. Gilden, I. Peake, C. Brennan, L. Danner, G. Iles, J. Low
5:20 Influence of immersion in a space-like environment on taste and odour perception. A. Tran, J. Low, **L. Duizer**
5:45 Concluding remarks.

VIRTUAL SESSION
AGFD General Poster Session and Undergraduate Poster Competition K. Deibler, E. Kreger, J. W. Soares, *Organizers*
12:00 Exploring Taiwan citrus extract's potential in inhibiting colorectal cancer growth. **Z. Su**, C. Chiang, G. Wei
12:00 General overview of intoxications by wild toxic mushrooms, case study: Algeria. **M. Souna**
12:00 Phytochemical properties, processing, and applications of juvenile Ginger (*Zingiber officinale*). **B. Sylla**, V. Volkis
12:00 Photocatalytic visible light active Co doped ZnO/cellulose acetate nanofiber membranes for functional food packaging. **S. Deshapriya**, I. Munaweera
12:00 Comparison of phytochemical and antimicrobial activity of leaf, stem and root of *Terminalia avicennoides*. **O.O. Onawumi**, **A. Sodamade**, D.L. Abiona, O.A. Onawumi
12:00 Novel approaches of microscopes application on the development of comparison of fruit flies. E.J. Parish, **H. Honda**, Y. Lo, G. Ren, H. Shyu, T. Wei
12:00 Untargeted and targeted metabolomics reveal the chemical characteristic of pu-erh tea (*Camellia assamica*) during pile-fermentation. **P. Long**
12:00 Enhancing potato storage efficiency: A blend of essential oils. **H. Almutairi**, V. Jeliazkov, C.L. Cantrell

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MONDAY EVENING
Morial Conv. Ctr. Hall C
AGFD Sci-Mix
See first 23 posters listed under the Sunday Evening AGFD Poster Session

TUESDAY MORNING March 19
Morial Conv. Ctr. rm 343
Toward Precision Nutrition - Holistic View of Relationship Between Food, Food Components Contribute to Taste, Aroma, Color, and The Gut Microbiome in Health Promotion T. Wang, *Organizer* L. Liu, K. Mahalak, *Organizers, Presiding*
8:00 Introductory Remarks.
8:05 Chronic dietary zinc deficiency alters gut microbiota composition and function. **E. Tako**
8:35 Dietary carbohydrates, gut microbes, satiety, and health. **M. Kable**, D. Lemay, N. Keim
9:05 Comparative analysis of western diet and chronic alcohol consumption shows dramatic alterations in the gut and plasma metabolome using non-human primate model. **C. Christopher**, H.F. Castro, S.R. Campagna, L. Simon, R. Siggins, P. Molina, D. Welsh
9:35 Advances in neuroimaging to explore the microbiota-gut-brain axis. **S. Eldeghaidy**
10:05 Intermission.
10:20 Effect of Allyl Isothiocyanate on the gut microbiota of different age groups. **K. Mahalak**, A. Narrowe, L. Liu, P. Van den Abbeele, A. Baudot, J. Firrman, J.M. Lemons
10:50 Analysis of fenugreek supplementation reveals significant alterations in large intestinal metabolome and microbiome of Western Diet fed mice. **K. Jones**, A.J. Richard, J.M. Salbaum, S. Newman, R. Carmouche, S. Webb, A.J. Bruce-Keller, J.M. Stephens, S.R. Campagna
11:20 Hydrogen sulfide modulates gastrointestinal metabolome, an *ex vivo* study. **L. Liu**, K. Mahalak, J. Firrman, A. Narrowe, J.M. Lemons, A. Baudot, S. Deyaert, P. Van den Abbeele
11:50 Concluding Remarks.

Morial Conv. Ctr. rm 357
Mycotoxins: Challenges and Future Perspectives Financially supported by CCC Food Security: Tackling Hunger H. Humpf, L. Jackson, *Organizers, Presiding* B. Cramer, *Presiding*
8:00 Introductory Remarks.
8:10 Quantitative biomarkers for exposure and risk from aflatoxins in high-risk regions of the world. **J.D. Groopman**
8:40 Aflatoxin and growth: A complex relationship between exposure intervention and measures of infant growth. **P.C. Turner**, E. Phillips, N. Kassim, E. Makule, L. Smith, F. Ngure, N. Makori, R. Nelson, R. Stoltzfus
9:05 Aflatoxin exposure is a potential risk factor for mortality in acutely ill children in the CHAIN network cohort. **Y. Gong**, L. Xia, H. Wu, A. Saleem, S. Ali, E. Mupere, C. Lancioni, A. Diallo, I. Potani, W. Voskuijl, M. Chisti, A. Sayeem, M. Timbwa, S. Mwaringa, C. Tigoi, M. Ngari, B. Singa, R. Bandsma, T. Ahmed, J. Njunge, K. Tickell, J. Walson, J.A. Berkley, M.N. Routledge
9:30 Metabolomic changes associated with aflatoxin exposure in children from the CHAIN cohort. H. Wu, C. Bourdon, L. Xia, R. Mandal, A. Saleem, E. Mupere, C. Lancioni, A. Diallo, I. Potani, W. Voskuijl, M. Chisti, A. Sayeem, M. Timbwa, S. Mwaringa, C. Tigoi, M. Ngari, B. Singa, K. Tickell, J. Walson, D. Wishart, R. Bandsma, J. Njunge, J.A. Berkley, Y. Gong, **M.N. Routledge**
9:55 Intermission.
10:15 Human mycotoxin exposure: From biomonitoring towards exposomics. **S. De Saeger**, R. Pero-Gascon, M. De Boevre
10:40 Estimating aflatoxin exposure by use of LC-MS/MS: Twenty years of CDC laboratory innovations and investigations. **N. Zitomer**, M.E. Rybak

11:05 Optimization of aflatoxin B_1-lysine analysis for public health exposure studies. **J. Renaud**
11:30 Discussion.

Achieving Environmental Justice in the Chemistry Enterprise: Connecting Innovation, Global Impacts and Burden Integrating Science with Community Partnerships to Address Environmental Justice
Spons. ENVR, Cospons.AGFD, AGRO, CEI, CHAL, CHED, CPRC, SCHB, SOCED

TUESDAY AFTERNOON
Morial Conv. Ctr. rm 343
General Papers E. Kreger, J. W. Soares, *Organizers, Presiding*
2:00 Introductory Remarks.
2:05 Biochemical changes during spoilage of milk with different fat content. **P. Iyer**, C.J. Blowers, F. Medina, A. Khan
2:25 Chemical characterization of bioactive compounds of Uva caimarona(Pourouma cecropiifolia) fruit by LC-MS non-targeted analysis. **C.A. Correa Lozano**, C. Osorio Roa, T.D. Stark, C. Dawid, G.M. Méndez Callejas
2:45 Foliar Nanoparticles Application Alleviate Cadmium Toxicity in Wheat (*Triticum aestivum* L.) via Long Distance of "Leaf-Root-Microorganism" Regulation. **M. Wang**, D. Zhou
3:05 Preparation and characterization of sodium alginate-carboxymethyl cellulose based essential nutrient slow release nanohybrids. **K.R. Maduwanthi**, I. Munaweera, P.T. Perera
3:25 Electrospun nanofiber membranes infused with essential oils for extending the shelf life of perishable produce like grapes and tomatoes. **M.C. Sethunga**, I. Munaweera, R. K.K.D.S., P. Gunathilake
3:45 Electrochemical quantification of capsaicin levels: A novel approach to assessing chili heat consistency in culinary applications. **A. Rudokaite**, A. Baradoke, N. Zilinskaite
4:05 Pesticide-induced biochemical changes in tomatoes by FTIR spectroscopy: Implications for Food Safety and Agriculture. **P. Yerra**, J. P, K. S, J. R, S. A, M.A. P, R. A
4:25 Concluding Remarks.

Morial Conv. Ctr. rm 336
Paring Flavors with Health and Wellness Food Products
Financially supported by CCC Food Security: Tackling Hunger
X. Du, D. Wang, *Organizers, Presiding*
2:00 Introductory remarks.
2:05 Role of flavor in health and wellness food products: An overview. **X. Du**, D. Salta
2:35 Physicochemical factors that affect baked sweetpotato textures and sweetness. **M. Allan**, S. Johanningsmeier, M. Nakitto, O. Guambe, M. Abugu, K. Pecota, C. Yencho
3:05 Multi-omics discovery of aroma-active compounds formation in three different mango cultivars. **X. Liu**, Y. Wang
3:35 Intermission
4:00 Detection of smoke-derived volatile phenols in grapes using a portable easy to use biomimetic sensor. **A. Khan**, A. Rumbaugh, S. Andreescu
4:30 Chemical composition and bioactive compounds of γ-irradiated stable chamomile accessions (*chamomilla recutita* (L.) Rauschert.). **Y. Pant**, K. Yadav, R.K. Lal, C.S. Chanotiya
5:00 Advancing stem in agriculture with active experiential learning engagement for high school and college students focused on creation of health product from super-fruits and medical herbs. W. Weaver, S. Grebenyuk, A.G. Ristvey, **V. Volkis**

Morial Conv. Ctr. rm 357
Mycotoxins: Challenges and Future Perspectives
Financially supported by CCC Food Security: Tackling Hunger
H. Humpf, L. Jackson, *Organizers, Presiding* H. Abbas, *Presiding*
2:00 Introductory Remarks.
2:05 From AflaZ to SoLFOOD and beyond: German-Kenyan World Nutrition Projects aimed at reducing food losses due to mycotoxin contamination in sub-Saharan Africa. C. Roder, **M. Schmidt-Heydt**
2:30 Dynamic geospatial modeling of mycotoxin contamination of corn in Illinois: Unveiling critical factors and predictive insights with machine learning. **L. Castano-Duque**, E. Winzeler, J. Blackstock, C. Liu, N. Vergopolan, M. Focker, K. Barnett, P. Owens, H. van der Fels-Klerx, M. Vaughan, K. Rajasekaran
2:55 Peptide natural products from the fungus *Aspergillus flavus*: Potential virulence factors?. **M. Lebar**, J. Cary, B. Mack, C. Carter-Wientjes, M. Kumarihamy, Q. Wei, R. Majumdar, V. Uka, S. De Saeger, J. Diana Di Mavungu
3:20 Innovative research on mycotoxins in grains from Costa Rica to guarantee quality for human consumption: Research Center for Seeds and Grains of University of Costa Rica. **A. Irias-Mata**, M. Viñas-Meneses
3:45 Intermission.
4:00 Management of aflatoxins and fumonisins in corn using biocontrol with non-toxigenic strains of Aspergillus flavus, bioplastic, and biochar. **H.K. Abbas**, **R. Paulk**, C. Accinelli, N. Little, N. Bellaloui, W. Shier
4:25 Evaluating Acheta domesticus for the reduction of fumonisin B1 in livestock feed. H.K. Abbas, **R. Paulk**, G. Rojas, J. Morales-Ramos, M. Busman, N. Little, W. Shier
4:50 Bioinformatically informed evaluation of *Sarocladium zeae* biocontrol agent viability. **S.M. Schoellhorn**, T.H. Lim, T. Nguyen, I.G. Sartor, E. Skellam
5:15 X-ray irradiation of *Aspergillus flavus* and Aflatoxin B1 contaminated maize. **H. Glesener**
5:40 Stable, sustainable, and edible Chitinase formulation for biocontrol of fungal rot. **F. Deeba**, D.W. Wood, D.L. Watkins, C. Rappleye

Achieving Environmental Justice in the Chemistry Enterprise: Connecting Innovation, Global Impacts and Burden We Can Do It: The Synergy of Safety, Green Chemistry, and Environmental Justice in Making Chemistry Safer, More Sustainable and Just Spons. ENVR, Cospons. AGFD, AGRO, CEI, CHAL, CHED, CPRC, SCHB, SOCED
State of the Art in Protein-Based Engineered Materials Protein-based Materials Engineering Spons. CELL, Cospons. AGFD, COLL, PMSE

WEDNESDAY MORNING March 20
Morial Conv. Ctr. rm 343
Michael Granvogl Memorial Symposium J. Beauchamp, R. Tardugno, Y. Wang, X. Zhai, *Organizers, Presiding*
8:00 Introductory remarks.
8:05 Spotlight on Michael Granvogl: Science and socializing. **T.D. Stark**
8:30 Formation of furan and furan derivatives in model systems and food products. **A. Schoepf**, C. Oellig, M. Granvogl
8:45 Enhancing sensory quality of Golden Delicious apple brandies: Identification of key aroma compounds for distillation parameter optimization. **S. Kramp**, C. Oellig, M. Granvogl
9:00 Exploring edible halophytes: Polyphenols extraction, characterization, and antioxidant activity of endemic sea

asparagus (*Salicornia europaea* L.) from the Apulian region of Italy. **R. Tardugno**, F. Limongelli, M. Muraglia, P. Crupi, M. Clodoveo, F. Corbo
9:15 Different wood – different smell? Elucidation of wood odors of different species. A. Baum, H.M. Loos, **A. Buettner**
9:30 Linking the dynamics of aroma release and flavor perception via *in vivo* analytics and time-resolved sensory assessments. **J. Beauchamp**, N. Cleve, M. Izaber
9:45 Intermission.
10:05 Odorants identified in Chinese dry-cured ham contribute to salty taste enhancement. **Y. Chen**
10:20 Mining and rapid screening model and database construction of umami peptide taste patterns based on amino acid sequences. C. Zhiyong, W. Wang, **Y. Liu**
10:35 Formation of volatile heterocyclic compounds and open-chain amides of theanine in model systems with glucose, tea leaves, and tea extract under tea roasting conditions. M. Li, **X. Wan**, **X. Zhai**
10:50 Consumer mushroom quality expectation and the impact of thermal process on mushroom desired flavor creation and nutrient retention. **X. Du**, Y. Xu
11:05 Influence of thermal treatment on the formation of dry jujube flavor: A new insight into pyrazines production with important bakery-type aroma compounds. **Q. Xiao**, C. Ho
11:20 Characterization of ethyl vanillin in nature and its potential impact on flavor industry. **X. Song**, M. Porter, V. Whitaker, S. Lee, **Y. Wang**
11:35 Concluding Remarks.

Morial Conv. Ctr. rm 335
General Papers E. Kreger, J. W. Soares, *Organizers, Presiding*
8:00 Introductory Remarks.
8:05 Withdrawn
8:25 Absorption, distribution, metabolism, and excretion (ADME) studies of [^{14}C]-nitrofurazone residues in broiler chickens. **A. Singh**, D.J. Smith
8:45 Determination of acrylamide content in common pelletized small animal food. **S. McComis**, **T. Tatum**
9:05 Exploring and understanding food emulsion systems with neutron scattering and spectroscopy. **T. Heiden-Hecht**, H. Frielinghaus, M. Müller, O. Holderer
9:25 Rekindling a cherished memory: The flavor of the American chestnut. **W. Yang**, S. Fitzsimmons, K.R. Cadwallader
9:45 Intermission.
10:00 Chitosan films made from food and agricultural waste as replacements for petroleum-based plastics. **K. Orcutt**, Z. McCaffrey, J.H. Kim, W. Hart-Cooper
10:20 Micro-thermography reveals new insights into ice nucleation and growth inside frozen food products. M. Zalazar, **R. Drori**
10:40 Developing humidity-sensitive pectin-based triboelectric devices for monitoring relative humidity as a food-quality indicator. **Z. Jin**, Y. Fu, L. Li, Y. Wang
11:00 Withdrawn
11:20 Thermogravimetric kinetics analysis of synthesized bio-lubricants from naturally derived oleic acid. **K. Mainali**, M.I. Sarker, B. Sharma, M.P. Yadav, H. Ngo, R. Ashby
11:40 Fungicidal constituents from phytopathogens against some agriculturally important fungi. **K.M. Meepagala**

Morial Conv. Ctr. rm 340
Mycotoxins: Challenges and Future Perspectives
Financially supported by CCC Food Security: Tackling Hunger
H. Humpf, L. Jackson, *Organizers, Presiding* C. M. Maragos, *Presiding*
8:00 Introductory Remarks.
8:05 Portable mass spectrometry as a tool for monitoring mycotoxin contamination. **C.M. Maragos**
8:30 Thermal degradation of the mycotoxin citrinin. L. Brückner, **B. Cramer**, H. Humpf
8:55 Fluorescent DNA aptamer sensor platforms for ochratoxin A detection. **R.A. Manderville**
9:20 Novel aptasensor for the ultrasensitive mycotoxin detection. **M. Shoaib**, H. Li, Q. Chen
9:45 Intermission.
10:05 Emerging mycotoxins in the food chain: Challenges and perspectives. **D. Marko**
10:30 Realistic follicular fluid concentrations of *Fusarium* toxins trigger apoptosis and activate NLRP3 inflammasome in bovine primary theca cells. **I. Alassane-Kpembi**, G. Cai, I.P. Oswald, C. Price
10:55 Aflatoxin B_1 metabolism *in vitro* and *in vivo:* New insights by HPLC-MS/MS analysis in combination with intravital imaging. A. Gerdemann, B. Cramer, M. Behrens, A. Ghallab, R. Hassan, G. Degen, J. Hengstler, M. Esselen, **H. Humpf**
11:20 Data delivery from the US-EPA Center for Computational Toxicology and Exposure to support mycotoxin researchers. **A.J. Williams**, G. Janesch, E.T. Carr, V. Tkachenko
11:45 Concluding Remarks.

State of the Art in Protein-Based Engineered Materials
Protein Waste Revalorisation for Sustainable Materials
Spons. CELL, Cospons. AGFD, COLL, PMSE

WEDNESDAY AFTERNOON
Morial Conv. Ctr. 335
General Papers E. Kreger, J. W. Soares, *Organizers, Presiding*
2:00 Introductory Remarks.
2:05 Fluorine-19 NMR analysis of polymers used in food packaging. **C. Ridge**, F. Chen, K. Carlos, P.F. Scholl
2:25 Microfibrillated cellulose (MFC) barrier coating for extending banana shelf life. **J. Zhu**, J. Geng, N. Stark, P. Kitin, X. Zhang
2:45 Dissipation of Pendimethalin and Clomazone in sugarcane soil in Louisiana. **D. Wayment**, D. Bergeron, A.A. Wright, G.A. mccollam, P. White
3:05 Comparative study of cannabis moisture techniques. **K. Blake**, E. Simoes
3:25 Intermission.
3:40 Waterpipe (shisha) tobacco packing density and product performance. **J.H. Lauterbach**
4:00 Spoilage kinetics of vegetable products: Making sense of fluorescence fingerprints to gain insights into stability and nutritional losses. **M. Singh**, X. Liu, M. Zhang, H. Zou, X. Jun, J. Shi, M. Corradini
4:20 Withdrawn
4:40 Comparison of volatile aroma compounds between cricket (*Acheta domesticus*) powder and cricket protein isolate. E. -, T. Wongprasert, **I. Suppavorasatit**
5:00 Rapid analysis of sugarcane quality parameters by Near-Infrared Spectroscopy. **S. Imbachi-Ordonez**, K. McPeak, G. Eggleston
5:20 Constituents isolated from Brazilian propolis as natural pesticides. **V.P. Ribeiro**, J.K. Bastos, A.S. Estep, K. Meepagala

State of the Art in Protein-Based Engineered Materials
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AGFD TECHNICAL PRESENTATION ABSTRACTS

SUNDAY MORNING March 17

Food Allergen Characterization, Modification, and Detection

Natural/artificial mutations and nitrogen/sulfur metabolism control for hypoallergenic buckwheat production Tomoyuki Katsube-Tanaka, tanakato@kais.kyoto-u.ac.jp, Yasuo Yasui. Kyoto Daigaku, Japan To reduce allergy risks on plant-based food, allergen reduction and elimination or lowering allergenicity are necessary and effective in edible crops. Approaches to attain hypoallergenicity at the upstream of food supply in cereal and pseudo-cereal crops include genetically removing allergens, improving digestibility through the structural modifications of allergenic proteins, and compositional alterations of seed storage proteins (allergens) by controlling the availability of sulfur against nitrogen. Common buckwheat (Fagopyrum esculentum Moench), which is a pseudo-cereal crop cultivated traditionally in east and south Asia and east Europe but recently utilized worldwide, sometimes causes sever allergenic reactions and has two major seed storage proteins (allergens), 13S globulin (Fag e 1) and 2S albumin (Fag e 2). 13S globulin is consisted of Met-rich (4.8% Met+Cys) and Met-poor (less than 0.9% Met+Cys) subunits. 2S albumin is basically rich in Met+Cys (14.2-29.8%). Thus, it is anticipated that 2S albumin and the Met-rich subunit of 13S globulin can be reduced under sulfur poor environments. Meanwhile, our research found natural mutations such as trypsin-digestible types (0rep+10aa and g11_3rd DBL) and non-functional types (GlbNB2, g13null, and g28null). Recently we produced artificial null mutant on g14 (2S albumin) by double treatments of chemical mutagen, ethyl methanesulfonate (EMS) with the mutation detection method of NGS-TILLING. The g14null type has a single nucleotide polymorphism (C245A) leading to an immature translation in g14 polypeptide. Therefore, exploration and utilization of natural/artificial mutations as well as nitrogen/sulfur control in cultivation could be effective for producing hypoallergenic buckwheat.

Gluten in fermented or hydrolyzed foods: Challenges and opportunities for quantitative analysis Rakhi Panda, rakhi.panda@fda.hhs.gov, Christina Galanis. FDA, College Park, Maryland Celiac disease affects approximately 1 in 141 individuals in the US, requiring adherence to a strict gluten-free diet. In 2013, the FDA issued a final rule defining the term ‘‘gluten-free’’ for food labeling. In 2020, FDA issued a final rule establishing the “gluten-free” compliance requirements for fermented or hydrolyzed foods, and foods that contain fermented or hydrolyzed ingredients. The 2020 rule acknowledged that there were no scientifically valid analytical methods for accurately quantifying the gluten content in fermented or hydrolyzed foods; this is primarily due to variable proteolysis and the lack of appropriate calibrants for these products. Addressing the variability in gluten quantitation from wheat, rye, and barley is another inherent challenge of all gluten detection methods. To fill this gap, a multiplex-competitive ELISA was developed that utilizes gluten specific G12, R5, 2D4, MIoBS, and Skerritt antibodies from commercial sources. The method generates antibody reactivity profiles depending on the types of fermented or hydrolyzed foods analyzed, which ultimately provides guidance on selecting appropriate calibrant(s) and quantitation strategies for the accurate estimation of the gluten concentration. Such profile determination is not possible with conventional ELISAs that use a single gluten-specific antibody. As such, relying on single antibody ELISAs will most likely lead to over or under estimation of gluten concentration, depending on the gluten epitope(s) the method targets and the type of fermentation/hydrolysis involved. This presentation will cover the challenges in quantitating gluten in fermented or hydrolyzed foods and recent efforts to accurately quantitate gluten, derived from wheat, rye, and barley, in fermented dairy products and sourdough by the multiplex-competitive ELISA.

Chemical and molecular analysis of heated pecan nuts C. Nacaya Brown1, nacaya82@aol.com, Rebecca A. Adams Dupre1, rebecca.dupre@usda.gov, Phoebe Anne Zito2, pazito@uno.edu, Brennan Smith1, brennan.smith@usda.gov, Christopher P. Mattison1. (1) Food Processing Sensory Quality, USDA Agricultural Research Service, New Orleans, Louisiana (2) Chemistry, Univ. of New Orleans College of Sciences, Louisiana Heating causes denaturation, aggregation, and precipitation of food proteins and this can alter allergen content. Changes in the chemical composition and protein content of microwave and oven heated pecans nuts were accessed using analytical methods. Optical spectroscopy of whole acid solubilized pecans revealed increases in absorbance at both 280 and 358 nm wavelengths after microwave heating suggesting an increase in the occurrence of aromatic ring structures. Oven heated pecan samples were extracted with borate buffer, digested with trypsin, separated by reverse phase liquid chromatography, and analyzed by mass-spectrometry to characterize soluble protein content. Although differences in allergen peptides were noted, more than five candidate marker peptides from Car i 2 and Car i 4 were identified in both heated and unheated pecans, while only one distinct peptide from Car i 1 was consistently observed. Insoluble material from heated foods is less tractable and has not been well characterized. To focus on the insoluble material, microwave heated and unheated pecans were stripped of soluble components by sequential extraction with borate buffered saline, sodium chloride, and 1% SDS. The remaining insoluble material was first extracted with 2:1 methanol:chloroform and the resulting supernatant was termed fraction 4 (F4). F4 material isolated from unheated pecan nut is colorless while F4 from heated pecan is yellow/brown in color. Thin layer liquid chromatography (TLC) of F4 indicated that heated pecan nut samples produced a dark smear between the application site and the terminal end of the solvent front that was absent in controls. Continued analytical analysis of insoluble heating-induced pecan nut material, such as F4, will

expand our knowledge of processing induced changes to allergens and other food components.

Transfer of shrimp proteins in shared batch fryers Xingyi Jiang1, xy1521@outlook.com, Robert Beverly1, Jeremiah Kidd1, Jane Cluster2, Karen Swajian2, Lauren Jackson1. (1) Center for Food Safety and Applied Nutrition, Office of Food Safety, US FDA, Bedford Park, Illinois (2) Center for Food Safety and Applied Nutrition, Division of Seafood Safety, US FDA, College Park, Maryland Batch fryers are used by the food industry to produce par-fried shrimp products which are subsequently frozen. Some manufacturers also employ the same frying oil for other par-fried food items. Concerns have been expressed over the potential for shrimp allergens to transfer to frying oil and other foods prepared in reused frying oil. The objectives of this study were to (1) Develop protein extraction methods from reused oil, (2) Validate protein extraction efficacy, (3) Evaluate oil post-treatments on allergenic protein removal from frying oil. Two experimental models were established. In the first model, low (800 ppm) and high (8000 ppm) levels of black tiger shrimp powder were spiked into soybean oil, respectively, and a portion was fried (182 °C, 3 min). In the second model, ten batches of shrimp (40 g/batch) were fried in 1 L soybean oil under the same condition. The contaminated oil from both models was filtered through metal sieves or cellulose filter paper of various pore sizes. The total protein content, protein profile and tropomyosin concentrations in oil were determined using the Pierce bicinchoninic acid (BCA) assay, gel electrophoresis and by enzyme-linked immunosorbent assay (ELISA), respectively. The developed protein extraction method could recover more than 80% of total protein and tropomyosin from the unheated oil at two spiking levels. However, such recoveries from fried oil were reduced. Gel electrophoresis identified two major proteins in the used frying oil, namely tropomyosin (36 kDa) and sarcoplasmic calcium-binding protein (18 kDa). The total residual protein and tropomyosin content of the frying oil increased with the number of frying batches. Post-treatment such as sieving and filtration reduced oil residual tropomyosin content. This study demonstrated that the shrimp proteins can be transferred to frying oil, with tropomyosin being a prominent allergenic protein of concern. However, the amount of allergenic protein was likely underestimated due to the decreased extractability and detectability of tropomyosin after frying. Future research will involve (1) improving recovery of shrimp proteins in reused frying oil; and (2) quantifying the transfer of shrimp tropomyosin to subsequently fried food items.

Effectiveness of cleaning treatments for removing nut butter residue from shared processing equipment Hilary Green1, hsgreen@ucdavis.edu, Jeremiah Kidd1, Josh Warren2, Lauren Jackson1. (1) Center for Food Safety and Applied Nutrition, Bedford Park, Illinois (2) Illinois Inst. of Technology, Chicago In recent years, the variety of products nut/seed butters available on the market has increased due to their high nutritional value and the shift from animal-protein based diets to those rich in plant protein. In the case of nut/seed butters, products may be processed on the same equipment and cross-contact can occur during manufacturing if equipment is not effectively cleaned. Allergen-related recalls for nut and seed butter products have become more frequent, indicating that research is needed to determine the effectiveness of dry sanitation methods for removing nut butter residue from food-contact surfaces and processing equipment. This study performed sanitization trials to determine their effectiveness at reducing cross-contact when manufacturing on pilot-plant scale equipment. Almond butter was manufactured from whole, roasted almonds using a nut butter mill. Subsequently, the mill was cleaned with a designated method and then used to produce peanut butter from whole, roasted, blanched peanuts. Samples of peanut butter were collected at varying timepoints and each sample was tested for almond protein using a quantitative, almond-specific ELISA. The most effective cleaning method involved scrubbing the mill with hot water and detergent. However, wet cleaning cannot easily be utilized by industry as water can allow microbial pathogens to grow and contaminate products. Therefore, this treatment was used as a control and other dry-cleaning methods more commonly used were evaluated. It was found that using peanut butter as a push-through material was the least effective method, while a combination of methods, including manually cleaning using scrapers/brushes and an alcohol-based detergent were more effective at removing almond residue from the mill. These results demonstrate it is imperative for industry to test method effectiveness and improve sanitary design given the limited number of dry-cleaning methods available. A combination of methods may be the best way to minimize allergen cross-contact.

Investigation of in silico allergen identification methods based on nano-UHPLC-ESI MS/MS characterization data Naryttza Diaz-Fortier1, naryttza.diaz-fortier@jti.com, Daniel Mucs1, daniel.mucs@gmail.com, Tadashi Hirata1, Asuka Daikoku2, Irene Baskerville-Abraham1. (1) Scientific and Regulatory Affairs, JT International SA, Geneve, Switzerland (2) Scientific and Regulatory Affairs, Nihon Tabako Sangyo Kabushiki Kaisha, Minato-ku, Tokyo, Japan Identification of substances that can cause allergenic responses in complex matrices such as food or consumer products is a crucial part of toxicological risk assessment due to the severity of the responses they can induce. While characterization methods such as nano ultra-high performance liquid chromatography (UHPLC)-electrospray ionization (ESI)-tandem mass spectrometry (MS/MS) are available, the rapid identification of specific characterized components of toxicological concern remains a challenge. While many in vitro methods exist for small molecules, such as Amino acid Derivative Reactivity Assay (ADRA), Direct Peptide Reactivity Assay (DPRA) or human Cell Line Activation Test (h-CLAT), these usually have limited applicability for larger biomolecules such as proteins, which are often found in natural extracts. Like for small molecules, various in silico methods are available to identify proteins based on structures (amino acid sequences), however, no suitable holistic reviews to date were identified from a risk-assessment perspective which could guide the integration of these methods into a day-to-day toxicological risk assessment process. Here we present the result of our investigation on various available in silico tools to identify potentially allergenic proteins from genome sequence and also proteome characterization data generated using a nano UHPLC ESI MS/MS method reported in the literature.

Biosimilar protein immunotherapy: Tolerance inducing immune response in patients with cow milk anaphylaxis Nathan Marsteller1, nmars3@yahoo.com, Inderpal Randhawa2. (1) Research, TPIRC, Long Beach, California (2) Clinic, The Food Allergy Inst., Long Beach, California Rationale: Oral immunotherapy remains a limited form of treatment for food allergic children. Limitations primarily stem from small study sizes, significant adverse events, unclear long-term immunological outcomes and the inability to reach tolerance. In our cohort of anaphylaxis patients undergoing biosimilar protein immunotherapy (BPI) in the Tolerance Induction Program (TIPTM), we sought to determine the rate of decline in skin prick testing (SPT) and specific IgE (sIgE) results following one year of BPI. Methods: The study comprises 214 cow milk anaphylactic children who underwent TIP TM at the Translational Pulmonary & Immunology Research Center/ Food Allergy Inst.. Post intervention changes in cow milk sIgE, component resolved diagnostics and specific IgG4 (sIgG4) were assessed. Results: After one year of 10 g dairy protein weekly dosing, eosinophil count decreased from 558.38 to 409.26 cells/uL, the mean Cow Milk IgE decreased from 16.91 kU/L to 9.10 kU/L,

the mean Boiled Cow Milk IgE decreased from 12.89 kU/L to 6.03 kU/L, the mean Bos D4 decreased from 7.38 kU/L to 3.52 kU/L, the mean Bos D5 decreased from 6.79 kU/L to 3.16 kU/L, and the mean Bos D8 decreased from 13.55 kU/L to 6.62 kU/L. Adverse events were rare. Conclusions: TIP ™ cow milk immunotherapy significantly reduced cow milk sIgE and component resolved diagnostics while increasing sIgG4 in cow milk anaphylactic children. TIP ™ demonstrates remarkable safety and clinical efficacy in cow milk anaphylaxis treatment.

FDA regulatory update on food allergens Lauren Jackson, Lauren.Jackson@fda.hhs.gov. FDA, Bedford Park, Illinois Food allergies affect an estimated 10-12 million people in the U.S., and the prevalence appears to be increasing, particularly in children. Allergens are a leading cause of food recalls in the U.S., and represent one of the most commonly reported hazards to the FDA Reportable Food Registry (RFR). These allergen-related recalls and RFR reports are attributed mainly to labeling errors, improper handling of rework, cross-contact, and inadequate supply chain controls. In the U.S., the Food Allergen Labeling and Consumer Protection Act of 2004 (FALCPA) defined the priority allergens (known as major allergens) as peanut, milk, egg, fish, crustacean shellfish, tree nuts, soy and wheat, and required these food allergens to be declared on the food packaging when they are intentionally added to food. Sesame has been added as the ninth major allergen in the U.S. due to passing of the Food Allergy Safety, Treatment, Education, and Research (FASTER) Act of 2021. The food allergen labeling requirements of the FALCPA and FASTER Act only apply to a major food allergen that is an ingredient of the product; they do not apply to allergen presence due to cross-contact, the unintentional incorporation of a food allergen into a food. The Food Safety Modernization Act (FSMA), which was signed into law in 2011, added requirements for food manufacturers to have a food safety plan in place that includes an analysis of hazards and risk-based preventive controls to minimize or prevent the identified hazards. With regard to allergens, FSMA required food manufacturers to develop preventive controls to prevent allergen cross-contact. This presentation will provide a review of the FDA regulatory requirements for food allergens under FALCPA, the FASTER Act and FSMA, as well as provide an update on current FDA regulatory activities on food allergens.

Food Security: Tackling World Hunger CCC: Highlighting Chemistry from Multiple Divisions

Graphene synthesized from a microbial culture as a nanocarrier for plants Nandini Bhattacharya1,2, nandini.biochm@gmail.com, Mandira Kochar3, Himadri B. Bohidar2, Wenrong Yang1, David Cahill1. (1) Faculty of Science Engineering and Built Environment, Deakin Univ., Geelong, Victoria, Australia(2) Sustainable Agriculture, TERI-Deakin Nanobiotechnology Centre, Gurugram, Haryana, India(3) Sustainable Agriculture, The Energy and Resources Inst., Gurugram, Haryana, India Reduced graphene oxide (rGO) synthesized from a microbial source, that had been biofunctionalized by the microbial cell components was employed as a nanocarrier for crop plants. The phytohormone, Indole acetic acid, was loaded on the rGO via physical adsorption. The synthesized nanocomposite was characterized by standard techniques to assess its properties. Results of the characterization indicated the successful formation of the indole acetic acid loaded rGO nanocomposite. Furthermore, the adsorption kinetics, loading efficiency, release percentage and release behavior of indole acetic acid on rGO was determined. Lastly, the biologically synthesized rGO and loaded rGO nanocomposite were applied on maize seeds by seed priming approach to determine their effect on plants. The green synthesized rGO as well as the indole acetic acid loaded rGO, displayed significant positive growth effects and biochemical changes in the maize plants. Research presented in this study shows that the microbial synthesis of reduced graphene oxide is efficient and further suggests the promising potential of reduced graphene oxide as a nano-delivery vector for the exogenous introduction of plant growth regulators into crop plants.

Silica nanomaterials to improve crop production Christy L. Haynes, chaynes@umn.edu. Chemistry, Univ. of Minnesota Twin Cities, Minneapolis Achieving food security on our warming planet with a growing population is going to require a collection of human behavioral changes and technological innovations. Among the potentially impactful technological innovations is the application of engineered nanomaterials that promote crop health. This work focuses on designing porous silica nanoparticles to maximize plant uptake and distribution as well control delivery of cargo molecules and the nanoparticle dissolution rate. Porous silica nanoparticles can be synthesized with a range of primary nanoparticle sizes and pore sizes, controlled by the synthetic precursors and conditions. The nanoparticle surface is easily functionalized to present appropriate electrostatic and hydrophobic properties. Nanoparticle size and surface chemistry significantly impact uptake by plants or seeds. In some cases, small molecule cargo, can be loaded into the nanoparticles for intraplant delivery. Finally, the silica nanoparticles transform within the aqueous intraplant environment, dissolving to produce silicic acid, a molecule most plants can use to strengthen their cell walls; the rate and profile of this dissolution process can also be tuned based on synthesis conditions. Overall, porous silica is a very promising platform for nano-enabled agriculture. Silica nanoparticle formulations with systematically varied properties have been applied to exemplar crop plants, both in greenhouse and field studies; results to date show limited unintended toxicity and several positive impacts on plant health and crop production.

Assessment of the antioxidant potential of Indian spice extracts for enhancing the oxidative stability of salmon fish oil Nutan Kaushik3, kaushikn2008@gmail.com, Asha Kumari3, Rasa Slizyte1, Revilija Mozuraityte1, Heidi Johnsen2. (1) SINTEF Ocean, Trondheim, Norway(2) SINTEF Industri, Trondheim, Trøndelag, Norway(3) Amity Food and Agriculture Foundation, Noida, Uttar Pradesh, India
The consumption of oils containing omega-3 fatty acids have numerous health benefits, including blood pressure regulation, brain development, and protection against coronary heart disease. However, the oxidative stability of fish oil is often compromised by various factors such as heat treatment, light exposure, oxygen availability, moisture, and the absence of antioxidants. Thus, there is a pressing need for strategies to enhance the oxidative stability of fish oil. In this study, the antioxidant potential of eighteen spice extracts was assessed. Notably, among all the spice extracts evaluated, the ethanolic extract of clove exhibited the highest antioxidant activity at 300 ppm (90.2% ± 0.6%), followed by the turmeric ethanolic extract (79.4% ± 0.5%), the ethyl acetate extract of black pepper (88.7% ± 2.4%), and the ethyl acetate extract of turmeric (83.9% ± 2.2%). Subsequently, these selected spice extracts, were utilized for fortifying fish oil with the aim of extending its stability. Response Surface Methodology (RSM), using Design Expert software, was employed to optimize the concentration of these extracts based on indicators such as free fatty acid content, peroxide value, and TBARS value. The stability of Salmon fish oil alone, blended with spice extracts, and blended with the commercial antioxidant BHT was assessed under accelerated conditions using the Schaal oven test at 60°C for 12days. Remarkably, Salmon fish oil containing the spice extracts at their optimized concentrations exhibited prolonged stability for 8 days, which is equivalent to 8 months of storage at normal room

temperature. The key parameters measured during this period were within acceptable limits of free fatty acid value (1.3% ± 0.2), peroxide value (4.3 meq/Kg ± 0.1), and TBARS value (3.8 mg malondialdehyde/Kg ± 0.1). The results demonstrated that Salmon fish oil fortified with the spice extracts is more stable than fish oil alone and fish oil with BHT.

Incorporation of dairy by-products into hydrogel structures for cultivated meat production Patrick Charron2, Christopher Foley2, Irfan Tahir2, Rachael Floreani1, Floreani@uvm.edu. (1) Mechanical Engineering, Biomedical Engineering, Materials Science, Food Systems, Univ. of Vermont, Burlington(2) Mechanical Engineering, Univ. of Vermont, Burlington Global food insecurity has led to recent developments in biotechnology, giving rise to alternative foods and proteins, including cultivated meat. Cultivated meat is produced in vitro using animal cells grown on a 3D structure (i.e., scaffold). Alginate was chosen as the base material, due to the tunability of their mechanical properties. Whey protein isolate (WPI), a by-product of the dairy industry, has recently been shown to encourage cell adhesion in bone and cartilage tissue engineering. Herein, we use WPI to provide cell adhesion ligands to an alginate network. Notably, there is a lack of information on its use in muscle tissue engineering, including cultivated meat. The objective of our study was to investigate the effect of WPI-based scaffolds on muscle cell adhesion and viability for cultivated meat production. AlgMA was synthesized by dissolving sodium alginate in deionized water, and WPI was dissolved in PBS; an excess of methacyrlic anhydride was added and the reaction was carried out for 24 hours. Photo-crosslinked AlgMA, WPI/AlgMA, and WPI-MA/AlgMA hydrogels were made using a custom made green light crosslinking system. Aqueous polymer solutions were prepared iat room temperature. One mM eosin Y, 125 mM TEAO, and 20 mM VP were mixed with the control (AlgMA) and experimental samples (WPI/AlgMA, WPI-MA/AlgMA) and exposed to the green light Scanning electron micrographs, equilibrium water content and hydrolytic degradation, and unconfined uniaxial compression tests were performed. Murine muscle cells were cultured on the scaffolds, and cell viabity and adhesion were examined. A 3D interconnected porous network was created, showing differences compared to an AlgMA control. The incorporation of non-modified and chemically modified WPI in alginate scaffolds shows encouraging data that supports the use of WPI-based scaffolds for engineering muscle tissue in vitro. Also, the tunability of composition and mechanical properties will allow these materials to be fine-tuned for other properties such as texture and flavor. Scaffolds were formulated using methacrylated alginate (AlgMA), WPI, and methacrylated WPI (WPI-MA). The resultant scaffold product was a photo-crosslinked, porous network that displayed marked differences compared to the AlgMA control scaffold. In summary, our study provides compelling evidence supporting the use of WPI-based scaffolds in 3D cultivated meat production, highlighting its substantial prospects and benefits.

Pioneering sustainable food packaging: Biodegradable anti-bacterial silk coating for enhanced food safety and waste reduction Yagmur Yegin, yyegin@mit.edu, Benedetto Marelli. Civil and Environmental Engineering, Massachusetts Inst. of Technology, Cambridge With the global population projected to reach 10 billion by 2050, ensuring food security amid limited resources is critical. Shockingly, one-third of food for human consumption is annually wasted due to safety and quality concerns. This extensive food waste harms the environment, contributing significantly to energy consumption and greenhouse gas emissions. Remarkably, the discarded food could nourish about 1.6 billion people, yet it's responsible for a quarter of global freshwater use and ranks as the third-largest greenhouse gas emitter, contributing to approximately 10% of total global greenhouse gas emissions. Redirecting this surplus food to alleviate hunger and mitigate environmental harm is imperative. To address this challenge, we've pioneered an innovative solution: an antimicrobial-embedded biodegradable silk coating. This intelligent coating effectively curtails foodborne bacteria growth, preserving perishables, and reducing the environmental impact of food packaging. Encapsulating antimicrobial essential oils within silk nanoparticles eliminates the need for solvents and surfactants. The resulting edible silk coatings serve as robust barriers against gases and moisture, safeguarding product freshness. Our biodegradable antimicrobial food coating also acts as a proficient moisture sealant, excluding oxygen and inhibiting pathogen proliferation. Delivered as dried films, it simplifies transportation, offering enduring stability and streamlining application to food surfaces. This innovation enhances food quality and safety without refrigeration or single-use plastic packaging. In summary, our research develops biodegradable polymers for functional agri-food materials. We aim to create biopolymers surpassing synthetic counterparts in performance while preserving essential attributes. The silk coating is a formidable shield against gas intrusion, retaining moisture and inhibiting pathogens. It's an innovative, scalable, and sustainable solution to combat food insecurity, reduce waste, and address climate change.

SUNDAY AFTERNOON

Withycombe-Charalambous Graduate Student Symposium

3D-printed hydrogel-based nanocomposites for sustainable food packaging Oluwatosin Popoola, popoolos@clarkson.edu, Abraham Finny, Ivy Dong, Silvana Andreescu. Chemistry and Biomolecular Science, Clarkson Univ., Potsdam, New York Yearly, about one-third of the food produced worldwide is wasted due to spoilage. Food contamination and spoilage, as well as the use and disposal of non-degradable packaging, affect human health and have substantial economic and sustainability implications. Achieving sustainability within the food system requires innovative solutions to both extend the food shelf life and reduce the environmental footprint. This presentation will describe the development of a 3D-printed ink, the printing process, and the functional properties of the resulting film as a potential substitute for food packaging. The ink was prepared from edible biopolymer hydrogels such as alginate and gelatin and formulated to provide antimicrobial action against food-spoilage bacteria. The film was reinforced with nanocellulose, a green and sustainable nanofiller, which enhances the overall mechanical performance of the hydrogel. Characterizing the resulting 3D-printed film reveals excellent durability, flexibility, and robustness. The formulation is also compatible with pH dyes and biomolecules, which provides opportunities for adding sensing functions with capabilities to visually assess spoilage when this occurs. The material formulations developed in this work are biodegradable, eco-friendly, easily sourced, and inexpensive, making them suitable candidates for next-generation sustainable food packaging.

Untargeted flavoromics provides new insight into the impact of high-tunnel and open-field production on the variations of aroma profiles of industrial floral hemp Zixuan Gu, zixuan.gu@ndsu.edu, BINGCAN CHEN, bingcan.chen@ndsu.edu. Plant Sciences, North Dakota State Univ., Fargo Currently, the research on industrial floral hemp (IFH) is burgeoning, primarily focusing on the functional properties of its cannabinoids, essential oils, and proteins. However, the influence of production systems on the aroma characteristics of IFH remains unclear. In this study, two IFH cultivars SB1 and CJ2 from Sunrise Genetics were employed to investigate the impact of open-filed and high-tunnel production systems on the changes of their aroma profiles via HS-SPME-GC-MS based untargeted flavoromics. The results indicated that the

aroma profile of IFH mainly consisted of mono- and sesquiterpenoids, and their respective oxygenated terpenoids. Untargeted flavoromics demonstrated a stronger impact of cultivar variations brought to the aroma profile of IFH than that of production systems, in which more oxygenated terpenoids were developed by CJ2 while sesquiterpenoids were more favored and generated by SB1. With the characterizations of relative odor activity value (ROAV) and aroma character impact (ACI), β-caryophyllene (spicy) and α-Humulene (woody) were outstood as two dominant key aromas contributing to the overall odor of all IFHs. In all, this study revealed variations in the aroma of IFH grown in different environments, providing valuable insights for producers and researchers, and holding potential values for commercial applications and product development.

Development of a microfluidic device to enrich and detect zearalenone in food using quantum dot-embedded molecularly imprinted polymer Marti Z. Hua, marti.a.hua@gmail.com, Xiaonan Lu. McGill Univ. Faculty of Agriculture and Environment, Sainte-Anne-de-Bellevue, Quebec, Canada Mycotoxins are fungus-produced chemicals prevalent in 60-80% of food crops and many processed products. Consuming mycotoxin-contaminated food and feed can lead to various adverse effects on humans and livestock. Therefore, testing mycotoxin residue levels is critical to ensure food safety. Gold standard analytical methods rely on liquid chromatography coupled with optical detectors or mass spectrometry, which are high-cost with limited capacity. This study reported the successful development of a microfluidic "lab-on-a-chip" device to enrich and detect zearalenone in food samples automatically based on fluorescence quenching effect of quantum dots and selective affinity of molecularly imprinted polymer. The dummy templates and functional polymers were synthesized and characterized, and the detailed design of the enrichment module and the optimization of the flow conditions in the microfluidic device were discussed. This device achieved an enrichment factor of 9.6 (±0.5) with a quantification range of 1-10 mg/kg (91-105% recovery) for zearalenone in dried corn kernel and wholewheat flour samples, covering the concerned residue level in the regulation. The entire analysis was completed in 20 min, involving 3 min of manual operation and no advanced equipment, providing a novel, rapid, portable, and cost-effective tool for monitoring mycotoxin contamination in food.

Solubilization of limonene by phospholipid vesicle dispersions Ann-Dorie Webley1, arwebley@ucdavis.edu, Stephanie R. Dungan1,2, Susan E. Ebeler3. (1) Food Sci. & Tech., Univ. of California, Davis (2) Chemical Engineering, Univ. o(3) Viticulture and Enology, Univ. of California Davis, Davis, California, US The efficacy and quality of food products is affected by the distribution of hydrophobic solutes such as flavours. We seek to determine the local distribution of these solutes and the factors affecting their stability, incorporation, and release, in order to improve food design. We focus on colloidal assemblies of phospholipids as they are safe and widespread natural amphiphiles that can solubilize hydrophobic compounds. Short-time headspace microextraction is used to determine the local distribution of hydrophobic solutes and the effects of structure, while keeping the system intact. We have extended our previous work on micellar solutions by developing a quantification method for the solubilization and retention of volatile nonpolar compounds in phosphatidylcholine vesicles. The local partitioning of the aroma molecule limonene was investigated in vesicles of various structures, lipid compositions, and at different temperatures. Vesicles were found to be much more effective at solubilizing limonene than short-chain phosphatidylcholine micelles. They yielded vesicle-water partition coefficients of ~104M–1 that were 3–8 times larger than micelle-water partition coefficients. In addition, they can solubilize limonene up to solute-lipid mole ratios of ~3 before the system becomes saturated, compared to <0.9 for micelles. With saturated lipids, a higher concentration of limonene fluidizes the gel membrane and lowers the phase transition temperature. When this effect was removed by using sufficiently low concentrations of limonene, a decrease in the partition coefficient for vesicles in the gel phase was observed. Furthermore, we see a range of phases - fluid, gel, and a coexisting fluid/gel phase - depending on the mole fractions of limonene added. When above the gel transition temperature, lipid composition and vesicle size did not have a significant effect on the partitioning properties, however, the partition coefficient increases with higher limonene concentrations. Applying an interaction parameter with regular solution theory accounts for the enhanced solubilization.

Developing polymer-based delivery systems to improve bioaccessibility and bioefficacy of procyanidin dimers Zhiya Yin, zy169@scarletmail.rutgers.edu, Qingrong Huang. Food Science, Rutgers The State Univ. of New Jersey, New Brunswick, New Jersey Procyanidins, also known as condensed tannins, have recently attracted a great deal of attention because of their promising health-promoting effects. However, their oral bioavailability and subsequent bio-efficacy are hindered by their poor gastrointestinal stability and low intestinal absorption. In this study, polymer-based delivery systems were developed to encapsulate procyanidin dimer A2 (PAC A2) and B2 (PAC B2) with the encapsulation efficiency reaching 84.9% and 88.2%, respectively. The in vitro dissolution study and ex vivo permeation study (Franz cells) were performed, and it was found that the encapsulation significantly improved the transmembrane rates of PAC A2 and B2 by 1.4-fold and 1.47-fold, respectively. Moreover, the cellular uptake study indicated that both encapsulated gliadin-carboxymethyl dextran (G-CMD) nanoparticles and whey protein-cellobiose Maillard conjugates (WPI-CE) could enter Caco-2 cells within 2 hours and were observed surrounding the cell nuclei. Furthermore, G-CMD nanoparticles slightly increased the anti-lipogenic activity of PAC A2, which reduced lipid accumulation in differentiated 3T3-L1 cells in a dose-dependent manner. It was determined that PAC B2 loaded in WPI-CE conjugates exhibited a higher antioxidant ability than the free PAC B2 at all concentrations (0-50 μM) on the Hep-G2 cell line. In vitro microbial fermentation was conducted to investigate the metabolic pathways of the encapsulated and the free procyanidin dimers, and a high-throughput UHPLC-QqQ-MS/MS method combining QuEChERS and (EMR)-lipid technology was successfully developed for sample preparation and analysis. It was found that PAC A2 and B2 have different metabolism pathways and encapsulated dimers showed a slower metabolism rate and better retention during fermentation. In conclusion, polymer-based delivery systems were successfully developed for two procyanidin dimers, and the encapsulated procyanidin dimers showed improved bioaccessibility and bio-efficacy compared to their free forms.

Food Security: Tackling World Hunger CCC: Highlighting Chemistry from Multiple Divisions

Iron-based amendments decrease bioaccumulation of arsenic in lettuce grown in a contaminated soil Adeyemi S. Adeleye, asa2296@columbia.edu, Ziwei Han. Dept. of Civil and Environmental Engineering, Univ. of California Irvine Hunger is perpetuated by the occurrence of toxic substances in soil, which make it unsafe for food crop cultivation. Arsenic is a particularly challenging soil contaminant because it exists naturally in several geological formations and was historically used as a pesticide. Unsurprisingly, arsenic is frequently detected in foods, and approaches to decrease uptake by plants are needed to decrease food loss. We hypothesized that reactions with iron will decrease

arsenic's availability in soil and its bioavailability to food crops. To test this hypothesis, we amended two forms of iron—nanoscale zerovalent (NZVI) and sulfidated nanoscale zerovalent iron (SNZVI)—into an agricultural soil that was contaminated with 0, 5 and 50 mg/kg arsenic. Lettuce (Lactuca sativa) was then cultivated in the soils from the seed stage to maturity and thereafter analyzed for arsenic bioaccumulation. Both NZVI and SNZVI significantly ($p < 0.05$) decreased arsenic bioaccumulation in lettuce tissues. Arsenic concentration in lettuce leaves decreased from 91.7 mg/kg in untreated contaminated soil to 55.1 and 47.4 mg/kg when treated with 0.3 wt.% of NZVI and SNZVI, respectively. The iron amendment had no significant ($p > 0.05$) impact on essential nutrients, such as Na, K, Mg, and Ca in lettuce leaves. X-ray diffraction (XRD) revealed that the iron particles immobilized arsenic in soil via reduction, adsorption, and substitution reactions. Furthermore, iron increased the iron plaque on lettuce roots, which adsorbed and precipitated arsenic as FeAsO4. This study shows the potential of iron in decreasing hunger by making it possible to safely grow food crops in arsenic-impacted farm soils.

***Blighia sapida,* a versatile fruit, alleviating hunger and** promoting good health Andrea Goldson-Barnaby, andrea.goldson03@uwimona.edu.jm, Debbie Ann L. Phillips. Chemistry, The Univ. of the West Indies, Kingston, Jamaica Food wastage and food loss total a third of the world's food. This waste can be reduced through its conversion into value-added products. Fruits and vegetables are good candidates for reprocessing. The fruit, *Blighia sapida (*ackee), originally from West Africa, has for centuries been a staple in Jamaica. During canning, a significant quantity of arilli is discarded which can be converted into other food products. In our study we investigated the conversion of ackee arilli into an edible oil. The oil was characterized utilizing NMR spectroscopy, GC-MS and UV spectroscopy. The oil is rich in oleic acid, contains carotenoids (44 ppm), is thermally stable with a smoke point of 232 °C and exhibits high free radical scavenging activity (98 %). 1,3- Dioleylpalmitin was identified as the main triacylglycerol present. Thermal processing positively impacts the available beta carotene. The ackee, economical and versatile, can be further processed to aid in hunger alleviation.

Flavors of specialty crops from controlled environment agriculture Yun Yin1, yunyin2@vt.edu, Jingsi Liu1, Isabel Gutierrez1, Michael Evans2. (1) Food Sci. & Tech., Virginia Polytechnic Inst. and State Univ., Blacksburg (2) School of Plant and Envir. Sci.s, Virginia Polytechnic Inst. and State Univ., Blacksburg, Virginia Controlled environment agriculture (CEA) is reaching a high market momentum as it enables sustainable crop cultivation with reduced inputs and growing space. Environmental factors, including growing systems, lighting, temperature and fertilizers, all largely influence the growing dynamics, plant quality and accumulation of flavor, bioactive compounds and more. All these quality matrices directly determine the consumer acceptance of the final product. The skillset and toolbox owned by food chemists will largely assist successful CEA production of specialty crops, from varietal selection, growing system evaluation, and the influences of abiotic stress (lighting, salinity, etc.). This oral presentation will, in particular, showcase the findings from our on-going projects evaluating the quality of CEA-produced specialty crops from chemistry perspectives.

Novel nanoparticle platforms for improved plant genetic engineering Gozde S. Demirer, gdemirer@caltech.edu. California Inst. of Technology, Pasadena Anthropogenic climate change has made the need for more nutritious and stress-tolerant plants indisputable for providing food security. Climate change has decreased the global agricultural productivity by 21% since 1961, and will continue to drop crop yields by 7.4% for every degree-Celsius increase in temperature. CRISPR genetic engineering can enable previously inaccessible crop tolerances to meet the demand for nutritionally-balanced and high-yielding crops. However, plant biomolecule delivery and transformation are two important bottlenecks, which we address using novel nanomaterial platforms. In this presentation, I will describe the development and use of virus-like particles (VLPs), which are self-assembled protein nanoparticles capable of delivering cargoes into plant cells for DNA-free plant genetic engineering. These VLPs produced scalably and sustainably in plants enter plant cells, disassemble in cytosol to deliver biomolecules, and can potentially allow rapid, efficient, species-independent, and tissue culture-free genetic engineering of crops by targeting meristems to help eliminate world hunger.

Development of phage-CRISPR nexus for microbial food safety Juhong Chen1,2, jhchen@vt.edu. (1) Bioengineering, Univ. of California Riverside (2) Biological Systems Engineering, Virginia Polytechnic Inst. and State Univ., Blacksburg Current food production faces a tremendous challenge from the growing human population. It is estimated that the global population will reach 9 billion by 2050, and 70% more food is required. Due to the clean resource drain and climate change, it is challenging to increase food production. Thus, there is an urgent to improve food safety and reduce food waste for a sustainable food system. With a focus on improving microbial food safety, my research program is to develop advanced and innovative phage- and CRISPR-based approaches to detect foodborne pathogens, including bacteria and viruses. In these detection strategies, we have achieved excellent detection sensitivity and specificity to detect foodborne pathogens, which will be extremely important in solving critical and emerging issues in microbial food safety and ensuring enough better quality and safer foods for human consumption.

Sustainable technologies for protein ingredient production from alternate crops: A path forward for zero hunger Nandika Bandara, nandika.bandara@umanitoba.ca, Thilini N. Dissanayake, Anuruddika Hetti Hewage. Univ. of Manitoba, Winnipeg, Canada Achieving the zero-hunger target is critical to feed the growing world population. Plant protein ingredients, such as flour, protein concentrates, and protein isolates, must exhibit improved functionality to mimic animal proteins and to be used in food applications. The conventional protein processing methods employed in the industry often result in excessive denaturation of proteins, leading to compromised functional properties. To address these challenges, novel and sustainable protein extraction and modification technologies must be developed to produce functionally superior protein ingredients. In line with this objective, our research group currently focuses on developing eco-friendly extraction methods using deep eutectic solvents (DES) and reverse micelles (RM) extraction. DES-based extractions, relatively new systems, offer milder extraction conditions than traditional methods, making them less invasive. The novel DES technology shows great potential in enhancing extraction yield, purity, and protein functionality in multiple crops such as mung bean, fava bean, yellow pea, canola, etc., which prompt alternate protein sources to be used in human foods.

Functional foods in the daily diet: The potential of plants and fruits traditionally consumed in the Yucatan peninsula Luis M. Pena-Rodriguez, lmanuel@cicy.mx. Centro de Investigacion Cientifica de Yucatan, Merida, Mexico Currently functional foods include fruits and plants that contain bioactive components and their health benefits are obtained through their consumption as part of a balanced diet. In this investigation we evaluated the potential of 16 species of plants and fruits consumed traditionally in the Yucatan

peninsula. All fruits/plants were collected or purchased mature and the edible pulps or leaves dried by lyophilization. The lyophilized and ground materials were extracted by maceration with a mixture of water-ethanol and the corresponding crude extracts were evaluated for their antioxidant, anticancer, antimicrobial and antidiabetic activity. The results obtained in these evaluations will show that the fruits of Byrsonima bucidifolia, Melicoccus bijugatus, Phyllanthus acidus, Spondias purpurea, Cucurbita moschata, Cordia dodecandra, as well as the leaves of Cnidoscolus aconitifolius, can be considered as potential functional foods and important species to be produced, consumed and commercialized outside the Yucatan Peninsula.

SUNDAY EVENING

AGFD General Poster Session and Undergraduate Poster Competition

note – first 23 posters in this session are also scheduled for presentation at Monday Evening Sci-Mix

Poster01 Effects of ethylene exposure on Hass avocados (Persea americana) during ripening in the presence of Cavendish bananas (Musa acuminata) over a five-day period Andrew Gao, agao4389@gmail.com, Andrew Lee, Senming Hsia, Lucas Qu, Rhea Choksey, Addison Burgos, Ishan Choksey, Liam Jannotti, Emily Lopez-Couto, Chang Yiyuan, Romina Jannotti. Chemistry, Trinity Preparatory School, Winter Park, Florida Background Avocado ripening is a notoriously complex process. Hass avocados, in particular, are known for their sensitivity to external factors, including temperature, humidity, and the presence of other fruits. Minor deviations in storage conditions can significantly impact their ripening rate and quality. This study aims to explore how the density and mass of Hass avocados change over a five-day period when stored alongside Cavendish bananas. Methods 30 Hass avocados were purchased randomly from a local supermarket. Each avocado was marked from 1-30 with a wax marker, and had its volume and mass measured. Volume was measured using the water displacement method. The avocados were then stored in an opaque bin with 10 Cavendish bananas. Daily, for five days, the mass and volume of avocados were recorded. Avocado density was calculated from the data. The density and mass of avocados are compared with respect to time. Results The data show a strong linear negative correlation between time elapsed and the weight of avocados ($r = -0.93$, Figure 1), with an average rate of change of -0.42 grams per day. The volume of the avocados displayed a negative relationship with respect to time elapsed ($r = -0.39$). Lastly, the density of the avocados increased with respect to time, albeit with a significantly weaker correlation than either volume or mass ($r = 0.22$). Conclusion The researchers hypothesize exposure to ethylene gas led to an increase in the metabolism of the plant cells, and subsequently a loss of weight through cellular respiration, in addition to moisture loss. The loss of volume was likely caused primarily by moisture loss, but such minute changes in volume would require significantly more precise methods to measure. The density increased overall, which indicates that the proportional amount of volume lost, mostly through water, was greater than the proportional amount of mass lost, mostly through metabolism.

Poster02 Genetically-encoded nanoparticles for siRNA-mediated crop genetic engineering Virginia H. Pistilli, gigipistilli7@gmail.com, Mark Legendre, Gozde Demirer. Div. of Chemistry and Chemical Engineering, California Inst. of Technology, Pasadena Genetically-engineered crops are a critical solution to food insecurity amidst our growing global population and changing climate. However, plant genetic engineering is challenged by inefficiencies in biomolecule delivery and transformation bottlenecks. While nanoparticle-mediated delivery of biomolecules to plants offers a promising solution to these challenges, previously developed inorganic nanocarriers threaten environmental health given their potential cytotoxicity and non-biodegradable nature. To address these concerns, we engineered genetically-encoded delivery vehicles (GDVs) from virus-like particles of Tobacco Mosaic Virus. Synthesized in and purified from plants, these high-aspect ratio, rod-shaped GDVs offer a biodegradable, scalable, and programmable platform alternative to conventional crop engineering methods. Most notably, Agrobacterium-mediated transformation is limited to delivering specific cargoes to narrow host ranges and require genomic integration, thus raising regulatory concerns and limiting field applications. In contrast, our nanoparticles are uniquely suited to deliver small interfering RNA (siRNA), protecting siRNA from degradation, targeting a variety of crops, and providing a useful tool for field applications of siRNA-based treatments. First, we verified that our GDVs can enter or associate with plant cells to deliver cargoes. For this, I performed a copper-catalyzed alkyne-azide cycloaddition reaction between Cy3-azide fluorophores and native glutamic acid residues on the GDV internal channel. Infiltration of Cy3-labeled GDVs into tobacco leaves verified cell wall entry/association needed for siRNA delivery. Next, bioconjugation of cationic peptides to the exterior surface resulted in functionalized GDVs that electrostatically adsorbed nucleic acids. We are currently assessing the ability of this nanocarrier-siRNA complex to successfully deliver siRNA to the cytosol and silence protein expression, demonstrating that GDVs are promising delivery vehicles for critical plant genetic engineering applications.

Poster03 All-natural healthy power aid drinks from specialty crops rich by antioxidants, essential oils, and terpenes Ludan Osman1, lhosman@umes.edu, Bokary Sylla1, Andrew G. Ristvey2, Victoria Volkis1. (1) Natural Sciences, Univ. of Maryland Eastern Shore, Princess Anne (2) Wye Research & Education Center, Univ. of Maryland Extension, College Park Aronia mitschurinii is a deciduous shrub native to North America. Aronia, along with hascaps, elderberries, and mulberries, makes a new generation of super fruits with the content of phenolic antioxidants much higher than for well-known assai berries. The unpopular taste of tannins can be balanced when berries are used in juices, jams, or other sweetened products. Another obstacle is a high content of sorbitol, that limits recommended per-day consumption. This research is focused on now being patented all-natural, colorants-, preservantes-, and sugar-free power aid drinks using aronia juice. The typical power aid drinks on the market has high sugar content, calories overload, and cardiovascular risks. Aronia juice naturally has a high content of potassium, magnesium, selenium, iron, and zinc. Organic mineral drops complement it by other cations from natural minerals. Adding young ginger, freeze-dried organic berries, earl gray and/or medical herbal brews to the basic power aid drink, sweetened by organic stevia, helps avoiding the tannins' flavor, and allows variety of flavors, while adding more health benefits to the drink. Here we present the phytochemical characterization of all developed drinks, along with best processing practices after performing thermal decomposition experiments. Qualitative screenings have shown the presence of Flavonoids, Glycosidases, Polyphenols, and Saponins. Drink characterization analysis on the basic ginger drink has indicated pH (3.82), Conductivity (47.44µS/cm), and brix percentage (3.3%). Further quantitative research has shown a sufficient amounts of Anthocyanins (37 mg/g C3G), Polyphenols (10mg/g GAE), Flavonoids (1.00mg/g QE), Tannins (0.45mg TA/g) in the pasteurized drinks.

Poster04 Exploring flavors of edible ants: A path to sustainable gastronomy and consumer acceptance Selene Alvarado Martinez1,

salvaradomarti8855@sdsu.edu, Ali Raza1, Daisy Lopez1, Victoria Esparza1, Jing Zhao1,2, Changqi Liu1,2, changqi.liu@sdsu.edu. (1) School of Exercise and Nutritional Sciences, San Diego State Univ., California (2) Center for Better Food Futures, San Diego State Univ., California Edible insects are gaining popularity as a sustainable solution for the rising global demand for proteins, owing to their low environmental impact and high nutritional value. However, solely emphasizing the environmental and health advantages of consuming insects might not be sufficient to encourage widespread acceptance. Investigating the flavor profiles of edible insects holds the potential to shift marketing strategies towards hedonic-focused campaigns that will be more successful in boosting consumer acceptance and therefore, insect consumption. Certain insects are already considered delicacies. For instance, Formicine ants are utilized as a sour flavoring agent in some cultures, and the leaf-cutting chicatana ants are highly favored in Mexican cuisine. To explore the flavor profiles of these edible ants, the aroma compositions of common black ants (Lasius niger) and chicatana ants (Atta mexicana) were analyzed using headspace solid-phase microextraction and gas chromatography-olfactometry-mass spectrometry (HS-SPME/GC-O-MS). Our study revealed distinctive odor profiles for different ant species. Common black ants were characterized by a pungent, acidic, and vinegary smell primarily due to their high formic acid content, a secretion from their venom glands. In addition, numerous Dufour gland alkanes such as tridecane, undecane, and pentadecane, known to act as alarm pheromones, were detected in common black ants. In contrast, chicatana ants exhibited nutty, roasty, woody, and fatty notes. Unlike common black ants, chicatana ants did not contain formic acid. Instead, they had alarm pheromone 4-methyl-3-heptanone and trail pheromone 2,5-dimethylpyrazine. The fatty aroma of chicatana ants was probably attributed to their abundant presence of aldehydes such as hexanal, octanal, and nonanal. Understanding these flavor profiles is essential for the food industry to create appealing insect-based products that can overcome psychological barriers, such as disgust-based aversions, associated with insect consumption.

Poster05 Developing an Ochratoxin A nanoaptasensing screening system with a plasmonic platform Andres Fabian, abfabian@pucp.edu.pe, Angeline Saldana, Sara Córdova, Yulan Hernandez, Betty C. Galarreta. Ciencias - Sección Química, Pontificia Univ. Catolica del Peru, Lima, Lima, Peru Ochratoxin A (OTA) is a low molecular weight metabolite that contaminates various food products (e.g. coffee, wheat, among others) and is highly dangerous because it generates adverse health effects even at low concentrations (in the ppb region). This has led to rigorous regulation and the development of new methods that allow simple, rapid, and selective detection. Given this situation, biosensors based on gold nanospheres (GNPs) are a promising alternative to conventional detection methods. GNPs exhibit excellent optical properties due to localized surface plasmon resonance (LSPR). The position of the LSPR band is determined by the shape, size, and refractive index of the medium around the nanoparticle. The latter, together with the functionalization of the surface of the nanoparticles with recognition agents, such as aptamers, allow the development of highly selective methods. Herein, GNPs have been immobilized on a solid substrate, such as glass, and integrated into a microfluidic system to build a plasmonic platform to detect OTA. Polyethylene glycol (PEG-SH) and ochratoxin A aptamer (Apt-SH) have been used as part of the developing process. The effect of their concentration and flow rates have been modulated as part of the optimization process of the system. All the adsorption steps are monitored by changes in real-time of the LSPR band in the visible and near-infrared range. This study shows that diffusion processes of thiolated molecules to the surface of GNPs govern their functionalization. Preliminary results of food samples spiked with OTA and the improvement of the detection method are shown. This work may allow the establishment of real-time detection protocols for ochratoxin A in food samples that are highly sensitive and selective in an accessible manner.

Poster06 Comprehensive comparison of the dynamics of kombucha fermentation in a silicone bag and a glass jar Kortnie Chamberlain, kc0143@ship.edu, Emily Swartz, John N. Richardson, Jeb Kegerreis. Chemistry, Shippensburg Univ. of Pennsylvania Kombucha is a fermented tea beverage popular all around the world and known for its distinctly sour taste. The brewing of kombucha relies on a symbiotic culture of bacteria and yeast (SCOBY). One of the most important processes that occurs during a kombucha fermentation is the production of acetic acid. The yeast in the SCOBY convert a food source to ethanol, and the bacteria (when exposed to oxygen) convert ethanol to acetic acid. For non-alcoholic kombucha to be sold commercially, the alcohol by volume (ABV) must be less than 0.5%, so understanding ways to maximize bacterial activity becomes paramount. In our study, two different types of brewing vessels were analyzed to determine which produces more desirable ABV values. One vessel was an air-permeable silicone bag, and the other vessel was a one gallon mason jar. An equivalent batch of kombucha was brewed in each vessel, and pH, ABV, titratable acidity, dissolved oxygen concentration, and a benchtop Nuclear Magnetic Resonance (NMR) spectrometer was used to monitor sugar concentration. The sugar concentrations were validated by comparing the NMR results to those obtained using an enzymatic sugar testing kit. The air permeability of the bag increases dissolved oxygen levels, increasing the activity of the bacteria relative to the jar and lowering the ABV.

Poster07 Investigating the impact of sugar source variation on kombucha fermentation Ian Loscher, il5708@ship.edu, Abigail Czarnecki, John N. Richardson, Jeb Kegerreis. Chemistry, Shippensburg Univ. of Pennsylvania Kombucha is a fermented tea beverage that has become increasingly popular in recent times due to its health benefits related to its probiotic properties. The main components of a kombucha brew are tea, a SCOBY (Symbiotic Culture of Yeast and Bacteria), and a sugar food source. Because of the many fermentation products that create the unique flavor profile of each kombucha brew, information about the optimization of the brewing process has become important to members of the kombucha industry. Using glucose, sucrose, and fructose as different starting sugar food sources was found to produce different metrics in the completed brews that may be more favorable to kombucha brewers. Time dependent data was acquired using potentiometric titrations, gas chromatography, NMR, HPLC, and other techniques.

Poster08 Semi critical CO2-ethanol assisted extraction of photoinduced bioactive pigments from seaweed algae: Advances in renewable dyes production for food supplements and pharmacy applications Angelo Chatmon, achatmon00@student.coppin.edu, Viviana Wamiru, Tulio Chavez-Gil. Natural Sciences, Coppin State Univ. College of Arts & Sciences and Education, Baltimore, MarylandSeaweed algae biomass has been identified in the food supplements and pharmacy sectors as sustainable producers of renewable bioactive pigments with potential for commercialization. To perform photosynthesis, algae use pigments to harvest sunlight energy. The natural pigments found in algae are classified as chlorophylls, carotenoids, and phycobilin’s. Natural dyes such as carotenoids are the most found in micro algae and includes astaxanthin, lutein, fucoxanthin, canthaxanthin, zeaxanthin, and β-cryptoxanthin which are credited to possess medicinal applications as antioxidants, anti-inflammatory, antitumor, immunoprophylactic, among others. Because the presence of several olefinic double-bonds in the carotenoids chemical structure, they also exhibit wide

health applications while protecting other essential molecules from oxidative stress induced by active radicals using various biochemical mechanisms. Scenedesmus obliquus is a micro algae strain with high levels of astaxanthin, lutein, and carotenoids production. This research provides insights into a new extraction approach formed by a CO2-ethanol biphasic solvent applied to algae natural pigments extraction, in an effort to standardization of a protocol for scale up and commercial production. Two cultures of Scened. obl were subjected to (a) unstress and (b) stress photophysical growth for three weeks. The pigments were accessed via semi critical assisted extraction (SmCAE) technology, purified through column chromatography, and characterized by NMR, UV-VIS, FTIR, Raman, and GC-MS. The pigments content (carotenoids, mg/g) were determinate by Kirk and Allen method. Carotenoid (μg/g) = A480 + (0.114 × A663) – (0.638 × A619) (eq. 1) (a) Unstressed growth (0.3537g). SmCAE-CO2-ETOH – Glass-Thimble (1 h). Carotenoid (μg/g) = 0.1001mg/g (b) Stressed growth (0.4521g) SmCAE-CO2-ETOH – Glass-Thimble (1 h). Carotenoid (μg/g) = 0.0109 mg/g. We will discuss the induced photophysical factors related with pigments production, pharmaceutical application, marketing potential, bottlenecks, and future endeavors.

Poster09 Development of a high-performance thin layer chromatography (HPTLC) method for the qualification and quantification of soya saponin compounds Genesis Chavarria, genesis.chavarria.montero@est.una.ac.cr, Angélica Sibaja-Salazar, Sergio Nates, Victor Alvarez-Valverde, Pablo Jimenez-Bonilla. Univ. Nacional, Heredia, Costa Rica Saponins are glycosides of triterpenes and steroids. They are a group of secondary metabolites that are mainly produced by plants. The applications of saponins are directly related to their chemical structures; the hydrophobic and hydrophilic parts of the molecule provide them with emulsifying and stabilizing properties that have been exploited in the pharmaceutical and food industries. According to numerous scientific studies, saponins can boost the immune system, lower cholesterol, reduce inflammation, fight bacteria and viruses, and inhibit different stages of cancer development or progression. The discovery of new saponins could provide new avenues to treat these and other diseases. However, quantification of saponins is considered rather challenging because they do not have chromophores in their structure which restricts their detection in UV light. Also, saponins are hard to separate and resolve because of their amphiphilic nature. The most relevant quantification strategies available nowadays rely on the application of evaporating-light scattering detection, there has also been reported an LC electrospray MS method. Herein, we report the development of a high-performance thin-layer chromatography method that was able to qualify and quantify soyasaponins in different soy extracts. Samples were applied on a precoated silica gel 60 F254 and derivatized using an anisaldehyde/H2SO4 solution thus, allowing their detection under UV illumination at 366 nm. Previous protocols for HPTLC utilize 550 nm wavelength, which contains several limitations such as low color stability and different molar absorptivity for each compound. The HPTLC analysis showed several advantages compared to other analytical methods including a low detection limit down to ng, the use of a small amount of a single mobile phase, the automated sample application, and the ability to run several samples at the same time

Poster10 Categorization of organic compounds in agricultural soils Noah Reilly, reillyn@aquinas.edu. Chemistry, Aquinas College, Grand Rapids, Michigan This study aims to understand the main question of "how much carbon is absorbed by soil and particular land uses". In this study, 8 different agricultural fields were studied throughout West Michigan. A positive correlation between less disruptive tilling practices and an increase in sequestered carbon was found as well as a positive correlation between larger amounts of organic compounds and a larger amount of sequestered carbon. The proposition that less disruptive tillage practices lead to more sequestered carbon within the agricultural soil was present in the literature and reaffirms the results that we found. Carbon is a large part of the foundation of agricultural problems regarding how researchers and scientists can be able to solve them. One way tillage practices can impact the amount of carbon being sequestered in the soil is through harsh and disruptive tillage practices. While that may be a seemingly obvious or well-known idea, the organic compounds present within the soil, and the characterization of them, are more complicated.

Poster11 Unraveling the health implications of modified sucralose Isabella Beasley, isabella.beasley@lyon.edu, Dailyn Crain, Michael Jorgensen, Téa Mason, Irosha N. Nawarathne. Chemistry, Lyon College, Batesville, Arkansas Sweet tasting food enhances the human appetite. However, high sugar intake shows evidence in increasing the risk of developing obesity, prediabetes, type 2 diabetes, and cardiovascular disease. Consequently, non-nutritive sweeteners (NNS) such as sucralose, acesulfame potassium (Ace K), saccharin, aspartame and stevia are recommended as dieting tools. Consumers are instinctively choosing NNS in place of sugar to maintain or lose weight despite emerging evidence of unanticipated health implications of NNS that include but not limited to weight gain, glucose intolerance, increased appetite, altered taste sensitivity. Sucralose is a general purpose synthetic sweetener, a tri-chlorinated derivative of sucrose, which is about 320–1000 times sweeter than sucrose and shows incredible heat stability and shelf life. The sucralose market is continuously growing at a compound annual growth rate of 5.43% to reach US$5.357 billion in 2024 fromUS$3.901 billion in 2018. The bacteriostatic effects of sucralose on both aerobic and anaerobic bacteria are repeatedly reported. These effects lead to various modifications in the intestinal microbiota causing inflammation in the host. In this study, the solubility, reactivity, and other analytical aspects of sucralose and sucralose derivatives that contain tosyl, amino, and azido functional groups were investigated. Next, the effects of sucralose derivatives on common gut microbes will be unraveled while focusing on their potential as bacteriostatic agents. Can sucralose be altered for healthier human consumption and/or as a novel antibacterial agent? In this presentation, we will answer these bitter-sweet problems.

Poster12 Comprehensive metabolomic profiling for elderberries (Sambucus spp.) in uncovering bioactive compounds Nadia Bostick1, Nadia.Bostick@uhsp.edu, Pietro Martano1, Micaela Uy1, Samira Mahdi2, Xavier Jones2, Qingbo Yang2, Ray Mu1. (1) Basic Sciences, Univ. of Health Sciences and Pharmacy in St Louis St Louis College of Pharmacy, Missouri (2) Agriculture and Envir. Sci. & Cooperative Research, Lincoln Univ. of Missouri, Jefferson City Elderberries (Sambucus spp.) are recognized as a rich source of bioactive compounds with the potential to offer substantial health benefits. In our initial investigation, we employed various solvent extraction methods and state-of-the-art high-resolution mass spectrometry (HRMS) for the identification of both targeted and untargeted metabolites. Additionally, we performed various statistical analyses, including differential analysis and hierarchical cluster analysis, and more, to gain deeper insights into elderberries' metabolomic profile. In this study, we have delved deeper into the metabolomic profiling of elderberries, focusing on the qualitative and quantitative assessment of different bioactive compounds. Our exploration successfully uncovered a diverse array of bioactive compounds within elderberries, including anthocyanins, phenolic acids, flavonoids, vitamins, and triterpenoids. By combining the HRMS, Compound Discoverer for metabolite

identification, and the insights garnered from statistical analyses, we further elucidated the intricate web of bioactive compounds within elderberries. These efforts not only contribute to expanding our understanding of elderberry metabolites but also hold significant promise for harnessing their health benefits. Furthermore, we harnessed the rich resources of the KEGG and BioCyc databases for comprehensive biopathway identification. This database-driven approach helped us reveal significant insights into the transformation mechanisms of these bioactive compounds. In conclusion, our study represents a pivotal step in metabolomic profiling of elderberries and underscores the importance of employing multiple analytical techniques and statistical analyses. These findings carry substantial implications for the development of elderberry-based products and pave the way for a more in-depth exploration of elderberries' potential as a natural health-promoting resource

Poster13 Creating a glucometer-based device to observe the ripening of Aronia mitschurinii Ryan Buzzetto1, rrmore@umes.edu, Ezra Cable1, Andrew G. Ristvey2, Victoria Volkis1. (1) Natural Sciences, Univ. of Maryland Eastern Shore, Princess Anne (2) Wye Research & Education Center, Univ. of Maryland Extension, Queenstown Aronia mitschurinii is a super-fruit renowned for having exceptionally high antioxidant content. Research has shown that the peak for antioxidants in Aronia occurs early in the ripening process when brix content is low. Harvesting the crops during the peak of antioxidants is important for pharmaceutical applications, yet harvesting when the fruits are fully ripened would be preferable for use in food products. The issue with harvesting Aronia is that there is no visual difference to show the ripening of the fruit. Our approach involves using a glucometer to assess both antioxidant and brix content. The most valuable antioxidants found are anthocyanins, with a majority consisting of Cyanidin-3-Glucoside (C-3Glu), which undergoes glucoside bond hydrolysis under acidic conditions. Research data indicates that at neutral pH conditions the reading on the glucometer is proportional to brix readings on a refractometer, whereas under acidic pH conditions the reading is proportional to the C-3Glu content read using a UV/Vis spectrophotometer. A device was developed for in-field testing with the accuracy being evaluated and compared to laboratory results. To accommodate the glucometer's range, juice dilution was employed, and data analysis determined an optimal dilution ratio. The data shows that the values of anthocyanins and brix are consistent regardless of if the glucometer, UV/Vis, or refractometer was used. Additionally, glucose and C-3Glu standards underwent testing on the glucometer with various dilutions to observe the relationship between glucometer measurements and concentration. This study presents the findings of the methodologies, and the calibration curve results.

Poster14 Effects of betulin derivatives from birch and sycamore bark on Drosophila melanogaster Faith Davies, daviesf1@newpaltz.edu, Mendy Gross, Lucia Speranza, Miles Wilklow-Marnell. Chemistry, SUNY New Paltz, New Paltz, New York, US White Birch (Betula papyrifera) and American Sycamore (Platanus occidentalis) bark contain tannins, polyphenols, and lupane triterpenoids such as betulin, betulinic acid, and lupeol. Methanolic extracts of these barks have been found to be biologically active in assays on the common fruit fly (Drosophila melanogaster). The activity of crude extracts and more purified fractions is divergent, demonstrating protection against oxidative stress, larval growth enhancement, larval growth inhibition, or no-activity as compared to a control. Extracts were characterized by GCMS, 1H-NMR, and IR spectroscopy, and antioxidant activity was assessed by DPPH free radical scavenging assay. While crude birch extract, composed mostly of betulin, lupeol, and trace amounts of an unknown triterpenoid, was found to enhance larval growth and increase survivorship of adult flies in oxidative-stress and starvation assays, both purified betulin and lupeol displayed no statistical difference from control. However, after removal of what appears to be polyphenols and/or tannins, recrystallized sycamore extract (> 85% betulinic acid) showed enhanced proliferative/protective effects compared to both crude sycamore and birch extracts. Due to the relative ease of extracting/purifying betulinic acid and its apparent greater biological activity, it has been chosen for further investigation of these effects. There have been only several reports on bioassays of betulin derivatives in insect models, all showing antifeedant properties. However, a report on structurally related oleanane triterpenoids (again as antifeedants) indicates that glycosylation of the carboxylic acid moiety greatly enhances activity. To conduct a structure activity relationship and gain insight on these effects, a selection of esters derived from betulinic acid, including glycosylated versions, is being synthesized. Sycamore bark was removed of hydrophilic impurities via extraction with boiling water and dried/pulverized prior to betulinic acid extraction with methanol. Crude extract was obtained by precipitation from this methanolic solution following concentration and storage at 5 °C, which was then treated with activated charcoal in boiling methanol and recrystallized, providing a white solid with a minimum betulinic acid content of 85%. Through further recrystallization ≥ 95% betulinic acid can be obtained, which will be used for synthetic modifications.

Poster15 Molecular cloning of bacterial exopolysaccharide forming enzymes in sugarcane processing and biological and agricultural impacts Jack Fein1,2, jfein@tulane.edu, Yunci Qi1, Gillian O. Bruni1, Evan Terrell1, evan.terrell@usda.gov. (1) USDA-ARS Southern Regional Research Center, New Orleans, Louisiana(2) Tulane Univ., New Orleans, Louisiana In the postharvest processing of sugarcane to raw sugar, microbial activity results in the loss of sucrose and the production of contaminant exopolysaccharides (EPS). The most studied producers of EPS in the context of raw sugar production are Leuconostoc spp., which produce a dextran EPS constructed of repeating glucose units, using dextransucrase enzymes. Analogous levansucrase enzymes are also present many microorganisms, which produce levan fructan EPS during sugar crop processing. Levan producing bacteria include Gluconobacter, Bacillus, and Pseudomonas, among other microbes. These EPS introduce engineering challenges for processing facilities, particularly related to viscosity, crystallization, and the presence of biofilms. Leuconostoc lactis strain LASM16 was previously isolated from a raw sugar factory in Louisiana and characterized as a dextran-producing strain and its genome was sequenced. To further study the dextran produced by this strain, the DNA sequence coding for its singular/lone dextransucrase enzyme (dsrLASM16) was inserted into the pET21a expression vector. This plasmid was then transformed into E. coli strain BL21 (DE3) for protein production, from which the resulting dextransucrase enzyme was purified by Nickel affinity chromatography. Additional isolations of other dextransucrases and levansucrases is ongoing. Heterologous expression of these enzymes forms the basis for further investigations for biological and agricultural engineering, as it relates to sugar crop processing. Future work will explore cell free synthesis of dextran and levan EPS and rigorous characterization of the resulting EPS. Inhibition studies for dextran- and levansucrases enzymes are also planned. These results will also be used to inform microbial control and EPS mitigation strategies for agricultural industry stakeholders.

Poster16 Understanding the flavors and aromas in wine and beer Brian Bartholomew2, bbartho2@msudenver.edu, Brieana Caggiano1, Michael B. Jacobs2. (1) Nutrition & Dietetics, Health

Sciences, Metropolitan State Univ. of Denver, Colorado(2) Chemistry & Biochemistry, Metropolitan State Univ. of Denver, Colorado Many historical records illustrate that beer, wine, and other alcohol-containing beverages are essential to human existence. There is a cornucopia of recipes and other relics dedicated to alcoholic beverages. Due to the chemical components, a rainbow of aroma and flavor characteristics enlightens our sensory receptors. The malted grains, hops, and adjuncts can influence the flavoring and aroma of beer. The environment, grape, and fruit varietals can influence wine's flavoring and aroma. Both beverages are affected by yeast and the fermentation/aging process. Presented herein are the science and chemistry involved in identifying some of the world's favorite drinks through analytical processes in chemistry, olfactory senses, and overall enjoyment found in each beverage.

Poster17 Determination of xanthophyll carotenoid content in vegetables recommended for macular degeneration prevention through high performance liquid chromatography and heat exposure Madison Tarrance1, met36@students.uwf.edu, Karen W. Barnes2. (1) Biology, Univ. of West Florida, Pensacola(2) Chemistry, Univ. of West Florida, Pensacola The primary objective of this project is to extract the carotenoid content from different vegetables before and after cooking by either sautéing or microwaving. After extraction, a comparison of 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 and compare whether different cooking methods have a significant impact on carotenoid retention.

Poster18 Dr. Pepper Vanillin Flavor Compound determination and analysis using SPME and Headspace Analysis Madison Tarrance1, met36@students.uwf.edu, Karen W. Barnes2. (1) Biology, Univ. of West Florida, Pensacola(2) Chemistry, Univ. of West Florida, Pensacola The primary objective of this project is to identify the different flavor compounds within the soda Dr. Pepper following a recent lawsuit about possible fraudulent label claims. Dr. Pepper is a very popular soda brand that many people know and love for their formula containing a secret "Unique blend of 23 flavors". The company along with other soda brands recently faced a class action lawsuit over deceptive advertising of their flavors as "aged vanilla" since the products are made from artificial flavoring. The flavor is thought to come from synthetically developed Ethyl Vanillin. We aim to detect and identify the compound responsible for the vanilla flavor through SPME and Headspace analysis instrumentation. Samples of Dr. Pepper will be extracted through solid phase microextraction protocols and quantified through headspace and GC-MS analysis. Using the GC-MS, the compound will be separated and identified. Our project will allow us to determine whether the vanilla compounds used in the brand soda Dr. Pepper is able to be identified through laboratory testing and can be compared and identified as deceptively used in label claims.

Poster19 Analysis of heavy metals in dark chocolate Victoria Pipinich, pipinichv@wittenberg.edu, Raymond C. Dudek, rdudek@wittenberg.edu. Chemistry, Wittenberg Univ., Springfield, Ohio Dark chocolate, supposedly one of the healthier desert options, is rich in minerals and contains antioxidants. Higher percentages of cocoa can improve blood flow and lower blood pressure.8 However, previous research performed by Consumer Reports1 has found certain dark chocolate bars contain excessive amounts of lead and cadmium.1 To confirm these results, dark chocolate bars were tested using atomic absorption spectroscopy. The results of the investigation showed exorbitant levels of lead and cadmium in dark chocolate bars. The levels of lead were unusually high in the dark chocolate bars sampled. 1. Loria, K. Lead and Cadmium Could be in Your Dark Chocolate. Consumer Reports, Feb 2023. https://www.consumerreports.org/health/food-safety/lead-and-cadmium-in-dark-chocolate-a8480295550/.

Poster20 Characterization of purple star apple (Chrysophyllum cainito L.) as a promising functional food Gabriela Rubi R. Tapia-Alvarez1, dra.gtapia@gmail.com, Élida Gastelum-Martínez2, Karlina García-Sosa1, Lia S. Valencia-Chan3, Rosa Moo-Puc3, Inocencio Higuera-Ciapara4, Luis M. Pena-Rodriguez1. (1) Biotechnology, Centro de Investigacion Cientifica de Yucatan, Mérida, Yucatán, Mexico(2) Food Technology, Centro de Investigacion y Asistencia en Tecnologia y Diseno del Estado de Jalisco, Mérida, Yucatán, Mexico(3) Research, Instituto Mexicano del Seguro Social, Mérida, Yucatán, Mexico(4) Nutrition, Universidad Anahuac Mayab, Merida, Yucatán, Mexico Certain fruits are classified as functional foods due to their possession of antioxidant properties and their contribution to mitigating the effects of aging and various chronic health issues. Among these functional fruits, berries have gained prominence worldwide owing to their delightful flavor and potent disease-fighting properties. Nonetheless, their consumption in Mexico faces constraints due to limited availability and elevated market prices. Given Mexico's rich biodiversity, we advocate for the adoption of an alternative functional fruit produced in Mexico as a sustainable dietary approach, considering this shift can lead to numerous positive impacts on the environment, economy, and society. The purple star apple fruit (Chrysophyllum cainito L.), commonly known as caimito, shows promise as a functional food due to its polyphenol-induced antioxidant effects in a range of in vitro models, which significant prevent the increase of intracellular ROS levels and promote cell viability, similar to quercetin, in a H2O2-induced stress model.

Poster21 Evaluating chemical catalysts' thermal and kinetic effects on starch gelatinization Saeed Dupree, srdupree.2020@mymail.jcsu.edu, Thanh-Thuy Nguyen. Johnson C Smith Univ., Charlotte, North Carolina Starch gelatinization is utilized to enhance textures and properties for various food products. Food manufacturers can maximize food production and elevate food quality by examining starch gelatinization speed. Chemical catalysts are used to expedite gelatinization by modifying the pH environment and breaking starch bonds. Through the use of Differential Scanning Calorimetry (DSC), it is possible to identify different times, temperatures, and heat flow needed for starch to gelatinize when introduced to different catalysts. These studies will analyze white rice soaked into an edible chemical catalyst for 24 hours: Acetic acid (vinegar), Citric acid (Lemons), and Kefir (lactic acid) to understand if gelatinization speed increases. Additionally, we can calculate the kinetic parameters using a linear regression analysis of thermogram data, yielding the activation energy and pre-exponential factor. These parameters provide insights into the energy needed for starch bonds to break and water molecules to be absorbed, shedding light on collision events that break these bonds inside the white rice.

Poster22 Increasing desirable aroma compounds in Pennsylvania wines by treating post-harvest grapes with elemental sulfur Jacob J. Messner2, messner.jacob@gmail.com, Morgan Vincent2, Ryan Elias1, Misha Kwasniewski1. (1) Food Science, The Pennsylvania State Univ., Univ. Park(2) Chemistry, The Pennsylvania State Univ., Univ. Park Grape-derived polyfunctional thiols contribute positively to the aroma quality of wines, especially aromatic white wines. These thiols, such as 3-mercaptohexanol (3MH), 3-mercaptohexyl acetate (3MHA), and 4-mercapto-4-methylpentant-2-one (4MMP), have very low aroma thresholds (ng/L), but impart highly desirable aromas (e.g., grapefruit, passionfruit, blackcurrant) to finished wines. Recently, studies have

shown that the application of urea and micronized sulfur to the foliar during growing season in Pennsylvania resulted in a significant increase (73-300%) in varietal polyfunctional thiol content in finished wines. Unfortunately, the repeated application of these treatments can be time-consuming and expensive. In the present study, liquid-chromatography with tandem mass spectroscopy was used to investigate the impact of additions of elemental sulfur (S0), in combination with SO2, and/or ascorbic acid to grape juice on the concentration of polyfunctional thiols in finished wines. This approach relies on the recently elucidated mechanism by which S0 is biologically transformed (i.e., via yeast) to hydrogen sulfide during the primary fermentation, which is subsequently capable of reaction with juice-derived C6 alkenes (e.g., trans-2-hexanal, trans-2-hexanol, hexanol) via 1,4 Michael addition reactions to yield desirable polyfunctional thiols. These reactions have been shown to be effectively modulated through the addition of SO2 (a multifunctional antioxidant capable of quenching thiols, scavenging hydrogen peroxide, inhibiting polyphenol oxidase, and quenching carbonyl-containing oxidation products) and ascorbic acid (a strong reducing agent and oxygen radical scavenger). We hope to determine if the S0 addition technique is viable as a simple and cost-effective method of increasing the pool of desirable polyfunctional thiols in Pennsylvania wines.

Poster23 Sustainable formulation solutions for dsRNA-based biopesticides for next-gen agricultural pest control Sargun Malik, sargunmalik@outlook.com, Anil Kumar, anil@techaccel.net, Mosharrof Mondal, Adriano Pereira, Fred Moshiri, Kiran Nawaz, Tammy Zanker, Ida House, Dylan Gladson, Sydney Tomaschke, Jacob Shoemake, Jacob@techaccel.net, Lucas Nitcher. Rnaissance Ag, LLC, St. Louis, Missouri Twenty to 40% of global crop production valued at around $290 billion is lost to pests annually. Broad-spectrum chemical pesticides are extensively used by growers worldwide to protect crops against insect pests and plant pathogens. The extensive use of chemical pesticides contaminates air, soil, and water. Moreover, pesticide residues tend to remain in/on the crop for a long period consequently entering the food chain and affecting human health. Awareness among the consumers about harmful effects of chemical pesticides coupled with legislation like the European Green Deal is leading to the adoption of sustainable biological pest control measures. The use/adoption of biological pesticides however is associated with numerous challenges such as limited spectrum of activity, cost, variable efficacy, etc. RNA interference (RNAi)-based biopesticides are a new approach for controlling insect pests and vectors of plant pathogens wherein Double-stranded RNA (dsRNA) plays a central role in regulating gene expression at the post-transcriptional level. They offer a new mechanism of action to complement existing pest control strategies that are highly selective and present low risk to non-target organisms. However, in the field dsRNA is susceptible to degradation by temperature, UV radiation, rainfall, and microbial activity. RNAissance Ag, LLC (St. Louis, MO) has developed formulations to overcome these challenges. The developed formulation utilizes drying-based encapsulation technology and food-grade ingredients to protect dsRNA from degradation by environmental factors enabling enhanced delivery and efficacy of the dsRNA molecule. With this sustainable formulation solution, challenges associated with chemical pesticides such as food safety, environmental impact, and ecological imbalance can be eliminated ensuring efficient pest management and food security.

Publishing trends in journals of the ACS Agricultural and Food Chemistry portfolio Coralia Osorio Roa1, cosorior@unal.edu.co, Laura L. McConnell2, Thomas Hofmann3. (1) Departamento de Química, Univ. Nacional de Colombia, Bogota, Colombia(2) Crop Science Division, Bayer US, LLC, St. Louis, Missouri(3) Food Chemistry and Molecular Sensory Science, Technische Univ. Munchen, Freising-Weilhenstephan, Bavaria, Germany Since 2020, the ACS portfolio related to food and agricultural sciences has expanded and launched two new journals, additional to the Journal of Agricultural and Food Chemistry, with Dr. Thomas Hofmann as the Editor-in-Chief of all three journals. The two new journals, ACS Food Science & Technology and ACS Agricultural Science & Technology are managed by the Deputy Editors, Dr. Coralia Osorio and Dr. Laura McConnell, respectively. These journals provide the scientific community a fresh platform with a broader scope to lead the agriculture and Food Sci. & Tech. network to join forces between different researchers to fulfill the world's challenges, such as food security and sustainable use of land, among others. This poster will highlight representative publications from the journals.

Application of untargeted headspace solid-phase microextraction-gas chromatography-mass spectrometry for volatile metabolomics-based authentication of plant-based milk alternatives Renato Handoyo1, renatohandoyo@cmail.carleton.ca, Enea Pagliano2, Yaxi Hu1. (1) Food Science, Chemistry, Carleton Univ. Faculty of Science, Ottawa, Ontario, Canada(2) Chemical Metrology, National Research Council Canada, Ottawa, Ontario The growing demand for plant-based milk alternatives (PBMAs) has spurred the need for effective methods to ensure their quality and authenticity. As the market grows, concerns about potential adulteration have also intensified, requiring robust authentication methods to be developed. This study developed an untargeted volatile metabolomics-based approach that combines headspace solid-phase microextraction (HS-SPME) with gas chromatography-Triple Quadrupole mass spectrometry (GC-MS) to authenticate eight types of PBMAs (i.e., almonds, cashews, hazelnuts, walnuts, oats, peanuts, pistachios and macadamias). To achieve the maximum performance, optimization of the instrumentation (i.e., SPME fibre, GC column, desorption time and sample volume) was performed. The optimal method using a PDMS/DVB SPME fibre, a polar DB-1701 GC column, a desorption time of 60 s and a sample volume of 10 mL was applied to analyze 10 biological replicates of the eight types of PBMAs (i.e., 80 samples in total). The acquired untargeted GC-MS data were preprocessed by MS-DIAL and identification of metabolic features was achieved using the Kovats retention index. A total of 174504 volatile compounds were detected using this method . Unsupervised principal component analysis (PCA) was unable to identify clear distinctive pattern among different PBMAs. More advanced supervised machine learning algorithms, namely k-nearest neighbour (kNN), random forest (RF) and support vector machine (SVM), were then used in this study for accurate identification. All the three supervised learning models worked relatively well in predicting the PBMAs with RF providing the highest accuracy of 98.8 % in a 5-fold cross-validation model, followed by 97.5 % accuracy using SVM and 88.8% using kNN, indicating this HS-SPME-GC-MS method is highly promising to be applied for the authentication of PBMAs. An inter-laboratory validation of this method is currently ongoing and the preliminary data have demonstrated the feasibility for the methods to be easily adopted by testing laboratories even using different instrumentation set up.

Variation in the β-carotene content of *Blighia sapida u*nder various processing methods Debbie Ann L. Phillips, debbieann.phillips89@gmail.com, Andrea Goldson-Barnaby. Chemistry, The Univ. of the West Indies, Kingston, Jamaica *Blighia sapida,* also known as ackee, is a fruit originating from West Africa and is widely consumed in Jamaica. After harvesting, the edible arilli is separated from the seed and pod. The arilli is then blanched and sautéed with codfish. The impact of various processing methods (uncooked, cooked, uncooked frozen, cooked frozen, and canned) on the beta-carotene content of the arilli was

measured using a spectroscopic assay. The findings revealed a strong relationship between processing method and beta-carotene concentration. Canned ackee had the highest beta- carotene content (0.966 ppm). This is likely due to high-temperature processing breaking down cellular structures and releasing beta-carotene. Uncooked arilli had the lowest beta-carotene content (0.507 ppm). Temperature was a significant factor impacting beta-carotene concentration suggesting that processing methods play a crucial role in shaping the nutritional composition of *Blighia sapida* arilli

Mechanisms of arsenic immobilization by iron nanoparticles in a cultivated soil: Arsenic speciation and the role of iron sulfidation Ziwei Han, ziweih6@uci.edu, Adeyemi S. Adeleye. Dept. of Civil and Environment Engineering, Univ. of California Irvine Our recent study revealed that iron particles can decrease arsenic bioaccumulation in lettuce, but the mechanism is not well understood. To close this knowledge gap, 0.3% (w/w) nanoscale zero-valent iron (nZVI) and sulfidated nZVI (SnZVI) were applied to an As(V)-contaminated soil for 60 days before growing lettuce to maturity in a greenhouse. Soil samples were taken at time points for X-ray diffraction coupled with the reference intensity ratio (RIR) method to determine fractions of different arsenic crystal phases. nZVI and SnZVI significantly ($p < 0.05$) increased lettuce biomass (76- and 160-fold, respectively) and decreased As bioaccumulation factor (BAFAs) in lettuce (2.2±0.3 and 1.8±0.2, respectively) compared to untreated soil (BAFAs = 5.1±1.6). RIR analysis revealed that nZVI reduced As(V) to As(III) and As(0) in the cultivated soil over time, while As2S3 was the dominant form of As in the soil treated with SnZVI, showing displacement of iron in SnZVI by As.

On-site fluorescent detection of microbial contamination using a graphene oxide CRISPR-Cas12a (GO-CRISPR) sensor Tom Kasputis, tomk21@vt.edu, Qiaoqiao Ci, Juhong Chen. Biological Systems Engineering, Virginia Polytechnic Inst. and State Univ., Blacksburg Food waste remains the paramount challenge in combatting world hunger, with approximately one-third of all produced food going to waste annually. Microbial contamination significantly exacerbates food waste, underscoring the urgency of discovering and addressing contamination sources to reduce global hunger. Rapid identification of pathogens is essential to tackle contamination in a timely manner. However, most currently developed on-site biosensors are overly complex, costly, or lack the ideal sensitivity. Therefore, it is crucial to develop rapid and reliable biosensors for the on-site detection of microbial contamination contributing to food waste. Herein, we developed a CRISPR-Cas12a graphene-oxide (GO-CRISPR) biosensor for Salmonella detection in food sources. Under optimal conditions, our GO-CRISPR biosensor can specifically detect Salmonella Typhimurium in milk, with a detection sensitivity as low as 3 × 102 CFU/mL. This cost-effective biosensor generates a fluorescent signal in under one hour, providing a significant advantage for on-site bacteria detection to combat food waste.

Mung bean protein isolate: A novel food ingredient with enhanced functional properties extracted by a deep eutectic solvent Thilini N. Dissanayake, dissanat@myumanitoba.ca. Dept. of Food and Human Nutritional Sciences, Univ. of Manitoba Faculty of Agricultural and Food Sciences, Winnipeg, Canada Feeding the growing global population has become a challenging task today. Developing sustainable, functional food ingredients is crucial for quality, cost, consumer acceptance, and sustainability in food product development as it directly impacts food quality, cost, consumer acceptance, and sustainability. Despite its excellent functional properties, mung bean protein extraction relies on alkaline-based methods, resulting in protein denaturation due to undesirable conditions. The study aimed to optimize mung bean protein extraction using a DES system and compare functional properties with alkaline-extracted proteins. Remarkably, the outcomes demonstrated that both methods yielded similar quantities of protein with equivalent recovery rates. However, the protein extracted through the DES method exhibited significantly enhanced functional properties, including improved oil retention, emulsification activity at pH 5, and foaming capacity at various pH levels (3, 5, 7). These improved properties will benefit food product development, enhancing the industry's economic, environmental, and social sustainability.

Sustainable plant protein ingredient production from fava bean using choline chloride and glycerol deep eutectic solvent system Anuruddika Hetti Hewage, hettihea@myumanitoba.ca. Food and Human nutritional sciences, Univ. of Manitoba, Winnipeg, Canada The ever-increasing population growth has created significantly higher protein demand resulting need for alternative proteins to satisfy the nutritional requirements of humankind. Fava bean (FB) (Vicia faba L.) is an emerging sustainable plant protein source that has greater potential to meet this increasing global protein demand. Conventionally, FB protein isolates are produced by the alkaline extraction method. This has a negative impact on both the environment and the protein quality. Therefore, the need for a sustainable green extraction method in the protein industry is crucial, thus Deep eutectic solvents (DES) have recently gained much interest in plant protein extraction. DES system containing choline chloride and glycerol was used to extract the protein from FB. Extracted proteins were characterized using Fourier-transform infrared spectroscopy (FTIR) for secondary structure analysis. In addition, proximate composition, amino acid (AA) analysis, and in-vitro protein digestibility corrected amino acid score (IV-PDCAAS) were performed according to established methods. Both DES (DES-FBPI) and alkaline-extracted proteins (ALK-FBPI) had a similar protein content (92.50±1.36%). FTIR analysis revealed that DES extraction increased α-helix content (21.37%) while ALK-FBPI showed intermolecular β sheets as protein aggregates (7.61%). Interestingly, DES extraction improved the AA score for sulfur-containing AA (89.9%) compared to alkaline-extracted protein isolates (77.5%). This demonstrates that DES could extract more SAA, thus improving the nutritional value of the protein isolates. Further, a significantly higher IV- PDCAAS was observed with DES-FBPI (76.4 ± 0.5%) compared to ALK-FBPI (71.1 ± 0.4%) indicating that DES extraction could improve the protein quality of FB. In conclusion, DES-based protein extraction, as a green approach, shows a promising technique that could potentially be used as an alternative to the conventional alkaline extraction method. This will allow industries to provide considerable opportunities for innovations in the plant proteins industry across the value chain, thereby increasing the utilization of FB for new food applications.

Narrow-wavelength red LED lighting on quality and aroma expression of hydroponic fennel (Foeniculum vulgare Mill.) Jingsi Liu1, jingsi@vt.edu, Adam Sumner2, Alex Harris2, Song Li2, Bastiaan Bargmann2, David Haak2, Yun Yin1. (1) Food Sci. & Tech., Virginia Polytechnic Inst. and State Univ., Blacksburg (2) School of Plant and Envir. Sci.s, Virginia Polytechnic Inst. and State Univ., Blacksburg It is believed that narrow-wavelength red LED is sensed by plant phytochromes and can regulate the accumulation of secondary metabolites. However, plant responses are species-specific and the influences of lighting on fennel remains unclear. Fennel (Foeniculum vulgare Mill. cv. Grosfruchtiger) is a culinary herb that is cultivated worldwide for its unique aroma profile. Our objective is to investigate the effect of supplemental red LED lighting on plant growth, aroma compounds, and gene expression in

hydroponically grown fennel. Fennel was cultivated with nutrient film technology (NFT) hydroponic systems under controlled environment. After fennel seedlings were transplanted to hydroponic systems, two treatments were applied: a natural (greenhouse) light control and a supplemental red LED lighting (PPFD 100 µmol m-2 s-1, 14h d-1). Whole plants were harvested six weeks after the transplanting. Results showed that supplemental red LED was beneficial for fennel growth and led to increased plant height and fresh weight. Headspace solid phase microextraction (SPME) gas chromatography-mass-spectrometry-olfactometry (GC-MS-O) was used for the identification and quantitation of aroma compounds in fennel leaves, and supplemental red LED increased the total concentration of aroma-active compounds in fennel. Specifically, the concentration of several most potent aroma compounds, such as trans-anethole (sweet, anise), estragole (anise, herbal), and p-anisaldehyde (floral, sweet) showed significant increase in fennel grown under supplemental red LED (t-test $p<0.05$). Preliminary results from RNA-seq gene expression analysis suggested that supplemental red LED also caused substantial changes to plant transcriptome. This study demonstrated the influence of narrow-wavelength LED lighting on the flavor and quality of culinary herbs and laid the foundation for future aroma expression research at molecular levels.

Identification of phytomarkers from Byrsonima bucidifolia fruits and their correlation with antioxidant activity: Chemometric approach Monica Anahi G. Poot, moniguillen7@gmail.com. Biotecnologia, Centro de Investigacion Cientifica de Yucatan, Mérida, Mexico Currently, there is particular interest in the identification of phytomarkers that can be used in the standardization of plant products consumed as natural alternatives for the prevention of chronic degenerative diseases. Recently, correlating data obtained from the chemometric analysis of metabolic and/or chromatographic profiles and the results of biological activity evaluations has been used to aid in the rapid identification of bioactive metabolites from plants. In this investigation, we have used chemometric tools to correlate the metabolic (1H-NMR) and chromatographic (UPLC-MS) profiles with the results of the antioxidant activity of extracts and semipurified fractions of Byrsoninia bucidifolia fruits. The results of the chemometric analysis allowed the identification of gallic acid as one of the metabolites responsible for the antioxidant activity of the extract, together with several glycosylated-polyphenolic metabolites. As the major bioactive component in the fruit extract, gallic acid can be considered as a potential phytomarker for B. bucidifolia-derived products.

Carbon nanodots for the delivery of biomolecules in N. benthamiana Jesus M. Galeana, jgaleana@caltech.edu. Chemistry and Chemical Engineering, California Inst. of Technology, Pasadena, California, US The increasing global human population has compromised food security and made world hunger an imminent threat. Food production must rise 70-100% by the year 2050, hence, it is essential to improve crop productivity rapidly and substantially. Plant genetic engineering is a promising approach to achieve this, but the delivery of biomolecules into walled plant cells has been a big challenge. Carbon nanodots (CNDs) has the potential to be efficient plant delivery vehicles given their small size and availability of surface modification chemistries, which can allow selective attachment and release of biomolecules in target plant cells and organelles. This poster will discuss the synthesis and characterization of CNDs for efficient donor DNA delivery into Nicotiana benthamiana leaf cells for gene insertion applications in plants. The species-independent and efficient plant genetic engineering enabled by CNDs can provide food security by making crops resilient to biotic and abiotic stresses that limit crop yields.

Carcass and meat quality characteristics of pasture-raised lambs as influenced by highly digestible fiber containing agro-byproducts Jung Hoon Lee1, leej@fvsu.edu, Stephan Wildeus2. (1) Agricultural Sciences, Fort Valley State Univ., Fort Valley, Georgia (2) Agricultural Research Station, Virginia State Univ., Petersburg Agro-byproducts such as soy hull and corn gluten have been recognized as economical sources of feeds for beef cattle because they can provide supplemental nutrients for pasture-raised cattle with highly digestible fiber. This study evaluated the effect of highly digestible fiber containing ago-byproducts as supplements for grazing lambs on the carcass and meat quality characteristics of lambs. Thirty-six, 7.5-month-old purebred hair (Barbados Blackbelly and St. Croix) and crossbred wool (Dorset) x hair lambs grazed predominantly Jesup tall fescue pasture. Lambs were randomly assigned to a pasture-only, or a soy hull (SH) or corn gluten feed (CGF) supplemented group balanced by breed type. Supplement was provided at 2% of body weight daily at individual feeding stations. Carcass traits were evaluated after slaughtering with standard procedures at the end of 77 days of grazing period. After 24 h cooler storage (2°C), each carcass was fabricated to obtain 2.5-cm thick loin chops for meat quality analyses. Loin eye area and all cuts from fore- and hind-saddle were greater ($P < 0.01$) in crossbred than purebred lambs, and greater ($P < 0.01$) in supplemented than pastured-only lambs. The CIE a* (redness) and b* (yellowness) values of lamb chops were not significantly influenced by the supplementation. However, chops from supplemented lambs had lower ($P < 0.05$) CIE L* (lightness) values than those from pasture-only lambs. Cooked chops from CGF supplemented lambs had lower ($P < 0.05$) shear values (3.13 vs 3.61 or 3.46 kg, respectively) than those from SH supplemented or pasture-only lambs. The longissimus muscle (LM) of loin chops from SH supplemented lambs had a lower ($P < 0.05$) level of thiobarbituric acid reactive substances (TBARS) than that of CGF or pasture-only lambs. Compared with lambs supplemented with SH or CGF, pasture-only fed lambs had higher ($P < 0.01$) amounts of moisture and ash contents, but a lower amount of total fat ($P < 0.05$) in the LM chops; higher concentrations of linolenic (C18:3n6), arachidonic (C20:4n6), eicosapentaenoic (C20:5n3) and docosahexaenoic (C22:6n3) acids, but lower ($P < 0.05$) concentrations of palmitic (C16:0) and oleic (C18:1n9) acids in the LM chops. Although supplemented with agro-byproducts did alter carcass traits and meat quality parameters of lambs in this study, fresh lamb from pasture-only lambs might have healthier nutritional properties compared to that from supplemented lambs.

Design of new and environmentally safe fungicides using AI and molecular modeling Micah Shaver, mlshaver@ualr.edu, Jerome A. Darsey. Chemistry, Univ. of Arkansas at Little Rock Fungi are biological organisms used that are detrimental to plants. A fungus negatively impacts the growth of plants such as crops and could cause the plant to die. Fungicides can either be contact, translaminar, or systemic. Few fungicides move to all parts of a plant. Some are locally systemic, and some move upwardly. Most fungicides can be bought in either the solid or a liquid form. Examples of fungicides are azoxystrobin, bitertanol, thiram etc. Fungicide residues have been found on food for human consumption, mostly from post-harvest treatments. The goal of this research is to take known fungicides and, using molecular modeling, modify these molecules in order to identify fungicides 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 Arkansas' economy. We will use the parameters computed in the quantum mechanical molecular modeling, along with the known binding affinities (IC50) 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 fungicides. We will make approximately 200+ modifications to the known fungicides. This should provide several molecules that will have superior "fungi-killing" properties but with much less environmental toxicity.

Incorporation of bioactive compounds from Melaleuca Alternifólia essential oil in pea, potato and rice starch films Farayde Matta Fakhouri1, farayde.matta@upc.edu, Justin O. Zoppe1, Vitor Augusto Garcia2, José I. Velasco1. (1) Materials Science & Engineering, Univ. Politecnica de Catalunya, Terrassa, Barcelona, Spain(2) Faculty of Agricultural Sciences, Sao Paulo State Univ., Botucatu, Brazil In recent years, a growing number of research activities involving packaging from renewable resources have been reported due to increasing environmental awareness regarding the impact of the disposal of materials from non-renewable sources. The essential oil of Melaleuca alternifolia, also known as the essential oil tree, has antimicrobial characteristics and antioxidants, which explains its wide use in research. The Melaleuca essential oil components, such as monoterpenes and sesquiterpenes, may present bioactivity, depending on its application. The incorporation of essential oils into edible films may be an alternative for maintaining antimicrobial and antioxidant characteristics, which are otherwise lost upon extensive processing. In the elaboration of bio-based films, some unconventional starches, such as from peas, potato and rice, present desirable characteristics in terms of processability. The objective of this work was to produce starch-based films from those unconventional sources and to incorporate different concentrations of Melaleuca A. essential oil (MEO) and evaluate the chemical characteristics by Gas Chromatography–Mass Spectrometry (GC-MS). Starch films were produced using a casting technique. The Melaleuca alternifolia essential oil presents several monoterpenes and sesquiterpenes, such as Terpine-4-ol, γ-Terpinene and 2-Carene, which attribute bioactive activity and after their incorporation into pea and rice, these compounds were not lost during processing and their concentration could be increased up to 30% wt. Thus, pea and rice films incorporating essential oil may be an alternative for the production of packages rich in bioactive compounds.

Mechanical properties of flexible films based on pea starch and cellulose nanocrystals produced by blown film extrusion Amanda Dambros2, Fabio Yamashita3, Justin O. Zoppe1, jozoppe@gmail.com, José I. Velasco1, Farayde Matta Fakhouri1. (1) Materials Science & Engineering, Univ. Politecnica de Catalunya, Terrassa, Barcelona, Spain(2) Lantmannen, Stockholm, Sweden(3) Univ. Estadual de Londrina, PR, Brazil Biodegradable and edible films can be used in food products to reduce moisture loss, to limit the oxygen absorption, to reduce the migration of lipids, to improve the mechanical properties and to provide physical protection, or to offer an alternative to the traditional packaging materials. Cellulose nanocrystals (CNC) have been extensively studied as a reinforcing filler in polymer matrices due to their desirable mechanical properties. The objective of this work was to elaborate a flexible film by blown film extrusion, based on pea starch with cellulose nanocrystals (CNC) as reinforcement, and to evaluate their mechanical properties. The cellulose nanocrystals were produced via acid hydrolysis and lyophilized. The flexible films based on pea starch, 25% glycerol as plasticizer (with respect to starch mass) and 1% CNC were successfully prepared, as well as a film without CNC addition. The samples were evaluated and the tensile strength increased when CNC was added in relation to the control sample (approximately 11.70 and 9.25 MPa, respectively), an increase of approximately 26%. However, the elongation at break decreased when CNC was added in relation to the control sample (approximately 68,15 and 309.28%, respectively).

Research on changes in aroma components derived from citrus essential oils in beverages by time passing Takeshi Sugawara, takeshi_sugawara@t-hasegawa.co.jp, Tadashi Yoshimoto, Kazuya Fukushima, Naoko Tanaka, Norio Miyazawa, Susumu Ishizaki. Hasegawa Koryo Kabushiki Kaisha, Chuo-ku, Tokyo, Japan Citrus essential oils are widely used as the most important ingredient for flavoring beverages. The aroma is highly desirable due to its naturalness and complexity. However, it is known that some aroma components derived from citrus oils are easily converted into other compounds in beverages. For example, citral, a characteristic aroma component of lemon, changes to p-methylacetophenone and p-cresol in acidic drinks, causing an unpleasant off-flavor. Therefore, the problem to be solved is to control changes in aroma components derived from citrus oils. Citrus essential oils are composed of a variety of volatile compounds. However, there are few studies that have investigated the increase or decrease of the multiple aroma components of citrus oils in beverages on the same time. In this study, we analyzed the change in aroma of three types of citrus essential oils (lemon cold pressed (CP) oil, orange CP oil, and lime distillated oil) during storage in four kinds of carbonated beverages(without(wo/)sugar-wo/acid, wo/sugar-with(w/)acid, w/sugar-w/acid, w/sugar-w/acid-w/ethanol), and report the changings of the aroma components. Each beverage was subjected to liquid-liquid extraction by adding an internal standard substance, and the extractions were performed immediately after preparation (0 weeks), and subsequent storage (25 degrees; 2 weeks, 4 weeks, and 8 weeks). The aroma extracts were analyzed by GC-MS to clarify the rate of change of various characteristic components of citrus essential oils. As a result, although there were no major differences in the changes of aroma compounds in beverages, there were differences in the degree of increase and decrease among the three types of citrus essential oils. Linalool, which has a floral aroma characteristic of citrus fruits, slightly increased in lemon oil, but decreased in orange and lime oils. The difference is thought to be due to differences in the aroma components of lemon, orange and lime essential oils other than linalool.

Characterization of metabolome alterations in barley (Hordeum vulgare L.) induced by Bipolaris sorokiniana Lisa Kurzweil, lisa.kurzweil@tum.de. Technische Univ. Munchen, Bayern, Germany Spot blotch caused by Bipolaris sorokiniana (teleomorph Cochliobolus sativus) is one of the most common foliar diseases of barley (Hordeum vulgare L.) worldwide and responsible for major losses of crop yield. Breeding resistant barley varieties has proven to be an effective countermeasure for protecting agricultural production. Plants react to pathogen attack by the upregulation or biosynthesis of secondary metabolites as one of their molecular defense strategies. So far, quantitative trait loci (QTL) affecting resistance against spot blotch have been mapped, but the molecular understanding of the metabolic defense responses in the plant still needs to be included. In this project, molecular marker compounds for an infection of barley with Bipolaris sorokiniana are examined by means of untargeted UPLC-TOF-MS metabolomics and lipidomics techniques. By the analysis of quantitatively resistant and susceptible barley genotypes, metabolites are identified and quantified that activate resistance on a molecular level. Co-chromatography with reference substances, chemical synthesis and chromatographic isolation followed by UPLC-TOF-MS, LC-MS/MS and 1D/2D-NMR experiments revealed the chemical structures of key phytochemicals. Their localization in the infectious hotspots were further mapped using desorption electrospray ionization mass spectrometry imaging (DESI-MSI). We examined changes in the metabolism of fatty acids, fatty acid oxidation

products as well as defense-related secondary metabolites, such as hordatines, phenolamides and flavone glucosides. These metabolites can serve as biomarker molecules in screening plants for disease and resistance. The combination of known genetic and novel metabolic understanding of plant-pathogen interactions and resistance meachanisms is essential for purposeful breeding of resistant barley cultivars in the future.

Biochar-Metal Organic Framework (BC-MOF) composites for the removal of rice fungicide(s) from water: An experimental and molecular simulation-based evaluation Chavali Sai kumar Reddy, bunnyreddychavali199@gmail.com, Neera Singh, Tirthankar Banerjee, Abhishek Mandal. Agricultural Chemicals, Indian Agricultural Research Inst., New Delhi, Delhi, India To investigate the potential groundwater contamination caused by three rice fungicides (tricyclazole, isoprothiolane, and carbendazim),we synthesised novel porous composites called Biochar-Metal Organic Frameworks (BC-MOFs). Specifically, we created Cu-BTC@BC, Fe-BTC@BC, MIL-53(Al)@BC, MIL88b-Fe@BC, and ZIF-8@BC. The BC-MOFs were subsequently subjected to characterization techniques, including (XRD), (FT-IR), (SEM), (DLS), and zeta potential analysis. The results obtained from Grand Canonical Monte-Carlo (GC-MC) simulations and in-silico adsorption experiments indicate that MIL88b-Fe@BC, MIL-53Al@BC, and ZIF-8@BC composites exhibit exceptional sorption potential for both single and ternary solute systems. The maximum capacities for adsorption of tricyclazole, isoprothiolane, and carbendazim, when present as single solutes, were found to be higher on MIL-53Al@BC (ranging from 98.97% to 99.94%) compared to MIL-88b-Fe@BC (ranging from 81.64% to 99.83%).In ternary, The MIL-53Al@BC compound exhibited a range of 75.3-99.4% efficiency, while the MIL88b-Fe@BC compound demonstrated a range of 64.1-97.8% efficiency in a 1 ppm aqueous solution. The confirmation of the adsorption of the rice fungicide onto the surface of BC-MOFs was achieved through the utilisation of (FTIR) and (XRD) spectroscopy techniques. The investigation on reusability indicated that MIL-53(Al)@BC exhibited superior regenerative properties for tricyclazole (90%) and isoprothiolane (approximately 80%) compared to other BC-MOFs. In the validation studies conducted using BC-MOFs, it was determined that MIL-88b-Fe@BC and MIL-53Al@BC exhibited superior performance in removing tricyclazole. Similarly, in the case of carbendazim, Cu-BTC@BC demonstrated a removal efficiency of 90.8%. Lastly, for the removal of isoprothiolane, MIL-53Al@BC exhibited a removal efficiency of 99.09%. These findings highlight the efficacy of MIL-88b-Fe@BC and MIL-53Al@BC composites in the purification of Hindon river water from these specific contaminants. Hence, it can be inferred that these newly developed BC-MOF composites exhibit potential adsorbents for the adsorption of tricyclazole, isoprothiolane, and carbendazim. In the future, it would be of great scientific interest to investigate the potential of BC-MOF composites as adsorbents for the effective removal of soil-water polluting pesticides, which are versatile foundation for various applications pertaining to the environment and energy.

Aflatoxin mitigation effect of 2,5-Diketopiperazines on Aspergillus flavus from Louisiana Mallika Kumarihamy, Geromy Moore, Yingqing Guo, Rebecca Sweany, Carol Carter-Wientjes, Matthew Lebar, matthew.lebar@ars.usda.gov. Food and Feed Safety Research Unit, USDA Agricultural Research Service, New Orleans, Louisiana Aflatoxin contamination from Aspergillus species (A. flavus and A. parasiticus) in food crops such as maize, peanuts, and various tree nuts is a significant global concern. Aflatoxins are highly toxic and carcinogenic metabolites detrimental to human and animal health. Additionally, adverse climate change will likely result in more contamination events. Application of nonaflatoxigenic A. flavus has been used as to mitigate aflatoxins in food crops, but biocontrol mechanisms are not fully understood. Preliminary screening of the extracts of the fermentation broth of nonaflatoxigenic A. flavus isolates from Louisiana showed a mitigating effect on aflatoxin production of aflatoxigenic strains, also isolated from Louisiana corn fields. Bioassay-guided fractionation of the extract led to the identification of proline-based 2,5-diketopiperazines (DKP) along with kojic acid as the main extrolites. Further investigation of one of the DKPs, Cyclo(L-Pro-L-Val), showed in vitro antiaflatoxigenic activity against toxigenic A. flavus strains at 2 mM concentration. Extrolites were identified by a mass spectrometry-based metabolomics (HPLC/MS QTOF) strategy through a global natural product social molecular networking (GNPS) platform. The production of diketopiperazines and other yet-to-be identified extrolites in nonaflatoxigenic A. flavus could contribute synergistically to its potential utility as a biocontrol agent.

Identifying sensory descriptors and aroma-active compounds in domestic edamame Rebekah Miller1, rebekahm20@vt.edu, Leah Hamilton2, Susan Duncan1, Thomas Kuhar3, Renee Boyer1, Bo Zhang4, Jacob Lahne1, Yun Yin1. (1) Food Sci. & Tech., Virginia Polytechnic Inst. and State Univ., Blacksburg, Virginia (2) Agricultural Research Station, Virginia State Univ., Petersburg, Virginia (3) Entomology, Virginia Polytechnic Inst. and State Univ., Blacksburg, Virginia (4) School of Plant and Envir. Sci., Virginia Polytechnic Inst. and State Univ., Blacksburg, Virginia A continued increase in US edamame consumption has created opportunities for domestic edamame development and production. Domestically bred and produced edamame, as they adapt to growing environment, are known to be more advantageous to the local growers and consumers. Research into the sensory and flavor attributes of domestic edamame is currently limited to edamame cultivars developed abroad and imported for use or consumption. This project worked to develop a list of sensory descriptors important to the domestic edamame market and identify aroma-active compounds contributing to these characteristics. Four edamame varieties (VT-Sweet, UA-Kirksey, Midori Giant, Chiba Green) were chosen based on commercial availability and grown at 3 locations (Blacksburg, VA; Painter, VA; Portageville, MO) providing replications. Two additional samples were purchased from a local grocery store. A general descriptive analysis (DA) sensory panel with 8 trained panelists developed a list of 27 edamame characteristics including taste, flavor, and texture attributes, and evaluated all edamame samples in triplicate based on the characteristics determined. Gas chromatography-olfactometry (GC-O) was completed by 7 additional panelists who were trained on 12 identified aroma-active compounds in edamame from literature and preliminary research. Pseudomixed ANOVA showed 12 of the identified characteristics through DA to be significantly different ($p<0.05$) between varieties including 3 taste attributes (“umami”, “sweet”, “bitter”), 6 aroma attributes (“fresh”, “salad”, “grassy”, “vegetable oil”, “alcohol”, “burnt toast”), and 3 texture attributes (“hardness”, “crunchy”, “juicy”). GC-O results underwent Kruskal-Wallis test revealing oct-2-enal as the sole compound displaying significant variability ($p<0.05$) across edamame varieties. Significant differences identified in taste, flavor, and texture suggested a diversity of sensory characteristics currently present in the domestic edamame market. The application of these sensory findings could help support further breeding and additional product development as domestic edamame production continues to flourish.

Does condensed tannin protect zein nanoparticles from digestion? Jules Jefferson, jefferj6@miamioh.edu, Sadeepa Mallikarachchi, Ann E. Hagerman. Chemistry and Biochemistry, Miami Univ., Oxford, Ohio Zein, the primary storage protein found in corn (maize) grain, forms nanoparticles on a carbonate scaffold

under anti-solvent conditions. These zein nanoparticles may be useful for drug delivery systems but the instability and digestibility of the particles limits their potential use. Tannins are high molecular weight polyphenols made by a variety of plants in leaves, fruits, flowers and roots. Tannins characteristically interact with protein by phenol-peptide hydrogen bonds and hydrophobic interactions. The two classes of tannin are hydrolyzable tannin (HT) and condensed tannin (CT, also known as proanthocyanidin). HT is made of galloyl groups linked with ester bonds to a core sugar, while CT is made of flavan-3-ol groups linked with carbon-to-carbon bonds. In earlier studies, the HT known as tannic acid was used to crosslink and stabilize zein nanoparticles. Condensed tannin has not been applied to nanoparticle synthesis. We coated zein nanoparticles with CT from cocoa bean, grape seed, or sorghum grain. Sorghum tannin (dp = 16) and cocoa tannin (dp = 4) are made up of (epi)catechin subunits and were quite pure. The grape seed extract contained monomeric flavan-3-ols as well as CT (dp = 4.5) comprising mixed subunits of (epi)catechin, (epi)gallocatechin and some 3-O-gallate esters. Digestibility was assessed in vitro with chymotrypsin using SDS-PAGE to monitor loss of the protein. Preliminary results showed that sorghum grain CT most effectively prevents digestion, with less protection by grape seed extract and much less by cocoa CT. We hypothesize that chain length and CT subunit composition both influence their interaction with the zein nanoparticles. Additional work with other CT might allow us to eventually tune the nanoparticle properties by using different tannins to achieve desirable properties.

Condensed tannin characterization by modified saw tooth HPLC system Kathryn Williams, will1233@miamioh.edu, Ann E. Hagerman. Chemistry and Biochemistry, Miami Univ., Oxford, Ohio Tannins are natural polymers that have broad applications in health, Envir. Sci., and agriculture. Of the two main classifications, condensed tannins (CT, also known as proanthocyanidins) are flavan-3-ol polymers with diversity in monomer identity, in interflavan bonding and in chain length. In reversed phase HPLC systems, CT gives large unresolved peaks, known as the "CT hump", which reveals nothing about the purity or structural details of the polymers. In this research, we examined the ability of a modified solvent system that was developed for synthetic organic polymers, on separations of sorghum, cocoa, blackbrush and bitter bush CT. In this gradient system each increment of increase in organic mobile phase is followed by a smaller decrease in organic phase, yielding a "zig-zag" pattern of increasing solvent strength. The system was optimized to transform the CT hump into 4-5 well resolved symmetrical peaks with different peak area patterns for each CT tested. However, the mechanism of the separation is still not well understood. In our study, two hypotheses were tested. The first dealt with classical adsorption of compounds to the column. Columns of differing alkyl chain lengths were used to investigate the interaction of the CT to the stationary phase. The second was based on compound aggregation and the prediction that aggregated compounds would not elute until the mobile phase solvent forced them to dissolve. Information obtained from Dynamic Light Scattering was used to alter the sample conditions to promote varying degrees of aggregation (or disaggregation). In comparing the effects of these changes on chromatogram patterns for CT, we hope to elucidate the mechanism behind their separation. Better separations and understanding of CT structure would benefit biomedical, food and biotechnology industries.

Evaluation of MIB and GSM reactivity using solid phase microextraction-GCMS Wayne Roussell2,1,3, wroussell1@nicholls.edu, Rebecca A. Adams Dupre1, Brennan Smith1. (1) USDA Agricultural Research Service, District of Columbia (2) Oak Ridge Inst. for Science and Education, Tennessee (3) Nicholls State Univ., Thibodaux, Louisiana Analysis of volatiles in water and food systems using solid phase microextraction (SPME) coupled to GCMS is a popular approach, particularly in the study of 2-methylisoborneol and geosmin. 2-Methylisoborneol (MIB) and geosmin (GSM) are odorous volatiles, attributing a “musty and earthy” taste to foods like fish, wheat, and wine. Because these compounds contribute to undesirable flavors in products, development of effective and efficient methods for removal of MIB and GSM would be beneficial for both agricultural and aquacultural industries. When measured by SPME-GCMS, MIB and GSM responses vary significantly depending on the environment of the sample solution. This study investigates how different variables, such as ionic strength and solvent composition, affect signal response of MIB and GSM. Attenuated MIB and GSM signal can be caused by chemical decomposition or by affecting fiber adsorption equilibrium in SPME. Distinguishing the two causes of attenuated signal is important in studies of MIB and GSM degradation. Innocuous salts used to increase ionic strength have different abilities to “salt out” volatiles and thus increase SPME efficiency. For example, use of MgSO4 in place of NaCl decreases MIB signal 2.5-fold. Biphasic solvent ratios (oil/water) greatly influenced the MIB and GSM signal, with behavior suggesting an effect on SPME equilibrium. Low pH values also decreased MIB and GSM signals. Byproduct formation and reversibility of the effects were studied to elucidate the mechanism of attenuated signal.

GC-MS determination of sterols in dried morel mushrooms Thomas W. Nalli, tnalli@inona.edu, Alix Overgard, Sumar Quint, Natalie Y. Walker, Chun W. Chu. Chemistry, Winona State Univ., Minnesota In this paper we report that commercially procured dried morel (Morchella) mushrooms have substantially similar sterol profiles to those reported previously for fresh morels with both types containing significant proportions of ergosterol 1 (17-33%), brassicasterol 2 (38-61%), and campesterol 3 (4-8%) as well as a number of other sterols (4-11). However, we only detected trace amounts (<0.5%) of two sterols reported in significant amounts (2-4%) in fresh morels, ergosta-5,7-dienol 4 and ergosta-7-enol 5,. A previously unidentified sterol reported in relatively high amounts (5-16%) in fresh morels was also detected (4-26%) and identified as 24-methylenecholesterol 6. Furthermore, five other previously unidentified morel sterols were identified as ergosta-5,22,24(28)-trienol 7, episterol 8, epiergosterol 9, ergosta-5,7,9(11),24(28)-tetraenol 10, and ergosta-5,7,9(11),22-tetraenol 11. The amount of the extremely rare sterol 7 was highly variable (mean = 4.0%, σ = 4.2, n = 30) and its presence in larger relative concentrations (6-11%) was associated with samples described as “sun dried” or as “burn” morels.

Almond shells: A natural bio-absorbent for reducing and recovering the phenolic content of winery wastewaters Elyse Doria1, eldoria@ucdavis.edu, Larry A. Lerno2, Alyson E. Mitchell1. (1) Food Sci. & Tech., Univ. of California Davis (2) Viticulture and Enology, Univ. of California Davis Almonds and wine are two of California’s largest exported goods. Both commodities generate enormous amounts of agroindustrial waste annually, including almond shells and winery wastewater (www) rich in phenolics. Finding new uses for these agroindustry wastes is critical for industry sustainability. Herein, we evaluate the use of powdered almond shells (asp) as an inexpensive and abundant bio-absorbent to decrease the financial impact, energy demand, and use of chemicals to reduce phenolics in www. A factorial design and surface area response plots were used to evaluate and optimize five binding parameters of the asp: asp to www ratio, asp particle size, contact time, pH of www, and water pretreatment of asp. Of these, asp particle size and asp to www ratio were critical factors in improving the phenolic binding capacity of the asp. Moreover,

phenolic compounds can be recovered from the asp with ethanol. ASP effectively reduced the phenolic concentration in model winery wastewater and may provide a new source for value-added compounds.

Chemical composition of different extracts of Conyza bonariensis Melissa Estrada1, mestrada141@toromail.csudh.edu, Isabelle Fabing2. (1) California State Univ. Dominguez Hills College of Natural and Behavioral Sciences, Carson (2) Univ. Toulouse III-Paul Sabatier, France The nematode, a parasite that attaches to plants, has a negative impact on agricultural production. Each year, this results in an estimated loss of yield of more than $80 billion worldwide. Unfortunately, fewer crops are edible because they do not survive this parasite. The overall objective of this research is to identify a specific compound from the endemic plant of Togo, Conyza Bonariensis, and to optimize the extraction method of this compound. Conyza Bonariensis was used because it was previously shown to have potential insecticidal and nematicidal activities. To initiate the research, four different extraction methods were used to obtain the crude extract of the dried plant: by a Soxhlet extractor, one by Clevenger, by sonication, and finally by supercritical fluid extraction (SFE). All the extracts were analyzed by ultra-high performance liquid chromatography (UHPLC) coupled with a photodiode array detector (PDA) and mass spectrometer (ESI-SQD). The compound of interest was detected, but it is now necessary to be able to extract it in large quantities or synthesize it in order to effectively combat nematodes.

Formation mechanisms and potential toxicity of oxidized triacylglycerols in food during thermal processing Hanshu Zhu1, Chenxu Wang1, Boyan Gao1, raphaelgao1985@gmail.com, Liangli Yu2. (1) Shanghai Jiao Tong Univ., Shanghai, China(2) Univ. of Maryland, College Park Oxidized triacylglycerols are significant byproducts that occur during lipid oxidation, yet their formation mechanisms and potential toxicology remain poorly understood. In this study, we investigated the oxidation progress of model compounds triolein and trilinolein. The oxidized products of these compounds were tentatively identified using UPLC-Q TOF MS. The mixture of oxidized triolein was orally administered to mice for a 90-day toxicity evaluation. Results showed that approximately 30% of triolein was oxidized after being heated at 180°C for 6 hours, yielding predominantly peroxide and epoxidate products. Trilinolein exhibited an oxidation rate exceeding 50% under the same thermal conditions. Regarding toxicity, oxidized triacylglycerols demonstrated slight hepatotoxicity, as evidenced by metabolomic differences in plasma and liver samples compared to the control groups. While this study sheds light on the formation mechanisms and potential toxicology of oxidized triacylglycerols, further research is necessary to elucidate the underlying toxicity mechanisms.

Nano-based modification of phosphorous fertilizers: A path towards sustainable phosphate supply Shirsa Mazumdar1, shirsa.mazumdar@ndsu.edu, Mohiuddin A. Quadir2, Achintya N. Bezbaruah1. (1) Civil, Construction and Environmental Engineering, North Dakota State Univ., Fargo (2) Coatings and Polymeric Materials, North Dakota State Univ., Fargo Phosphorus (P) is an essential nutrient for optimum plant growth and development. However, the conventional application of phosphorus fertilizers is characterized by low plant use efficiency (PUE) and environmental pollution. As phosphorus is crucial for crop production, our hypothesis posits that nano phosphatic fertilizers will enhance PUE and also effectively manage phosphorus runoff and leaching. In this research, we employed a high-energy ball mill to grind commercially available rock phosphate (RP) fertilizer, reducing its particle size to the nano-scale. Subsequently, we applied a layer-by-layer (LbL) deposition technique to coat these nano-sized RP particles with biodegradable polymers, including positively charged chitosan and a proprietary polymer. This coating strategy is aimed to achieve controlled release of P from the nano RP. The adhesion between the polymer layers was strengthened through physical crosslinking via electrostatic interactions between the negatively and positively charged groups on both the polymers. Characterization of the coated RP fertilizers was conducted using zeta potential measurements, Fourier transform infrared (FTIR) spectroscopy, and surface morphology studies, such as scanning electron microscopy (SEM). Furthermore, we investigated the release kinetics of P from the coated nano RP particles in distilled water over time. Our findings revealed that the initial chitosan coating effectively reduced P leaching, serving as a physical barrier. The subsequent coating with our proprietary polymer facilitated higher release of P than the control in a regulated manner over a long duration of time, thus would be supporting plants both during the early growth stages and their later development as well.

Cultural management and applications of Ocimum tenuiflorum (Holy Basil) grown in MarylandEzra Cable, eecable1@umes.edu, Henriette Den Ouden, Victoria Volkis. Natural Sciences, Univ. of Maryland Eastern Shore, Princess Anne Ocimum tenuiflorum, also known as Holy Basil, is a native plant in many Asian countries, especially India, where it plays a central role in Aurovedic medicine. It has been shown previously that holy basil can be grown in some parts of the US. However, the phytochemical composition of its extract is different from the one grown in India, and strongly depends on climate zone. This project is focused on cultural management and applications of holy basil grown in Maryland on the Eastern Shore. This study seeks to identify the yield and composition of essential oils and terpenes extracted by wet distillation and processed for applications in herbal medicine, as a natural pesticide, and as an active agent in antifouling protection formulations. Five subspecies of Ocimum tenuiflorum with four different soil types will be compared to see which yields the highest amounts of essential oils, as well as which part of the plant will provide the highest yield of essential oils. Phytochemical analysis of extracts and wet distillation crude oils, as well as the activity of these extracts in different applications will be discussed.

Protective effects of Citrus depressa peel extract on non-alcoholic fatty liver disease in mice fed a high-fat diet Zheng-Yuan Su1, zysu@cycu.edu.tw, Xuan-Ru Chen1, Guor-Jien Wei2. (1) Chung Yuan Christian Univ., Taoyuan City, Taiwan(2) National Yang Ming Chiao Tung Univ. - Yangming Campus, Taipei, Taiwan Citrus depressa (CD) contains an abundance of polymethoxyflavones (PMFs), including Nobiletin and Tangeretin. Its potential health benefits, such as anti-inflammatory, anti-cancer, and anti-atherosclerosis effects, have been highlighted by current research. This study aims to explore the protective effects and mechanisms of CD peel ethanolic extract (CD-EE) and its active components against non-alcoholic fatty liver disease induced by a high-fat diet in C57BL/6 mice. The mice were divied into the control group, high-fat diet group, low-dose CD-EE group (250 mg/kg body weight), high-dose CD-EE group (500 mg/kg body weight), Nobiletin group (50 mg/kg body weight), and Tangeretin group (50 mg/kg body weight). After 18 weeks of administration, the results revealed that both the low and high-dose CD-EE groups, as well as the Tan and Nob groups, demonstrated the ability to alleviate liver damage resulting from fat degeneration. The activity of AST and ALT in the blood was significantly decreased. Additionally, these interventions effectively reduced the size of lipid droplets that had accumulated in the liver. The low and high-dose CD-EE groups, along with the Tan and Nob groups, also ameliorated obesity induced by a high-fat diet, mitigated intermittent

weight gain, and suppressed the formation of adipose tissue. The findings of this experiment can be utilized to enhance the economic value of citrus fruit in the agricultural sector and contribute to the development of health products.

Plant maturity affects the phenolic composition and antioxidant properties of green basil (Ocimum basilicum L.) cultivars Holly P. Lawson, lawsonh@southwestern.edu, Emily D. Niemeyer. Chemistry and Biochemistry, Southwestern Univ., Georgetown, Texas Basil, a well-known herb of the Lamiaceae family, is noted for its antioxidant properties and ability to produce phenolic compounds. In the diet, these compounds have a variety of anti-inflammatory and other health benefits because of their ability to quench free radicals, relieving oxidative stress within the body. However, it is unclear how concentrations of phenolic compounds change over time throughout the development of the basil plant, and this information could be particularly useful in understanding the ideal harvest time for the herb. In this study, three cultivars of green basil, 'Tuscany,' 'Genovese,' and 'Spicy,' were harvested weekly over a period of 97 days to determine how phenolic composition and antioxidant properties are affected by plant growth. The total phenolic content (TPC) of the basil samples was measured using the Folin-Ciocalteu method, the antioxidant properties of the basil plants were determined using the cupric ion-reducing antioxidant capacity (CUPRAC) and the oxygen radical absorbance capacity (ORAC) assays, and high-performance liquid chromatography (HPLC) was used to identify and quantify individual phenolic compounds. Initial results show that harvest date significantly affected TPC values ($p < 0.001$). The total phenolic content for the first basil harvest at 15 days after germination was significantly lower than the TPC values for the last harvests, implying that phenolic content increases with basil plant maturity. Additionally, among the three cultivars in this study, phenolic content was affected differently by harvest date. This presentation will discuss the changes in antioxidant properties and phenolic composition that occur throughout the growth of these green basil cultivars, providing important information about when to harvest basil to optimize the dietary benefits of this popular herb.

Influence of cultivar and seed source on the phenolic composition and antioxidant properties of Monarda herbs Holly P. Lawson, Emily D. Niemeyer, niemeyee@southwestern.edu. Chemistry and Biochemistry, Southwestern Univ., Georgetown, Texas Lamiaceae herbs have been used for both culinary and medicinal purposes since antiquity. Even today, they are widely recognized for their value in producing essential oils, pharmaceutical ingredients, and flavoring agents. There have been numerous studies investigating the phenolic content and antioxidant properties of various Lamiaceae herbs; however, research has primarily focused on the more popular members of the family including basil, thyme, oregano, and mint. Monarda is a genus within the Lamiaceae family containing plants that are particularly noted for their high total phenolic contents, yet few comprehensive studies of the phenolic composition and antioxidant properties of Monarda species exist. In this study, seven Monarda cultivars, commonly known as bee balms, were grown under identical conditions using seeds purchased from four different commercial sources. Mature plants were analyzed using the Folin-Ciocalteu method to determine their total phenolic content, and their antioxidant properties were quantified with the cupric ion-reducing antioxidant capacity (CUPRAC) and the oxygen radical absorbance capacity (ORAC) assays. Additionally, high-performance liquid chromatography was used to characterize the individual phenolic compounds within each cultivar. This presentation will provide an overview of the similarities and differences in phenolic composition and antioxidant properties among Monarda cultivars, giving important insights into which varieties have promising antioxidant profiles for use in culinary, medicinal, and other applications.

Comparison of Headspace GC-MS techniques to characterize volatile phenols contributing to smoke taint in Pinot Noir wines Stephen J. Toth, stephen.toth@iff.com, Ashley Noble. R&D, International Flavors & Fragrances Inc, Union Beach, New Jersey A series of volatile phenols originating from smoke tainted grapes exposed to regional fires have been known to exhibit undesirable sensory characteristics such as smoky, burnt, ashy and medicinal flavoring in affected wines. This can be negatively perceived by consumers and often leads to an aftertaste of these characteristics lingering in the mouth after the wine has been swallowed. Wildfires plagued the counties in northern California and Oregon during the 2020 wildfire season from August through October. These fires severely impacted the grape harvest and challenged wine makers as many of their vineyards were either destroyed or their crops were contaminated with smoke taint. Numerous wineries opted to release limited amounts of 2020 Pinot Noir for this reason or produce rosé or white wines from affected grapes. Our research will look specifically at three different vintages (2019, 2020 and 2021) of Pinot Noir from the same vineyard in the Willamette Valley region of Oregon. It should be noted that "smoke" as an indicator of taste in wines is not always an indicator of smoke taint but can also be imparted into the wine by aging in oak barrels. We will compare headspace based GCMS techniques to characterize these wines and profile the volatile phenol content (cresols, methyl guaiacols, guaiacol, and syringol). Solid phase micro extraction (SPME) and stir bar sorptive extraction (SBSE) will be used to analyze both free volatile content and gylcosidically bound phenolic content. The free volatiles will be acquired in unaltered wine to best represent the consumer's initial experience. These samples will then experience a pH adjustment, sonication and heat treatment to release gylcosidically bound phenolic compounds which could potentially be released over time by aging the wine. Our research will characterize the phenolic compounds contributing to the smoke taint odor and flavor present in the Pinot Noirs against the sugar bound compounds that can potentially release over the shelf life of the wine utilizing SPME and SBSE extraction methods. Additionally, the comparison of vintages will indicate whether the phenolic characteristics obtained by GCMS can be used to capture the smoke defect in the wine profile from 2020.

Effects of thermal and non-thermal processing on allergen removal from pistachio shell waste Leila Fereidooni, leila.fereidooni@ku.edu, Ana Morais, Mark B. Shiflett. Chemical and Petroleum Engineering, Univ. of Kansas School of Engineering, Lawrence Pistachio (Pistacia vera L.) shells are the largest by-product of the pistachio industry and accumulate every year at harvest time. Applications for pistachio shells are needed. One example that may be promising is the use of pistachio shell powder as a functional ingredient in animal food. Pistachio shell powder contains several beneficial nutrients and compounds, such as dietary fiber, phytochemicals, minerals, proteins, and lignans. The presentation investigates the reduction of allergenic protein in pistachio shell powder for use as an ingredient in animal feed formulations. The overall goal is to diminish the IgE binding potential associated with pistachio shell allergens. Techniques that disturb the structure of allergens have the potential to reduce IgE binding and decrease the probability of experiencing food allergy reactions. The results of this study demonstrate that food processing (both thermal and non-thermal methods) can induce structural and/or conformational changes in proteins, thereby altering their allergenic capacity. The allergen content of pistachio shell powder was reduced from 5000 ppm to 20 ppm in this experimental work.

Assessing the biosynthetic inventory of the biocontrol fungus Trichoderma afroharzianum T22 Wenyu Han1, wenyuhan0609@gmail.com, Zhongshou Wu3,4, Zhenhui Zhong3,4, Jason Williams1, Steve Jacobsen3,4,5, Zuodong Sun2, Yi Tang2,1. (1) Chemistry and Biochemistry, Univ. of California Los Angeles(2) Chemical and Biomolecular Engineering, Univ. of California Los Angeles(3) Molecular Cell and Developmental Biology, Univ. of California Los Angeles(4) Howard Hughes Medical Inst., Univ. of California Los Angeles(5) Eli & Edythe Broad Center of Regenerative Medicine & Stem Cell Research, Univ. of California Los Angeles Natural products (NPs) biosynthesized from biocontrol fungi in the rhizosphere can have both beneficial and deleterious effects on plants. Herein, we performed a comprehensive analysis of natural product biosynthetic gene clusters (BGCs) from Trichoderma afroharzianum T22 (ThT22), which has long been utilized as biofertilizer and biocontrol agent for agricultural purposes. This fungus encodes at least 64 BGCs, which are proposed to encode plant-beneficial NPs. Although ~400 NPs have been isolated from Trichoderma, only seven compounds and four BGCs were previously characterized or genome-mined from ThT22. We correlated 21 BGCs of ThT22 with known primary and secondary metabolites through homologous BGC comparison and characterized one unknown BGC involved in the biosynthesis of eujavanicol A using heterologous expression. In addition, we performed untargeted transcriptomics and metabolic analysis to demonstrate the activation of silent ThT22 BGCs via the “one strain many compound” (OSMAC) approach by growing ThT22 on six different media, five of which were not reported for ThT22 NP isolation. Collectively, our analysis showcases the biosynthetic capacity of ThT22 and paves the way for fully exploring the roles of NPs of ThT22 in plant-fungi interactions.

Investigation of natural polyphenols as potential colorectal cancer (CRC) therapeutics Jaden Kardos, Thomas Rennie, trennie@wvstateu.edu, Jasmine Porter. Chemistry and Physics, West Virginia State Univ. College of Natural Sciences and Mathematics, Inst. Colorectal cancer (CRC) is the third most common type of malignancy that affects many individuals worldwide and is a leading cause of cancer mortality. Although this multifactorial disease is one of the most preventable cancers globally, treatments have been restricted due to their acquired chemoresistance and side-effect toxicity. Due to these limitations, novel anti-tumor strategies that reduce toxicity and improve tumor cells' chemosensitivity are necessary. One approach implemented in the design of adequate CRC clinical trials is combined drug therapy of anticancer drugs with natural compounds. Literature has shown significant benefits in CRC patients who combine natural dietary polyphenols with conventional chemotherapy. This pilot study aims to investigate phenolic compounds derived from parsley and assess their biological activity. Polyphenols from this plant source were extracted using various methods, followed by their phenolic content determined through the Folin-Ciocalteu assay. Phytochemical screening was conducted to identify the various classes of phytoconstituents in the crude extracts. The individual components of each crude extract were purified and analyzed via HPLC. The growth inhibition of each isolated phytochemical will be screened in vitro against human colorectal adenocarcinoma cells (HT-29) using an MTT bioassay. Based on this preliminary data collected, the antioxidant activity of each compound will also be assessed through a DPPH assay, and their antibacterial properties will be evaluated through a modified Kirby-Bauer disc diffusion method. Potential hit compounds will be further optimized through in silico studies to improve their biological efficacy.

Comparison of Logk', LogPoct and LogDoct values for the catechol flavones William L. Whaley1, whaley@tarleton.edu, Marcus Gregory2, Taryn Gibbs3, Sara Tuck4. (1) Chemistry, Tarleton State Univ., Stephenville, Texas(2) Chemistry, Univ. of North Texas, Denton(3) Nuclear Engineering, Oregon State Univ., Corvallis(4) Chemistry, Duke Univ., Durham, North Carolina Catechol flavonoids such as fisetin (3,7,3’,4’-tetrahydroxyflavone) and 7,8-dihydroxyflavone (7,8-DHF) have exhibited efficacy in preclinical models for several neurological diseases. For ingested catechol flavonoids to benefit brain conditions they must be absorbed in the small intestine, transported by the blood stream, and partition across the blood-brain barrier. The octanol-water partition coefficient (Poct) is a parameter for predicting the absorption, distribution, metabolism and excretion (ADME) properties of drugs. It is represented as LogPoct which is an index of the lipophilic character of a compound. A value of LogPoct between 1.38 and 1.80 is ideal for intestinal absorption, while a value near 2.00 is ideal to cross the blood-brain barrier. For phenolic compounds, LogPoct must be measured with an acidic aqueous phase to maintain the analyte in a single neutral form. Distribution coefficients (Doct), measured at pH values relevant to the digestive system, are also used to predict ADME properties. Flavone, the catechol flavones and 3,2’-dihydroxyflavone (3,2’-DHF) were assayed for chromatographic retention factor (Logk’), LogPoct (pH=1.5 and 3.0) and for LogDoct (pH=6.5, 7.4 and 7.8) values. The LogPoct values ranged between 2.87 (7,8-DHF) and 3.45 (flavone). Self-association was observed for 3,2’-DHF; however, estimates of LogPoct and LogDoct were obtained. LogDoct values for 3,2’-DHF and 7,8-DHF were lower than the LogPoct values due to ionization of hydroxyl groups with unusually low pKa1 values. These LogPoct and LogDoct values should facilitate the prediction of ADME properties for catechol flavonoids.

Beer we go! Analysis of carbonated and nitrogenated beers Alyx S. Frantzen, afrantzen@sfasu.edu, Sadie Atkins, Holly S. Gibson. Chemistry and Biochemistry, Stephen F Austin State Univ., Nacogdoches, Texas A flavorful crisp beer is a popular, worldwide beverage. Beer can be either carbonated or nitrogenated, each giving a different sensory outcomes. Carbonated beer, such as Budweiser, has a crispy and light texture, whereas nitrogenated beer, such as Guinness, has a creamy, smooth mouthfeel. A comparison study of these two different beer types was done using a Packaged Beverage Analyzer (PBA). The PBA is used to analyze the density, CO2, O2, N2, and alcohol contents of various beverages, such as beer, sparkling water, and soda. The carbonated beer chosen for analysis was Budweiser. It was readily available and came in different container types; aluminum can, aluminum bottle, and glass bottle. The parameters assigned to the carbonated beer were container type and the temperature at which it was stored. The carbon dioxide, oxygen, and alcohol contents were analyzed weekly over a six-month testing period for each different container type and storage temperature. In contrast, the parameters for the nitrogenated beer were container type and widget variation. The nitrogenated beers analyzed were varieties of Guinness and Left Hand Brewing Company. Consumers desire consistent tastes and longevity in their beverages, and these parameters could potentially impact the shelf stability and sensory outcomes of each type of beer.

Analyzing the effects of pulsed electric field in the winemaking process Matthew H. Lorentz, lorentzmatthew0150@gmail.com, Owen M. McDougal, Priscila Santiago-Mora. Boise State Univ., Idaho In recent years, research has increasingly focused on the application of Pulsed Electric Field (PEF) technology as a novel food processing technique, demonstrating its potential to revolutionize future wine production. This emerging technology has shown promise in expediting the vinification process and enhancing the extraction of desirable compounds, particularly polyphenols such as anthocyanins and tannins, during the maceration and

fermentation of Mouvedre grapes. These compounds significantly influence the unique chemical and sensory properties characteristic of red wine. This study aims to assess the presence of these polyphenols and measure total acidity, sugar content, and color in red wines. The PEF equipment was deployed on-site at a local winery in Garden City, Idaho, during the harvest production. Daily samples were collected over the initial 10 days to monitor dynamic changes using UV-visible spectroscopy analysis. During the maceration/fermentation process, notable increases were observed in the extraction of polyphenols, anthocyanins, tannins, and the enhancement of the wine's color pigment.

Analysis of flavor and aromatic compounds in whisky using both gas and liquid chromatography and mass spectrometry Emma Hendrix, eehendrix03@gmail.com, Christopher J. Monceaux. Chemistry, Radford Univ., Radford, Virginia Like any alcoholic beverage, whisky is known to have a broad range of flavors and aromatic components, which help to differentiate across brands and types. These components stem from how the whisky is made, how long it is aged, and what it is aged in. Before alcohol is ever aged, the biggest difference across types would be in the types of grain used. For example, in an Irish whiskey, the malt is composed most heavily of barley, while in most bourbons, the mash is consisted of approximately 50% corn. Aging times can usually be seen to dictate the price of the bottle, where shorter aged whiskies are usually cheaper. And the barrel that the alcohol is aged in is used to distinguish type, but also can be original to brand. All these factors play a role in the compounds that make up the alcohol, and thus, the taste and smell of the alcohol in the finished product, in theory. By using gas chromatography and liquid chromatography, coupled with mass spectrometry (GC/MS and LC/MS), these compounds that make each brand and bottle unique can be identified. This project used a wide variety of types and brands of whiskey to determine what compounds make each bottle unique and different from the rest of the market, spanning from well-known brands to small distilleries. The compounds that were identified in each bottle were compared to the flavor and aromatic profile of the whisky, to demonstrate how the chemistry of the whisky matched the consumer expectation for taste and smell.

Lipoxygenases in Costa Rican soybean seeds: Influence on oil nutritional profile Laura Vega Fernandez, laura.vegafernandez@ucr.ac.cr, Andrea Holst, Hans-Peter Mock, Andrea Irias-Mata. Center for Research in Grains and Seeds (CIGRAS), Universidad de Costa Rica, San Jose, In recent years, agriculture has been challenged to migrate to agricultural sustainability, meeting the needs of the present without compromising the future. It means not only contributing to the three dimensions of sustainability (environmental, social, and economy), but also to the four pillars of food safety (availability, access, usability, and stability). Soybeans are one of the most important crops in the world, with high demand due to their nutritional value. However, soybeans have a strong "beany" flavor that limits their direct consumption (only 2% is consumed directly of total production), struggling directly with food safety. This flavor is caused by lipid oxidation, which is catalyzed by enzymes called lipoxygenases (LOXs). LOXs combine with polyunsaturated fatty acids (PUFAs) to produce volatile compounds (VC), molecules that produce a rancid taste. Besides, the vitamin E inside the seed works as an oil stabilizer because works as a chain reaction terminator of polyunsaturated fatty acids (PUFAs); with the quality that one tocopherol molecule can act on the breakdown of the lipid peroxidation chain several times before degrading. Plant breeding has been used to develop soybean varieties with null or partially null LOXs, which have a lower production of VC that causes the rancid flavor. Molecular markers can be used to accelerate the selection process of these varieties. In Costa Rica, the Center for Research in Grains, and Seeds (CIGRAS) of the Univ. of Costa Rica (UCR), has a growing interest in developing Costa Rican soybean varieties for human consumption. This research aims to characterize the LOXs of the seeds of soybean varieties grown in Costa Rica and their influence on the fatty acid and vitamin E profile of their oil for human consumption. The use of molecular markers to characterize LOXs in Costa Rican soybean seeds could allow the selection of promising materials that are attractive to improve the quality of the oil of its seed. This research is aligned with strategic axes 1, 2, and 6 of the National Seed Policy of Costa Rica, objectives 2 and 12 of the United Nations Development Program, and finally, strategic axis 1 of the National Bioeconomy Strategy 2020-2030.

Discrimination of the geographical origin of various agricultural products by applying machine learning algorithms on data produced from different spectroscopic techniques John Kapolos1, jkapolos@teikal.gr, Konstantinos Papadimitriou2, Kalliopi Dalaklidi1, Athanasia Koliadima3, Marina Papadelli1. (1) Food Sci. & Tech., Univ. of the Peloponnese, Kalamata, Greece(2) Food Science and Human Nutrition, Geoponiko Panepistemio Athenon, Athens, Attica, Greece(3) Chemistry, Panepistemio Patron, Patra, Periféria Dhitikís Elládh, Greece Data from different spectrometric techniques as Fourier Transform Infrared (FTIR), Near Infrared (NIR), Nuclear Magnetic Resonarse (NMR) can be used as input to machine learning methods in order to clarify the geographical origin of various agricultural products. The authentication of foodstuffs has become a central challenge for all actors in food science, the food industry and consumers. For this purpose, non-destructive spectroscopy methods and emerging artificial intelligence tools canbe used. The aim of this study is to introduce a robust classification framework, combine data from spectroscopic techniques and machine learning algorithms for the authentication PDO products produced in the region of Peloponnese. The proposed machine learning framework by using either independently or combined Spectroscopic data with the aid of the nested cross fold validation scheme and adequate preprocessing of the raw data can serve as an efficient food authentication tool and generalize to new data as well, such as data from other food products or from other spectroscopic methods. Acknowledgment: This research has been co-financed by the European Union and Greek national funds through the European Regional Development Fund – ERDF and the Operational Program “Peloponnese 2021-2027” του NSRF 2021-2027 (MIS 6001408).

Algae as a precursor of seafood flavor in alternative seafood Ali Raza, araza@sdsu.edu, Ellie Cramton, Jesse Baker, Changqi Liu, Jing Zhao. School of Exercise and Nutritional Sciences, San Diego State Univ., California Algae is a sustainable protein source that has been increasingly incorporated into plant-based foods. Due to its inherent ocean-like odor, algae enrichment is a promising approach to delivering seafood-like flavors in alternative seafood. However, the aroma and taste of algae-enriched plant-based seafood remain unexplored. Our study aims to generate seafood-like flavors from algae through controlled protein hydrolysis and Maillard reactions. Instrumental analysis in combination with human sensory evaluation was used to identify flavor-active compounds. The aroma compositions of three kelp (Ascophyllum nodosum) and three microalgae (Arthrospira platensis, Chlorella vulgaris, and Dunaliella salina) powders were characterized using headspace solid-phase microextraction and gas chromatography-olfactometry-mass spectrometry (HS-SPME/GC-O-MS). Over fifty volatiles were detected, including pleasant aroma compounds such as D-limonene (citrus and fresh aroma) and 3-methyl-2-(2-methyl-2-butenyl)-furan (mint-like aroma), as well as undesirable volatiles like (E)-2-octen-1-ol (soap-like and plastic aroma). Numerous volatiles from seafood

were detected in the algae samples. For instance, 1-octen-3-ol, detected in all three kelp samples and A. platensis powder, delivers a mushroom and green aroma and serves as a key-aroma compound of crab, tuna, and salmon. Tetramethyl pyrazine, found in crab and shrimp and possessing a grassy and musty aroma, was detected in A. platensis and C. vulgaris. We further enhanced seafood-like flavor in algae through enzymatic and thermal treatments. Pretreating kelp with Flavoenzyme followed by heating it with ribose and cysteine resulted in Maillard reaction products with reduced bitter taste and a desirable crab cake-like and canned tuna-like flavor. New volatile compounds formed during the Maillard reaction included 1-(2-furanyl)-ethanone (nutty and almond-like aroma) and 5-methyl-2-furancarboxaldehyde (bread-like and coffee-like aroma). Our current study explored various Maillard reaction precursors and conditions to achieve diverse seafood-like flavors. Future research will delve into the mechanisms behind the formation of flavor-active compounds in thermally treated algae samples.

Isomerization of hop alpha acids during wort boiling Ian Hofland, ihofland@carrollu.edu, Michael D. Schuder. Carroll Univ., Waukesha, Wisconsin Alpha and iso-alpha acids were quantified to monitor concentrations throughout the wort boiling step in producing an IPA beer at a local microbrewery. The isomerization of alpha acids to iso-alpha acids during wort boiling contributes to the bitter taste in the final product. Alpha acid and iso-alpha acid samples taken at periodic times throughout the wort boiling stage were quantified using high pressure liquid chromatography (HPLC). A timeline of the concentrations of alpha acids and iso-alpha acids present throughout the wort boiling step was obtained using the results from the HPLC. Total conversion efficiency of hops added to iso-alpha acids in the finished beer were calculated.

Me**tabolomic analysis in organic and conventionally grown** elderberries Xavier Jones1, xavier.jones346@my.lincolnu.edu, Samira Mahdi1, Nadia Bostick2, Sarah J. Eber3, Nadia Navarrete-Tindall3, Ray Mu2, Qingbo Yang1. (1) Cooperative Research, Lincoln Univ. of Missouri, Jefferson City(2) Basic Sciences, Univ. of Health Sciences and Pharmacy, St Louis College of Pharmacy, Missouri(3) Cooperative Extension, Lincoln Univ. of Missouri, Jefferson City Organic produce has increasingly become the preferred choice in everyday food consumption because it avoids the use of chemical fertilizers, synthetic pesticides or other artificial substances, thereby improving food safety and being an effective practice to achieve sustainable agriculture. However, if Good Agricultural Practices (GAP) are not followed, the effectiveness of organic farming can be compromised, or even result in sub-standard food produced due to improper farming or management practices. Emphasizing the parallelism of GAP is equally or more important in traditional farming practices, especially among the underserved communities. Here, we report a continuous case study on elderberries (Sambucus canadensis) at Lincoln Univ. of Missouri. Through a developed metabolomic method via the state-of-the-art ultra-high performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS), we examined hundreds of small molecule compounds, including nutrients and contaminants. Results indicate that implementation of GAP is critical to achieving the desired nutritional quality and concentration of elderberries whether grown organically or conventionally. Notably, elderberries produced by conventional farming following GAP closely match the nutritional content of organically grown products. This once again illustrates the importance of implementing GAP and suggests that traditional agricultural products combined with GAP have sufficient nutritional content at relatively low prices, while maintaining the content of harmful chemicals below the threshold, and in some cases, do not contain harmful chemicals, as in some of the organic foods that lack GAP. The detailed results will be presented at the upcoming ACS Meeting. This study highlights the potential benefits of promoting GAP in conjunction with organic farming practices, while demonstrating the broad application potential of metabolomic methods in the field of food sciences and nutritional research.

Essential oils: A natural solution for preserving potato quality in storage Areej Alzarqaa, alzarqaa@oregonstate.edu, Valtcho Jeliazkov. Dept. of Crop and Soil Science, Oregon State Univ., Corvallis Potatoes (Solanum tuberosum), a vital global staple crop, require careful preservation during extended storage to ensure a year-round supply. Preventing potato sprouting during storage is crucial, as it threatens food security by contributing to increased food waste. Synthetic chemicals, with chlorpropham (CIPC) as the most widely used, have traditionally been employed to prevent potato sprouting. However, due to concerns about its impact on human health and the environment, CIPC has recently been banned in the European Union and other countries. Furthermore, CIPC and other synthetic chemicals are not permitted in certified organic production. While natural products have been used for sprout control in certified organic production, their use has been limited in conventional production systems. This study assessed 20 essential oils (EOs) and an untreated control to identify those capable of preventing potato sprouting in three potato cultivars (Terra Rosa, Ranger Russet, and Trail Blazer minitubers,) over a 90-day storage period at room temperature. Essential oils #179 and #184 emerged as the most effective in suppressing potato tuber sprouting. In addition, these two EOs showed the lowest percentage of weight loss relative to the control tubers in all three cultivars. These findings underscore the potential of essential oils #179 and #184 as efficient and environmentally friendly alternatives for potato sprout control during storage, offering promising solutions for sustainable potato preservation and reducing food waste.

Development of zein nanoparticles for encapsulating avocado seed extract as a functional ingredient Thanida Chuacharoen, thanida.ch@ssru.ac.th. Faculty of Science and Technology, Suan Sunandha Rajabhat Univ., Bangkok, Dusit, Thailand Avocado (Persea americana) seed is an exclusive source of the unique acetogenin compounds named avocadene and avocadyne that were found to induce leukemia cell death. In this work, pectin-zein nanoparticles encapsulated with extracted avocado crude (Avo-ZNPs) were developed using liquid-liquid dispersion and characterized in terms of diameter size, polydispersity index (PDI), zeta potential including entrapment efficiency (EE), and loading capacity (LC). Transmission electron microscopy (TEM) was used to image the particles. The release study was also evaluated under phosphate-buffered saline (PBS) conditions. Avocado seed powder was extracted using a total lipid extraction and analyzed by high-performance liquid chromatography-mass spectrometry (HPLC-MS) to confirm avocadene and avocadyne presented in the crude. The formation of avocado extract-zein nanoparticles (Avo-ZNPs) was confirmed by FTIR analysis. The Avo-ZNPs have a size ranging from 166.9 to 305.2 nm, 0.19 to 0.26 for PDI, and -59.5 to -32.9 mV of zeta potential. The EE was up to 82% and the highest LC was 14.8%. Encapsulated avocado crude expressed the efficiency in inducing leukemia cell death. Thus, ZNPs could be considered a promising delivery system for natural crude extracts to be used as biomedical ingredients.

Non-targeted volatile and non-volatile analyses of pectin samples to correlate molecular composition with sensory evaluation Christina Nauman1, christina_nauman@cargill.com, Dan Chambers1, daniel_chambers@cargill.com, Adam Zarth1, Li Jie Chan2. (1) Core R&D, Cargill Inc, Minneapolis, Minnesota(2) Shared Capabilities, Cargill Inc, Minneapolis, Minnesota Pectin is an important soluble fiber found in fruits with applications in food

as a thickener and bulking agent. Sensory evaluation has demonstrated that different pectin samples have significant differences in their flavor and aroma profiles. A non-targeted analysis was performed on six different pectin samples for non-volatile compounds by liquid chromatography- high resolution mass spectrometry and for volatiles by gas chromatography-high resolution mass spectrometry. The research presented here summarizes the flavor profile and sensory data collected from different geographies. A variety of volatile and non-volatile molecules were observed, and tentative identifications were made based on mass spectrometry data. Overall, our results indicate that we were able to determine major molecular differences in pectin that contribute to flavor and aroma. Based on these findings, we were able to predict the different sensory outcomes of pectin based on molecular profile. Leveraging mass spectrometry data may prove useful with future samples, as the analysis is faster, less labor intensive, and more reproducible than sensory panel evaluations.

Insecticidal potential of leaf extracts of Heliotropium indicum Linn (Boraginaceae) for control of insect pests of stored grains Boluwaji M. Adeniyi2,1, fowopee@gmail.com. (1) Chemistry, Benue State Univ. Faculty of Science, Makurdi, Nigeria(2) Perishable Crops Research Development, Nigerian Stored Products Research Inst.(NSPRI), Ibadan, Oyo State, Nigeria Grain beetles attack various grains and cause significant damage and reduction in commercial values. In this study, an eco-friendly approach was adopted by examining the insecticidal effect of Heliotropium indicum L leaf on the insect pests of stored grains.The plant is noted for its use in traditional medicine for the treatment of various disease. Column chromatography by gradient elution method and preparative thin layer chromatography were used in the isolation of column fractions from H. indicum. Further purification afforded a white crystalline needle-like compounds coded as IPM85 and IPM-65 in which IPM-65 was identified using LCMS as a mixture of Supinine, Echinatine, Lindelofine and Trachelanthine.The leaf methanolic extract of H. indicum L was screened for insecticidal activities towards the insect pests of stored grains at the dosage of (0.1, 0.2, 0.4 and 0.8) g/mL concentrations while the pure isolate coded as IPM-65 was screened for insecticidal activities at two concentrations of 1.0 mg/ml and 2.0 mg/ml on the substrates. The set up was laid out in a complete randomized design.The parameters assessed in this study were seed damage, percentage mortality and germinability. The extract showed the highest mortality of 60.2% on Sitophilus zeamais at 0.8 g/mL after 96 h of exposure. Mortality increased with increase in concentration and with days of exposure to H. indicum extracts, pure isolate and in Cypermethrin. There was significant difference ($p < 0.05$) between H. indicum extract (0.8 g/mL), and cypermethrin, but not with the isolate (0.1 mg/mL, 0.2 mg/mL) and Cypermethrin (0.05µ/L) at 72 and 96 h post-treatment. The cowpea seeds, paddy rice grains, sorghum and maize treated with H.indicum pure isolate at concentration of 1.0 and 2.0 mg/mL had no significant ($P > 0.05$) detrimental effect on seed germination after 60 days of storage.Acute toxicity test (LD-50) carried out on experimental rats did not reveal any mortality at a concentration of 100 mg/kg body weight throughout the 21 days of trial. The isolation and purification procedure of the methanolic extract was done on column chromatography and TLC while the characterization and structural elucidation were done using NMR spectroscopy and LCMS. Based on the findings of this study, the isolate of H. indicum L could be explored as a potential lead in the development of an eco-friendly biopesticide in the protection stored grains against weevils.

HS-SPME-GC-MS/Olfactometry-based sensory-directed flavoromics to uncover aroma boundary compositions of commercial barley malts with a wide Lovibond variation Zixuan Gu, zixuan.gu@ndsu.edu, BINGCAN CHEN, bingcan.chen@ndsu.edu. Plant Sciences, North Dakota State Univ., Fargo In this study, HS-SPME/GC–MS based untargeted and targeted flavoromics combing with olfactometry were employed to uncover aroma boundary compositions of five types of commercial barley malts with a wide range of Lovibond (L), including kilned base malts (1.8 L and 3.5 L) and roasted caramel malts (10 L, 60 L, and 120 L). Thirty-two compounds were identified as aroma-active with modified detection frequency (MF) > 50%. 3-Methylbutanal (malty), (2E)-nonenal (fatty, cardboard-like), and 2-furfural (burnt, bready) were recognized as the most influential odorants with MF > 70% in all the malts. After untargeted flavoromics, twenty-eight aromas were retained and quantitated. Furthermore, aroma boundary compositions inside/among malt groups were explored with PLS-DA. Eight aroma markers, 3-methylbutanal, 2-isopropyl-5-methyl-2-hexenal, (2E,4E)-Decadienal, 2-furfural, maltol, 2-acetylpyrrole, phenylacetaldehyde, and ethyl hexadecanoate were shortlisted for aroma boundary compositions regarding to the Lovibond of malts.

Toward a comprehensive understanding of ultracentrifugal milling on the processing properties and aroma profiles of yellow pea flour Zixuan Gu, zixuan.gu@ndsu.edu, Bingcan Chen, bingcan.chen@ndsu.edu. Plant Sciences, North Dakota State Univ., Fargo Yellow pea (Pisum sativum L., YP) grain is generally milled into flour for further processing or direct consumption. However, the comprehensive relationship between milling configurations and YP flour properties remains unclear. The aim of this study is to investigate the effect of configurations (screen aperture size and rotor speed) of ultracentrifugal mill on the physicochemical properties and aromatic profiles of YP flours. Starch damage, morphology, particle size distribution, pasting, thermal property, and aromatic profiles of YP flours were studied. Results show that starch damage increased significantly as the screen aperture size decreased. The YP flour produced with a 500 µm aperture screen had the most stable pasting and thermal properties. With untargeted flavoromics, 2-ethyl-1-hexanol could potentially be applied as an aroma maker to distinguish if an excessive milling or inappropriate configurations of ultracentrifugal mill are applied. This work has furnished fundamentals for the milling and application of YP flour.

Acidic degradation and byproduct formation of MIB and GSM in aqueous environments Rebecca A. Adams Dupre1, rebecca.dupre@usda.gov, Wayne Roussell2,1,3, Brennan Smith1. (1) USDA Agricultural Research Service, District of Columbia (2) Oak Ridge Inst. for Science and Education, Oak Ridge, Tennessee (3) Nicholls State Univ., Thibodaux, Louisiana 2-Methylisoborneol (MIB) and geosmin (GSM) are secondary metabolites of aquatic microorganisms, and their accumulation in fish and fish-rearing waters can be detrimental to the economics of aquacultural industries. MIB and GSM are classified as terpenoids, a designation of natural products which often have characteristic taste and odor properties. MIB and GSM are considered “musty” and “earthy” and can be identified by taste in drinking water at levels below 10 parts per trillion. As lipophilic compounds, these flavors readily concentrate in fish, which can lead to consumer dissatisfaction or rejection. There is a great need for treatment options to remove these flavors from fish, either through eliminating the compounds from fish-rearing waters or by treating fish with reagents to degrade MIB and GSM. Understanding of the reactivity of MIB and GSM towards degradation will aid in identifying treatment options. Acidic dehydration of MIB and GSM at pH < 2 has been reported, but parameters for practical applications have not been defined. The reactivity of MIB and GSM was investigated in aqueous solutions at pH values ranging from 1.2 to 8.6 using SPME-GCMS. Simultaneous SIM/scan data acquisition was utilized, which provided both sensitive tracking of MIB and GSM and the ability to

identify byproducts of degradation reactions. Significant degradation of MIB was observed at pH 2.4, while only moderate GSM degradation occurred at pH values below 2. Multiple dehydration products of MIB and GSM were identified by mass spectral data in pH 1.4 solutions. Analysis of acidified, then neutralized solutions showed dehydration reactions were partially reversible and exhibited a time-dependance for reversibility. Acidic degradation in biphasic solvent (<1% oil in water) was also studied, which can mimic the behavior of MIB and GSM in fish fillets.

Phosphorus reduction opportunities from animal agriculture utilizing a corn ethanol distillers grain feed substitute Kenneth Ruffatto2, ruffatt2@illinois.edu, Gerald Shurson1, Rebecca Muenich3, Roland Cusick2. (1) Dept. of Animal Science, Univ. of Minnesota Twin Cities, St Paul (2) Dept. of Civil and Environmental Engineering, Univ. of Illinois Urbana-Champaign (3) Univ. of Arkansas, Fayetteville Animal agriculture in the US (US) is a significant contributor to phosphorus (P) pollution, which can lead to the proliferation of freshwater algal blooms. Though technologies and best management practices have been developed for reduction of P from animal feeding operations, the dispersive nature of P loadings from and abundance of these sources has made them difficult to regulate. One technique that can better centralize P reductions from animals is through the generation of a distillers grain (DG) feed substitute with reduced P from corn ethanol biorefineries. However, a better understanding of the usage of DGs throughout the US is necessary to understand how a reduced P variety can lead to reductions. This study estimated an optimal county-level flow network of DG in the US to elucidate nutrient reduction opportunities from use of a DG feed substitute with reduced P. From this analysis, the total estimated P embedded in DG fed to livestock and poultry was nearly twice that estimated in human waste. The modeled flow network showed that a majority of DG usage was in the Midwest, with nearly three-quarters of estimated DG usage in the same state it was generated. This localized usage of DG also created the potential for a nutrient trading market between animal feeding operations using a DG with reduced P and water resource recovery facilities, as shown in a priority watershed for P pollution in Iowa. This study further demonstrated the pivotal role that corn ethanol biorefineries can have in sustainable P management in the US.

The era of chemical spaces: Mining relevant chemistry Christian Lemmen1, Daniel Comer2, Justin Holowachuk1,2, Justin@biosolveit.com, Alexander Neumann1. (1) BioSolveIT GmbH, Sankt Augustin, Nordrhein-Westfalen, Germany(2) BioSolveIT Inc, Boston, Massachusetts Over the past decade, there has been a significant transformation in small molecule discovery, driven by the continuous expansion of compound libraries. The emerging concept of "Chemical Spaces" relies on a combinatorial approach, utilizing in-house building blocks and well-defined reaction rules to create vast molecule collections for a variety of purposes including agriculture, fragrances, food chemistry and drug discovery. Consequently, this approach permits customization to meet specific requirements related to physicochemical characteristics and molecular composition in its field of application. We present novel computational methods aimed to mine respective relevant chemistry from the Chemical Spaces that is by design synthetically accessible.1-3 Those methods include fuzzy pharmacophore matching, Tanimoto-fingerprint screening, and substructure search to retrieve molecules based on the needs and challenges of the discovery campaign. Furthermore, the 3D ligand-based molecule superposition method FlexS can be employed to enhance the selection of potential compound candidates for further investigation. [1] Lessel, U.; Wellenzohn, B.; Lilienthal, M.; Claussen, H. Searching Fragment Spaces with Feature Trees. J. Chem. Inf. Model. 2009, 49, 270–279. https://doi.org/10.1021/ci800272a. [2] Bellmann, L.; Penner, P.; Rarey, M. Topological Similarity Search in Large Combinatorial Fragment Spaces. J. Chem. Inf. Model. 2021, 61 (1), 238–251. https://doi.org/10.1021/acs.jcim.0c00850. [3] Schmidt, R.; Klein, R.; Rarey, M. Maximum Common Substructure Searching in Combinatorial Make-on-Demand Compound Spaces. J. Chem. Inf. Model. 2022, 62 (9), 2133–2150. https://doi.org/10.1021/acs.jcim.1c00640.

Characterizing food profiles and detecting contaminants with hyperspectral imaging George A. Killian, gkillian2015@gmail.com. Applications, Headwall Photonics Inc, Bolton, Massachusetts Food product processing sites are faced with the challenge of removing foreign objects, detecting disease and contamination, and creating a consistent flavor profile of their product, and need to do so at growing speeds and demands. Hyperspectral imaging partnered with machine learning algorithms are shown to be able to solve these problems for a wide variety of different agricultural products. From sorting blueberries, to accurately predicting the brix content of a strawberry, or even estimating the surface concentration of histamine in a tuna steak, these different characteristics can be seen in the visible, near infrared, and short-wave infrared regions and their differences mapped with classification or regression models. This presentation will review push-broom hyperspectral imagers, hypercube-based machine learning algorithms, and three novel successful agricultural-based applications.

Characterization and quanitification of the polyphenols found in differing teas Maxwell S. Sykes, mssykes0@frostburg.edu, Matthew J. Crawford. Chemistry, Frostburg State Univ. College of Liberal Arts and Sciences, Frostburg, Maryland, US Aside from water, tea is the most widely consumed beverage in the world and has long been associated with health and vitality in many cultures. The secondary metabolites found within various plants (generally responsible for the defense against pathogens and UV radiation), known as polyphenols, have been postulated to possess various nutraceutical benefits and are believed to be the driving force behind the potential health benefits from teas; this is primarily in correlation to the antioxidant capabilities of polyphenols. The research herein focuses on the characterization and quantification of these polyphenols, extracted from differing tea varieties, by employing mass spectrometry and gas chromatography. The approach of this project is to use a gallic acid standard curve, coupled with a Folin-Ciocalteu assay, to gather absorbance data and a qualitative indicator for the presence of polyphenols within the tea-extract samples. Further characterization of these secondary metabolites will also aid in future research – allowing for antioxidant activity (as it relates to the different tea samples) to be quantified using a 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging capacity (DRSC) assay. The overall results of this study will hopefully illuminate beneficial aspects to the storage and utilization of the polyphenols found within plants, potentially leading to further, in-depth studies regarding their nutraceutical benefits.

Non-targeted analysis and standard free screening of PFAS using high-resolution mass spectrometry and ion mobility Samuel Putnam, Samuel.Putnam@bruker.com, Andrea Kiehne, Silke Bodendiek, Eva-Maria Niehaus, Brian K. Teeter. Bruker Daltonics Inc, Billerica, Massachusetts Per- and polyfluoroalkyl substances (PFAS) have been a health and environmental concern for more than 70 years, shortly after their development for use in many household and industrial products. At present, nearly 5000 compounds are included within the commercial PFAS family, all with at least one perfluorinated methyl group (-CF3) or at least one perfluorinated

methylene group (-CF2-). Accurate and comprehensive screening for this ever-growing list of PFAS is challenged by many factors, including a lack of reference standards. A broad, standard-free approach to directly screen for PFAS in water samples was tested using the timsTOF Pro 2 system. The use of trapped ion mobility separation improved resolution quality within the MS and MS/MS data pools, increasing the number of features detected while providing characteristic collision cross-section (CCS) values for each. PFAS signals were filtered from the complex data sets by applying Kendrick mass analysis. Based on the molecular structures of an assembled list of well-known and characterized PFAS contaminants, in-silico fragmentation patterns and CCS values were predicted and matched against the observed data, and corresponded to those which could be matched based on analytical standards. The data collected also enabled rapid separation and putative identification of untargeted PFAS in spiked water samples, using MetaboScape tools to mine public databases for candidate compounds for comparisons of elemental compositions, fragmentation patterns, and CCS values. Separation by trapped ion mobility using data-dependent MS/MS provided a broad pool of high-quality MS and MS/MS data, with MS/MS coverage near 95%. Kendrick mass analysis successfully filtered the data due to shared CF2 moieties and can be used for exploratory PFAS screening. Forty-six governmentally monitored PFAS were identified in the tested water samples from an extended target list created using structural information derived from InChI coding, with no standards needed. Statistical analyses within MetaboScape permitted clear differentiation between the control and spiked water samples for the putative identification of additional PFAS. This workflow shows excellent potential to push the analytical limits for standard-free PFAS screening to support improved environmental protection.

Food Analysis with Raman Microscopy Samantha Redes, samantha.redes@edinst.com. Edinburgh Instruments Ltd, Livingston, West Lothian, UK Raman spectroscopy has established itself as a versatile tool for the non-destructive analysis of food products, offering valuable insights into their chemical fingerprint and structural composition. In this poster presentation, we present an overview of Raman spectroscopy and microscopy techniques and their applications to food analysis, with a focus on how Raman can be utilized for enhancing quality control and safety assurance in the food industry. In quality control, the microstructure of food plays a critical role in its mechanical properties such as texture and firmness and ultimately consumer perception. In this poster, we will present the structural and chemical information that can be obtained on emulsions and pulps using confocal Raman microscopy. Rapid and accurate detection of contaminants in the supply chain is required to ensure safe food. We show how Raman spectroscopy used in conjunction with multivariate analysis methods can identify chemical, microbial and physical contamination in the food chain.

MONDAY MORNING March 18
Agnes Rimando Memorial International Student Symposium

Influence of complex coacervation on the structure and texture of plant-based protein-polysaccharide composites Xiaoyan Hu, xiaoyanhu@umass.edu, David J. McClements. Food Science, Univ. of Massachusetts Amherst Plant-based foods that mimic the sensory attributes of meat and seafood are being developed to address environmental, animal welfare, and health concerns linked to livestock production and processing. However, it is challenging to accurately replicate the structure, texture, and functionality of animal-based products by plant ingredients. Soft matter physics principles are therefore being employed to address this issue. In this study, coacervation and thermal gelation of gellan gum(GG)-potato protein(PP) were used to create biopolymer composites with meat-like textures. The main aim was determining whether the structural organization and rheology of biopolymer composites could be controlled by modulating the electrostatic interactions between PP and GG by controlled pH. The z-potential of the complexes was positive at pH 4, near zero at pH 5, and negative at pH 6, attributed to the reduction in the positive charge on PP when the pH was raised towards their isoelectric point, while GG remained strongly negative at all pH values. Large clumps were formed at pH 4 due to strong electrostatic attraction between PP and GG. However, fibril structures were formed after heating at pH 6, which was mainly attributed coacervate formation. Interestingly, a substantial quantity of air bubbles was generated within the biopolymer composites during the blending of the PP and GG mixtures at pH 4, which influenced the structure and rheology of the heat-set composite gels. At pH 6, fewer air bubbles formed due to disability to stabilize air-water interfaces. The electrostatic complexation of the PP and GG also influenced the dynamic shear modulus of the composite gels during heating and cooling, with the final shear modulus depending on pH: pH 4 > pH 6 > pH 5. By controlling the ratio of negative and positive molecules via pH, the electrostatic attraction or repulsion can be manipulated to create different microstructures in protein-polysaccharide composites. Our findings highlight the potential of using coacervation to create meat analogs with different fibrous structures and gel strengths, which may facilitate the design of plant-based foods with desirable textural attributes.

Phytotoxic activity of grammicin produced by Xylaria sp. infecting Handroanthus serratifolius (Bignoniaceae) Debora Barreto1,2, deborabarreto18@gmail.com, Camila Rodrigues de Carvalho1, Joanna Bajsa-Hirschel2, Sonia Queiroz4, Stephen O. Duke3, Charles L. Cantrell2, Luiz Rosa1. (1) Microbiology, Univ, Federal de Minas Gerais, Belo Horizonte, MG, Brazil(2) USDA-ARS Natural Products Utilization Research Unit, Univ., Mississippi, US(3) Univ. of Mississippi, Univ. Park, Mississippi, US(4) Empresa Brasileira de Pesquisa Agropecuaria, Jaguariúna, SP, Brazil
With the increase in the world population, there is a need for an increase in the agricultural production of food. In this scenario, weeds can sometimes be responsible for as much as 60% of crop losses, making agriculture highly dependent upon chemicals for weed management. Unfortunately, with indiscriminate, repetitive and continuous use of herbicides, the number of resistant weeds has increased. Currently, there are several types of herbicides available, but they all have mechanisms of action that were introduced 30 or more years ago, which helps explain the evolved resistance, leading farmers to sometimes increase application rates, putting human health and the environment at risk. Recent research shows that secondary metabolites produced by fungi are promising for the development of natural herbicides, as they exhibit activity at low concentrations, in addition to being considered by some safer than synthetic alternatives. We focused on evaluating the herbicidal activity of a phytopathogenic fungus isolated from leaf lesions of Handroanthus serratifolius (Bignoniaceae) seedlings showing signs of infection. The fungus was collected in Rio Doce State Park, a native fragment of the Atlantic Forest in the state of Minas Gerais, Brazil, and was isolated and grown in potato dextrose agar culture medium and identified as Xylaria sp. The dichloromethane extract of the culture displayed high phytotoxic activities against lettuce (Lactuca sativa) and bentgrass (Agrostis stolonifera), effectively inhibiting the germination of all the seeds at concentrations of 1 mg mL-1. Following different chromatographic steps, grammicin (1) and xylaric acid methyl ester (2) were isolated and identified. Grammicin was responsible for the phytotoxic activity, inhibiting growth of Lemna paucicostata (duckweed) by 50% at 87.7 μM. This is the first report of the phytotoxic activity of grammicin. Mode of action studies are in progress. These findings highlight the potential sourcing of phytopathogenic fungi found within the Brazilian

Atlantic Rain Forest's plant ecosystem to produce secondary metabolites with herbicidal properties. This discovery positions these fungi as valuable sources for investigating natural herbicides with potentially novel mechanisms of action.

RuBisCo: An edible and functional protein applied in emulsions Maren Müller, maren.mueller@tum.de, Henrich Frielinghaus, Olaf Holderer, Theresia Heiden-Hecht. JCNS, Forschungszentrum Julich GmbH, Garching, Nordrhein-Westfalen, Germany RuBisCo is the most abundant protein, which may be isolated from several sources like water lentils, alfalfa or sugar beet leaves. The protein isolation process is constantly improved to maintain the protein's molecular structure and functionality for food applications. Its functionality is an emerging and growing research topic, showing promising characteristics for applications in gels and emulsions. However, little information about the protein characteristics like molecular structure, solubility depending on pH, as well as emulsion stabilisation mechanisms are known. The emulsions stabilisation mechansims are affecting the emulsion characteristics on a macroscale like oil droplet size, and on a microscale like interfacial properties. Therefore, we investigated RuBisCo from different origin, and focused on properties of the protein and its emulsion on a macro- and microscale. The results of both -macro- and microscale- complete the understanding of RuBisCo stabilized emulsions, while static light scattering and CLSM focuses on properties of the macroscale; drop tensiometry and interfacial viscoelasticity analyse the microscale; and SANS and SAXS cover the whole length scale range. The results indicate that RuBisCo is a promising protein source for food applications with interfaces.

Metabolomic analysis with machine learning algorithms enables the evaluation of postharvest color stability in different pecan varieties Min Jeong Kang1, mk41285@uga.edu, Ronald B. Pegg1, Lenny Wells2, Patrick J. Conner2, Joon Hyuk Suh1. (1) Food Sci. & Tech., Univ. of Georgia, Athens (2) Horticulture, Univ. of Georgia, Tifton The color of nut kernels is an important indicator to determine nut quality as well as consumer's first impression on the product. In the postharvest stage, nut (e.g., pecans) kernels gradually darken with increasing red and blue colors, which have a negative impact on consumers' preference. Growing evidence has suggested that plant phenolics and their derivatives are responsible for the kernel color of nuts, while which compounds (biomarkers) play a key role in determining/altering kernel color (e.g., pecans) remains elusive. Here, pathway-based metabolomics combined with machine learning (ML) modeling was employed to identify key metabolites related to the postharvest color stability of pecans. Nine pecan cultivars were tested, and metabolites within phenylpropanoid, flavonoid, and anthocyanidin/anthocyanin biosynthesis pathways were analyzed using ultra-high performance liquid chromatography/mass spectrometry (UHPLC/MS). Different ML models (e.g., extreme gradient boosting, random forest, and support vector machine) were compared to find biomarkers for pecan color quality. Based on the results, potential markers associated with the color stability of different varieties of pecans were achieved. The selected markers included anthocyanidins, anthocyanins (majorly, contributing to red/blue colors), and their precursors in the pathways. Our work provides a novel insight and framework to understand complex color formation/regulation mechanisms in pecans. The collected biomarker information would be used as preliminary data for future pecan studies and pecan breeding programs for improving the color quality of pecan kernels.

Production and bioactivity of isoflavones from elicited hairy root cultures of pigeon pea Gaurav Gajurel1,2, gaurav.gajurel@smail.astate.edu, Amit R. Sharma2, Salma Abdel-Karim2, Mohammad A. Alam3, Fabricio Medina-Bolivar1,2,4. (1) Molecular Biosciences Graduate Program, Arkansas State Univ., Jonesboro (2) Arkansas Bioscience Inst., Arkansas State Univ., Jonesboro (3) Dept. of Chemistry and Physics, Arkansas State Univ., Jonesboro (4) Dept. of Biological Sciences, Arkansas State Univ., Jonesboro Isoflavones are a class of flavonoids that exhibit anticancer, antioxidant, anti-inflammatory, antibacterial, and pro-apoptotic properties. The extraction and purification of these bioactive phenolics from natural sources can be challenging and time-consuming. This project aimed to establish a hairy root culture system for pigeon pea via Agrobacterium rhizogenes-mediated transformation as a sustainable production platform for isoflavones. The hairy root cultures were co-treated with methyl jasmonate, methyl-β-cyclodextrin, hydrogen peroxide, and magnesium chloride for 192 h to study their effect on the accumulation of isoflavones in the culture medium and hairy root tissues. A total of two isoflavones, genistein and its prenylated analog isowighteone, were purified and identified from the elicited culture medium extract using column chromatography, semi-preparative high-performance liquid chromatography, tandem mass spectrometry, and 1D & 2D nuclear magnetic resonance spectroscopy. Most of the isoflavones were accumulated in the culture medium. The morphological differences between normal and elicited hairy roots were studied using scanning electron microscopy. Interestingly, the cells in elicited hairy root tips seemed to have a non-uniform shape along with some ruptures on the surface. The antioxidant activity of these isoflavones and extracts enriched in these compounds was determined using the DPPH antioxidant assay. The isoflavone-rich extract showed higher antioxidant activity compared to individual compounds at equimolar concentration. Additionally, the anticancer and anti-inflammatory activities of genistein and isowighteone were tested in MDA-MB-231 triple-negative breast cancer cells and RAW 264.7 macrophages at a concentration of 25 μM. Isowighteone exhibited higher cytotoxicity than genistein against MDA-MB-231 cells up to 72 hours and higher anti-inflammatory activity at 24 hours compared to genistein. Pigeon pea hairy roots provide a sustainable platform for producing bioactive isoflavones.

UHPLC-HRMS and GC-MS analyses of bioactive compounds in prairie berries in Canada and their antioxidant potential Chamali Kodikara2,1,4, kodikarc@myumanitoba.ca, Srinivas Sura4,1, Nandika Bandara2,3, Thomas Netticadan1,4,5, Champa Wijekoon1,4,5. (1) Science and Technology, Gouvernement du Canada Agriculture et Agroalimentaire Canada, Winnipeg, Manitoba (2) Dept. of Food and Human Nutritional Sciences, Univ. of Manitoba, Winnipeg, Canada(3) Richardson Centre for Food Technology and Research, Univ. of Manitoba, Winnipeg, Canada(4) Science and Technology, Morden Research and Development Centre, Morden, Manitoba, Canada(5) Canadian Center for Agri-food Research in Health and Medicine, Winnipeg, Manitoba Prairie berries are cold hardy fruits consumed by Canadians for their perceived health benefits. Phenolic compounds, fatty acids, and phytosterols are important groups of bioactive molecules present in berries. Assessment of the bioactive compounds and their antioxidant properties enable us to identify them as a potential functional food. The research examined the composition of phenolic compounds, fatty acid composition, phytosterols, and their antioxidant activity in fifteen different berries, grown in prairies. A liquid chromatography-high resolution mass spectrometry (UHPLC-HRMS) method was developed and used for the comprehensive and simultaneous analysis of 66 phenolic compounds in 15 different types of Canadian wild berries. In addition, gas chromatography-mass spectrometry (GC-MS) was used to analyze the fatty acids and phytosterols. Total phenolic content (TPC), 1,1-diphenyl-2-picrylhydrazyl (DPPH) free radical scavenging assay, ferric reducing antioxidant power assay (FRAP), and total flavonoid content were assessed for their antioxidant potential in respective

wild berries. Wild grapes were rich in phenolic compounds such as resveratrol, while gooseberries were rich in isoquercetin and para-coumaric acid. Saskatoon berries were rich in chlorogenic acid and quercetin. Rutin and chlorogenic acid were the most abundant phenolic compounds in chokecherries. Essential fatty acids such as linoleic and linolenic acids were found in wild grapes, seabuckthorn and Saskatoon berries. The highest TPC was in nanny berries while chokeberry had the highest FRAP activity.. Snowberry showed the highest DPPH activity. It is well established that diets rich in antioxidants can improve heart health and help prevent chronic diseases such as coronary heart disease. A novel UHPLC-HRMS method for phenolic compounds and a GC-MS method for fatty acids proved that the underutilized wild berries contain various beneficial phenolic compounds, essential fatty acids, and phytosterols. These berries, as sources of these important bioactive compounds, have the potential to be included in antioxidant-rich diets. The information from this study will help in finding applications for underutilized prairie berries as potential sources of functional food.

Optimization of ultrasound-assisted extraction of xanthophylls from Tagetes erecta L. using hydrophobic deep eutectic solvents (HDES) Soumyajit Ghoshal1, soumyajit.ghoshal99@gmail.com, Anirban Dutta1,2, Supradip Saha1, Aditi Kundu1, Abishek Mandal1,3. (1) Division of Agricultural Chemicals, ICAR-Indian Agricultural Research Inst., New Delhi, Delhi, India (2) Downstream Agro-processing Division, ICAR-National Inst. of Secondary Agriculture, Namkum, Ranchi, Jharkhand, India(3) Division of Basic Sciences, IACR-Indian Inst. of Horticultural Research, Bengaluru, Karnataka, India Hydrophobic deep eutectic solvents (HDES) prepared with two saturated fatty acids, namely caprylic (C8) and capric (C10) acid were employed as green solvents for extraction of xanthophyll pigments from marigold (Tagetes erecta L.) florets with the aid of an ultrasound-assisted technique. Eutectic mixtures with different molar ratios of the two fatty acids were prepared and characterized using FT-IR, NMR (H1 and C13), DSC, density and conductivity measurements, and molecular simulation studies. Experiment was carried out following Box-Behnken design (BBD) of response surface methodology (RSM) to optimize the extraction conditions for maximum extraction efficiency. The highest yield of xanthophylls (7.57 mg g-1 d.w. on the basis of lutein equivalence) was obtained by extraction with the HDES having molar ratio of 2:1 (caprylic acid: capric acid) at 60 mL g-1 solvent-to-solid ratio for 32.97 min of ultrasonication, which closely resembled the model predicted value (7.86 mg g-1 d.w.). At the same solvent-to-solid ratio and ultrasonication time, conventional organic solvents (hexane-acetone 1:1 v/v) could extract only 5.71 mg g-1 (d.w.) xanthophylls. SEM images suggested rupture of cells by cavitation process for high extraction efficiency of the technique. Switching the polarity of the DES from hydrophobic to hydrophilic facilitated the precipitation of the extracted lipophilic xanthophylls and their subsequent separation. This green solvent therefore can easily replace the hazardous organic solvents for efficient extraction of xanthophylls from marigold. The presence of lutein linoleate, an unsaturated fatty ester of lutein has been reported in marigold for the first time along with five monoesters and three diesters of lutein, and two diesters of violaxanthin.

Optimization of gluten-free bread's health benefits with Artichoke Leaf Extract and Sourdough Biotechnology Alessandro Annunziato1, alessandro.annunziato@outlook.it, Francesco M. Calabrese1, francesco.calabrese@uniba.it, Ruggiero Francavilla2, ruggiero.francavilla@uniba.it, Maria De Angelis1, maria.deangelis@uniba.it. (1) Food and Soil Science (DiSSPA), Univ. degli Studi di Bari Aldo Moro, Puglia, Italy(2) Dept. Interdisciplinare di Medicina (DIM), Univ. degli Studi di Bari Aldo Moro, Bari, Puglia, Italy The artichoke plant (Cynara cardunculus L.) is a compelling candidate for promoting health due to its rich nutritional content and numerous benefits. Despite this, artichoke by-products are often discarded, even though they contain valuable dietary fibers, phenolic acids, and other micronutrients. This study aimed to characterize a laboratory-made gluten-free bread (B) by supplementing rice flour with a powdered artichoke leaves extract (ALE) comprising 5% (w/w) chlorogenic acid. The ALE was incorporated into the experimental gluten-free bread. Four different bread batches were prepared using different combinations: i) gluten-free type-II sourdough bread (SB); ii) gluten-free type-II sourdough bread with ALE (SB-ALE); iii) Baker's yeast gluten-free bread (BY); iv) Baker's yeast gluten-free bread with ALE (BY-ALE). The study found that SB had the lowest glycemic index, while SB-ALE exhibited the highest antioxidant properties among the digested bread samples. Fermentation of the digested samples with fecal microbiota from healthy donors did not reveal clear microbial patterns based on plate counts. However, significant differences in volatile organic compounds were observed in SB-ALE, particularly with higher levels of hydrocinnamic and cyclohexanecarboxylic acids. Supernatants from fecal fermentation were recovered and tested for their beneficial properties on human keratinocyte cell lines against oxidative stress. In addition, the effectiveness in modulating the expression of proinflammatory cytokines in Caco-2 cells was evaluated. Results demonstrated that ALE contributed to protection against oxidative stress, and the combination of SB-ALE reduced the cellular expression of TNF-α and IL1-β. In conclusion, this preliminary study suggests that the synergy between ALE and sourdough biotechnology holds promise for enhancing the nutritional and healthy attributes of gluten-free bread.

Exploring novel magnetite nanoclay: A breakthrough composite for pesticide removal from water Anirban Sil1, sil.anirban2014@gmail.com, Neethu Narayanan1, Tirthankar Banerjee1, Neera Singh1, Niveta Jain2, Suman Gupta1. (1) Agricultural Chemicals, Indian Agricultural Research Inst., New Delhi, Delhi, India(2) Centre for Environment Science and Climate Resilient Agriculture, Indian Agricultural Research Inst., New Delhi, Delhi, India Across the world, the widespread pesticide dilemma and the enduring residues in surface and groundwater persist. To eliminate these minuscule contaminants from water, magnetite was reinforced with nano- and non-nano organoclays (with surface modification) and applied for removal of twelve mostly used pesticides (chlorantraniliprole, clothianidine, azoxystrobin, acetamiprid, fipronil, imidacloprid, thiamethoxam, dinotefuran, thiacloprid, tricyclazole and nitenpyram). From the screening experiment, most effective performance (>80% sorption for 12 pesticides) was achieved with a blend of 35-45 wt% Dimethyl Dialkyl Amine(DMDA) modified nanobentonite and magnetite. The novel composite was further characterized by Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM) and Fourier Transform Infrared Spectroscopy (FT-IR), Vibrating-sample magnetometry (VSM), X-Ray Diffraction (XRD) etc. Moreover, sorption tests indicated that the ideal adsorption occurred with 10 mg of the prepared material, exposed for 4 hours, in a 5 mL solution containing a pesticide mixture at a 1 µg/mL fortification level. The mechanistic analysis unveiled that a blend of physisorption and chemisorption played a role, with the rate-limiting step being controlled by film diffusion. The thermodynamic parameters suggest the sorption to be exothermic, spontaneous and enthalpically favourable. Economic viability of the composite was found suitable as regeneration and reusability can be carried out to three or more cycles. Further, this composite showed improved sorption of selected pesticides than commercially used granular activated carbon and when employed for removal of micropollutants and

additional pesticides from fortified and unfortified water samples of Yamuna river, it depicted almost 70-100% and ~100% sorption potential respectively. Therefore, magnetically separable novel magnetite-DMDA clay composite is proposed to be used as an efficient adsorbent for removal of pesticides and other micropollutants from wastewater sources

Ultrasound-assisted extraction of betalains from dragon fruit (Hylocereus sp.) peels: Optimization using response surface methodology-genetic algorithm (RSM-GA) hybrid model and chemo-profiling Dipsikha Mondal, dipsikhamondal555@gmail.com, Anirban Dutta, Aditi Kundy, Supradip Saha. Agricultural Chemicals, Indian Agricultural Research Inst., New Delhi, Delhi, India Dragon fruit, or Pitaya, is an exotic fruit crop grown currently on around 3,000 ha of land in India. The government has planned to increase its cultivation to 50,000 ha within the next five years. Its peels, constituting about 20% of the fruit's weight, are rich in betalain pigments, a group of natural antioxidants. The substantial peel waste generated by processing industries can be harnessed for betalain extraction, serving both environmental and economic purposes. This study focuses on optimizing the extraction procedure for betalains from red dragon fruit (Hylocereus costaricensis) peels using ultrasonication and to profile the compounds present in the extract. Ultrasonic probe-assisted extraction (UPE) technique surpassed the conventional solid-liquid, homogenization, and ultrasonic bath extraction techniques, in terms of yielding higher relative betalain content in comparatively less time using less solvent. UPE variables were statistically optimized for maximum betalain yield. Initially, response surface methodology (RSM)-predicted UPE conditions resulted in betalain extraction with a 5.89% error. However, combining the model with the genetic algorithm (GA) greatly enhanced accuracy. The GA-coupled RSM model predicted an extraction yield of 286.27 mg g-1 of betalains (dry weight) using ultrasonication for 40 min at 50% amplitude with 111.5 mL g-1 of solvent. Under experimental conditions, 286.85 mg of betalains per gram of dragon fruit peels (d.w.) were obtained, with an error value of only 0.20%. Betalains extracted from dragon fruit peels using different techniques, were evaluated for antioxidant potency via radical scavenging and reducing power assays to show comparable antioxidant activities. The chemo-profiling of the pigments present in H. costaricensis peels through UPLC-QTOF-ESI-MS showed that betacyanins, like betanin, betanidin, phyllocactin, apiocactin, hylocerenin, etc., were more prevalent than betaxanthins like indicaxanthin. Extracted betalains can further be used as natural colorants, with potential for functional roles in both the food and pharmaceutical industries, enhancing their value

Synthesis and fungicidal activity of novel indazolylchromones Riya Kundu, riyakundu708@gmail.com, Parshant Kaushik, Najam Akhtar Shakil, Virendra Singh Rana. Division of Agricultural Chemicals, Indian Agricultural Research Inst., New Delhi, Delhi, India The global agriculture faces a significant annual loss of 18%, amounting to roughly 1,300 billion INR, due to plant diseases caused by various phytopathogenic fungi. Sclerotium rolfsii is a detrimental soil-borne fungus leading to substantial crop losses ranging from 10% to 100%. In the case of tomatoes, this fungus typically attacks the lower stem near the soil surface, resulting in Southern blight. Another important soil-borne fungus affecting tomatoes is Fusarium oxysporum lycopersici, causing wilt disease. Despite advances in biotechnology and biological approaches, agrochemicals remain crucial in agribusiness due to increasing fungicide resistance over the past decade, resulting in the loss of several important fungicides globally. Chromones, naturally occurring compounds mainly found in plants, serve as pharmacophores in various natural and synthetic bioactive molecules, exhibiting diverse bioactivities . Indazole derivatives, though rare in nature, are prominent in synthetic drugs and offer a range of bioactivities. To address this, a series of 20 2-Indazol-1-yl-chromen-4-one derivatives were synthesized with yields ranging from 76.35% to 93.86%, and notably, 19 compounds (6b-6t) were reported for the first time in the literature. Comprehensive characterization was achieved through various spectroscopic techniques, including infrared (IR), nuclear magnetic resonance (1H NMR and 13C NMR). These newly synthesized indazolylchromones (6a-6t) exhibited substantial antifungal activity against S. rolfsii and F. oxysporum. Among the tested compounds, 6t and 6f showed excellent antifungal activity against S. rolfsii, with ED50 values of 10.10 ppm and 16.18 ppm, respectively. In the case of Fusarium oxysporum, compound 6f also exhibited good activity, with an ED50 value of 27.82 ppm. Based on these promising in vitro results, the two most effective compounds, 6f and 6t, were selected for pot experiments against S. rolfsii. In these pot trials, both compounds effectively controlled the disease at a concentration of 1000 ppm, achieving PDI values of 26.66% and 30%, respectively, which were comparable to the commercial fungicide Hexaconazole 5% SC (PDI 25%). However, in case of Fusarium oxysporum, compound 6f displayed lower activity, with a PDI of 35.00%, in comparison to the commercial Carbendazim 50% WP (PDI 24.00%). Consequently, there is potential to develop appropriate formulations of these two compounds for the effective management of Sclerotium rolfsii.

Bioactive phytochemicals from Litsea glutinosa bark for potential antifungal activity against Penicillim expansum Sourabh suman1, sourabhsuman551@gmail.com, Aditi Kundu1, chemaditi@gmail.com, Anirban Dutta1, Supradip Saha1, Amrita Das2. (1) Division of Agricultural Chemicals, Indian Agricultural Research Inst., New Delhi, Delhi, India(2) Division of Plant Pathology, Indian Agricultural Research Inst., New Delhi, Delhi, India Litsea glutinosa, a perennial tree belongs to Lauraceae family and commonly known as 'Indian laurel,'. It is widely distributed in tropical and subtropical regions, particularly in the Indo-Malesia terrains and China. Traditionally, the bark of this tree holds significant importance and is often utilized by practitioners due to its immense bio-functional properties. In the current study, the bark of L. glutinosa was subjected to sequential extraction using hexane, chloroform, acetone, methanol, and water to obtain respective concentrates. Bioassay-guided extraction revealed higher potency of chloroform soluble fraction to arrest the growth of the virulent strain of Penicillium expansum. Therefore, the ultrasonic probe assisted extraction (UPAE) process was optimized to intensify the chloroform soluble components using Box Behnken design (BBD) of response surface methodology (RSM). Higher extraction efficiency was determined by establishing extraction models which showed better fitting of dataset in 2nd order rate kinetic equation, signifying influence of more than one factors on extraction yield. Comparative assessment of extraction methods showed higher yield in UPAE over conventional technique, which was further confirmed through SEM image analysis indicating disruption of cell walls, facilitating better mass transfer. Bioactive compounds from chloroform extract were characterized using UPLC-QTOF-ESI-MS/MS, leading to the tentative identification of a total of forty-two phyto-constituents. The antifungal efficacy of the chloroform extracts was further proven through molecular docking studies generating concomitant data confirming favourable interaction with the target specific proteins responsible for sterol biosynthesis, correlating with the fungal ergosterol inhibition %. Keeping in view of the significant biofunctional properties of the compounds from L. glutinosa, huge opportunities lie for further development of standard formulations, which could be used for the protection against P.

expansum damage in temperate fruits under storage. Keywords-optimisation, RSM, UPAE, chemical profiling, modeling

Extraction & Biotechnology: A Natural and Sustainable Future for Flavors

Palm kernel oil: Physicochemical properties and volatile compounds Victor T. Wyatt1, vtwyatt@yahoo.com, Alberta Aryee2, Peace Asuzu2, Papa N. Asare-Okai3, Nii A. Tawiah2. (1) SBCP, USDA, Wyndmoor, Pennsylvania (2) Delaware State Univ., Dover (3) Univ. of Delaware, Newark Hexane (HEX) and dichloromethane (DCM) have been used to extract oils from various sources due to their expansive solubility and low volatility that ease removal at low temperatures. However, environmental and health concerns make them undesirable solvents. The aim of this study was to evaluate the extraction efficiency and physicochemical characteristics of palm kernel oil (PKO) extracted with the addition of acetone in HEX-acetone (1:1, v/v) and DCM-acetone (1:1, v/v) mixtures as alternative to DCM and HEX alone. PKO extracted with co-solvent systems had better quality characteristics compared to single solvent extracts. The oil recovered, free fatty acid content, peroxide value and other quality characteristics, and thermal properties were within the range for PKO, and similar oils as stipulated in standards. PKO contain up to 70% monounsaturated fatty acids of which lauric acid was the most abundant (48 to 52%). A total of 50 volatile compounds were identified by GC-MS and the results of principal component analysis (PCA) show that volatiles identification is dependent on the column, and acetone was a stronger DCM modifier than hexane. The results of this study can open new markets for palm kernel oil applications in several food industries and biofuel production.

Ionic liquids as green solvents of choice for the extraction of natural bioactive compounds Maliha Uroos, malihauroos.chem@pu.edu.pk. School of Chemistry, Univ. of the Punjab, Lahore, Pakistan Ionic liquids are designer green solvents with unique physical and chemical properties such as melting points, boiling points, vapor pressure, intoxicity, chemical and thermal stability and many others. They are solvents of choice due to their high dissolution abilities for organic, inorganic and even for biopolymeric compounds. Due to their dissolution as well as tailor-made properties, they can be designed for efficient extraction of biologically active compounds from natural products. One of such bioactive compound is thymoquinone found in the seeds of Nigella sativa. As an essential component of traditional medicine, Thymoquinone exhibits promising therapeutic potential in the treatment of various ailments, including inflammatory diseases, cancer, and neurodegenerative disorders. However, the efficient and sustainable extraction of thymoquinone remains a challenge. In our study, ionic liquids are specifically designed and used for cost-effective high purity extraction of thymoquinone from black seeds. The findings hold promise for the development of thymoquinone based therapies and the exploration of alternative, ecofriendly solvents, such as ionic liquids, in natural product extraction processes. The research work clearly depicts the disparity of results using organic solvents and ionic liquids. It also clarifies the interaction and solubility of thymoquinone in the solvents of different polarities.

From plant to palate: Refining cannabis extraction for flavor and fragrance Manuel E. Sosa, manny.sosa123@yahoo.com, Iain W. Oswald, Twinkle Paryani, Thomas Martin, Kevin Koby. R&D, Abstrax Tech Inc, Tustin, California Cannabis concentrates, especially those derived from solvents such as butane, are increasingly gaining popularity as a preferred mode of consumption in the US. Butane, due to its selectivity, has emerged as a leading solvent in cannabis extraction, with its efficacy being significantly influenced by extraction temperature. However, the predominant industrial methodologies lack rigorous scientific backing, particularly in understanding the intricate interplay between extraction parameters and the resulting product attributes. In this study, we delve deep into the impact of extraction temperatures on various properties of the extract. Notably, we observed a marked temperature-dependent increase in the undesired waxes—saturated carbon chains spanning from C26 to C30. Intriguingly, the concentrations of cannabinoids and terpenes remained largely unaffected across the temperature range, suggesting their high solubility even at temperatures below 30 °C. Crucially, we correlate the presence of these waxes to potential aroma off-notes, underscoring their influence on the overall sensory profile of the cannabis extracts. The insights garnered from this study not only shed light on optimizing cannabis extraction but also underscore its potential in flavor and fragrance applications, steering the narrative towards the sensory implications rather than merely the extraction process itself.

The Aroma of Vanilla Extracts Katrin Pechinger, Callum Helcke, Lewis Jones, Lewis.Jones@sensient.com. Sensient Flavours Ltd, Bletchley, Milton Keynes, UK Seen as a gift from the gods by the indigenous people of Central America, vanilla is now the world's most popular flavour. Hundreds of metabolites have been identified within a vanilla bean, yet the chemical compounds responsible for the complex flavour of vanilla are not yet fully understood (1). The flavour of vanilla extracts depends on the variety, origin and processing method of the beans used. While vanillin is the most abundant odourant found within vanilla extracts, at over 1% wt, it is not solely responsible for vanilla quality. Other compounds present at much lower concentrations, e.g. maltol and acetovanillone, significantly contribute to vanilla aroma (2). This presentation details how vanilla odorants were determined via chemical analysis and validated by sensory evaluation (Napping®). An aroma recombinant was created using analysis results and the audience can smell for themselves how this recombinant compares to the original vanilla extract. The presentation will then describe how the choice of extraction solvents affects aroma. Here, different solvents will be compared according to how effectively they extract odorants from vanilla beans. Again, the audience can smell the different extracts and compare solvent systems using their own senses. 1. Daphna Havkin-Frenkel; Belanger, F. C. Handbook of Vanilla Science and Technology; Hoboken, NJ Wiley Blackwell, 2019. 2. McCormick, D. Characterisation of vanilla extracts based on sensory properties and chemical composition. Doctoral thesis, Massey Univ., 2018.

Characterization of hybrid Vanilla beans using DTD-GC-MS analysis Stephen J. Toth, stephen.toth@iff.com, Ashley Noble. R&D, International Flavors & Fragrances Inc, Union Beach, New Jersey Vanilla is one of the most complex natural flavors with hundreds of compounds contributing in harmony to create that familiar and comforting aroma and taste. Currently the beans of the orchid Vanilla Planifolia produce the world's most popular flavor due to their high vanillin content and rich taste. Other species of vanilla such as Vanilla Tahitensis, Vanilla Pompona and hybridizations thereof are also used in flavoring and differ by their flavor profile and vanillin yield. These hybrids may be more robust and have a higher resistance to common diseases than traditional Vanilla Planifolia. There is considerable interest in the taste and aroma profile deviations produced by hybrid vanilla beans. To analyze the volatile and semi-volatile profile of vanilla beans, an improved direct thermal desorption gas chromatography mass spectrometry (DTD-GC-MS) method was developed and employed. This method involves cryo-grinding the cured vanilla beans in the presence of a chromatographic support material, packing the

pulverized material into a glass headspace tube using quartz wool and using a ballistically heated desorption inlet coupled to a GC-MS instrument to analyze the sample. We will use this method to characterize a series of hybrid vanilla beans to determine variations of the taste/aroma profile and discuss how geographic location, curing techniques and efficiency of hybridization affects the overall organoleptic quality and desirability.

Unified quantitation method enables the elucidation of cheese flavor Carolin J. Feyerabend1, carolin.feyerabend@tum.de, Verena K. Mittermeier2, Michael Gigl2, Corinna Dawid1,2. (1) Food Chemistry and Molecular Sensory Science, Technische Univ. Munchen, Bayern, Germany(2) Functional Phytometabolomics, Technische Univ. Munchen, Bayern, Germany Due to its characteristic flavor and nutritional value, cheese has been popular across the globe for centuries, with consumption still rising. Accordingly, it has been subject to extensive research, and amino acids, organic acids, fatty acids, and minerals have been identified as important tastants in Gouda and Parmesan cheese. Besides, their aroma is induced by aldehydes, ketones, organic acids, esters, lactones, and sulfur compounds. However, the full flavor code of other signature cheeses, such as Cheddar or Provolone, is not fully elucidated yet. Thus, a unified quantitation method was developed using mainly ultra-high performance liquid chromatography-tandem mass spectrometry (UHPLC-MS/MS), characterizing the concentrations of the key food odorants and tastants in different cheese products. It enabled the full re-engineering of Cheddar and Provolone flavor codes. We applied the Sensomics approach, combining human sensory experiments with quantitative analysis via UHPLC-MS/MS to investigate the flavor of Cheddar and Provolone cheese. A particular focus was placed on the combinatorial analysis of taste and aroma. First, sensory profiles of the cheeses regarding taste, orthonasal and retronasal aroma were recorded to establish a “golden standard”. Next, key flavor compounds were quantified using UHPLC-MS/MS, gas chromatography-mass spectrometry and high-pressure ion chromatography. For the simultaneous detection of the key tastants and odorants of cheese, a UHPLC-MS/MS-based unified flavor quantitation method was developed. Carbonyl compounds were derivatized with 3-nitrophenylhydrazine, enabling the quantitation of volatile analytes via UHPLC-MS/MS. Coupled with a simple sample workup and stable-isotope dilution analysis, this method allows for high-throughput quantitation of the key flavor compounds of Cheddar and Provolone cheese. Flavor recombination experiments confirmed the identification of the key flavor compounds, proving the applicability of the developed method. The newly established analysis procedure enables the fast, high-throughput quantitation of the key flavor compounds of Cheddar and Provolone cheese. As most of their key tastants and odorants also contribute to the flavor of other cheeses, the procedure can be broadly applied to elucidate the flavor of different cheese types. With these insights into cheese flavor, new plant-based cheese analogs can be developed in a targeted approach, catering to the increasing number of vegans.

Evaluation of different cell disruption methods to extract nutritional and flavor constituents of yeast biomass Keith R. Cadwallader, cadwlldr@illinois.edu, Nagiat Hwisa, Aqsa Chatha. Food Science and Human Nutrition, Univ. of Illinois Urbana-Champaign Yeast extracts are commonly utilized for their nutritional and flavoring properties. In this study, five cell disruption methods (autolysis, ultrasonication, ultrasonication-assisted autolysis, bead milling, and high-pressure homogenization) were applied to extract the cell components of Saccharomyces cerevisiae (Baker’s yeast). Extracts of the above-mentioned techniques were analyzed for their total protein and amino nitrogen contents. Results indicated that autolysis and ultrasonication-assisted autolysis facilitate efficient protein hydrolysis and could be the best extraction methods to release flavor components. On the other hand, high pressure homogenization and bead milling have minimal effect on protein which could be the optimum methods for nutritional components release. The effect of these methods on taste and flavor constituents and precursors such as ribonucleotides, amino acids, and the key odorants will also be discussed. The study will provide fundamental understanding on the impact of cell disruption technique on the potential nutritional value and flavor constituent released from yeast cells.

Chemistry of Alcoholic Beverages

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 in the chemical sector. Our symposium will present the latest research on the chemistry of alcoholic beverages. 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.

Beer foam: A chemistry wonderland Charles Bamforth, cwbamforth@ucdavis.edu. Food Sci. & Tech., Univ. of California Davis Most people who opt (correctly) to consume their beer from a glass rather than directly from the container expect to see a stable head on the product. For this to occur, the beer must be dispensed such that the carbon dioxide is released as bubbles and there must be the correct balance of foam stabilizing materials in the beer. These include polypeptides, bitter acids, certain cations, Maillard reaction products and, in darker products, molecules produced during roasting reactions. To add further complexity, the precise nature of the polypeptides is important, with some being adept at entering the foam but not being especially suited to stabilizing the foam and others being less "foamable" but better stabilizers. pH has a significant role to play. Furthermore, there are molecules, notably lipids and ethanol, that destabilize foam. The complex chemistry of beer foam will be described.

Chemistry underlying hangovers Alyson E. Mitchell, aemitchell@ucdavis.edu. Food Science & Technology, Univ. of California Davis Many people will experience a hangover at least once in their lifetime. Hangover refers to a collection of unpleasant and painful symptoms (headache, body aches, weakness, nausea) that can develop after excessive ethanol intake. Hangover symptoms vary depending upon many factors including hydration, blood glucose and genetic predisposition. Acute ethanol intoxication can affect the liver, gastrointestinal tract and central nervous system. Ethanol is oxidized via alcohol dehydrogenase (ADH) to form acetaldehyde; a highly unstable compound that quickly forms toxic free radicals. Acetaldehyde is further metabolized by aldehyde dehydrogenase into acetic acid. Methanol, a co-fermentation product undergoes the same metabolism to form formaldehyde. Acetaldehyde produces many of the symptoms associated with a hangover however, different types of alcohol can cause different hangover symptoms to manifest. Drinks with higher concentrations of methanol and/or congeners generally result in more pronounced symptoms. Red wines and dark liquors such as bourbon and whiskey contain greater amounts of congeners than white wines and clear liquors such as vodka. Whereas higher levels of methanol are found in beverages such as tequila, whiskey and cognac. Carbonation speeds the absorption of alcohol. Herein a general discussion of the biochemical effects of alcohol consumption and the chemistry underlying a hangover will be discussed.

Evaluation of rapid wort color method using caramel malt series and inclusion methods Nick O. Flynn, nflynn@wtamu.edu. Chemistry/Physics, West Texas A&M Univ., Canyon Studies in our lab continue to 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 for evaluating beers. Earlier studies have suggested that darker malts may benefit from inclusion of lighter grain or adoption of original ASBC methods for darker malts. In this study, we explored the applicability of this method to a caramel malt series from the same manufacturer as well as the use of other inclusion ratios on darker malts. This presentation will summarize current findings and present suggested modifications to the method as written.

Chemical and sensory evaluation of 40 hop varieties: Insights into the relationship between aroma properties and growing regions using two-dimensional gas chromatography Marcos A. Ojeda, marcos.ojeda@abstraxtech.com. Abstrax Tech Inc, Tustin, California Hops (Humulus lupulus) are regularly used in the brewing process as a bittering, flavoring, and aroma additive. Hops can generally be separated into two categories depending on use: Aroma hops or bittering hops. Aroma hops are usually low in α-acids and primarily used to impart a desired flavor. These varieties have seen a rapid rise in use as dry hopping becomes more popular. This has also increased the need for more diversity in available hops aroma profiles to impart new, unique flavors into beer. To understand the wide aromatic diversity of hops, we analyzed forty different varieties ranging in both geographical location of origin and genetic age. By employing advanced and comprehensive two-dimensional gas chromatography (GCxGC) in conjunction with mass spectrometry, flame ionization detection, and sulfur chemiluminescence, we obtain in-depth aroma profiles for each individual variety. We found similarities between the major aroma compounds in the samples measured, and key compounds: esters, alcohols, ketones, and volatile sulfur compounds (VSCs). The relationship between the chemical composition of the varieties and their aroma properties were then evaluated by a sensory panel to understand how these different growing regions affect aroma and flavor. Our results provide a comprehensive understanding of the relationship between the chemical and aromatic properties of a wide range of hops, which may help guide future cultivation, breeding, or brewing production in the future.

Markers on the ageing of hoppy ales and non-alcoholic beers Christian Schubert1,2, c.schubert@vlb-berlin.org, Scott Lafontaine2, Nils Rettberg1. (1) Versuchs- und Lehranstalt für Brauerei in Berlin (VLB) e.V., Germany(2) Dept. of Food Sciences, Univ. of Arkansas, Fayetteville Many consumers appreciate beer styles with distinctive characteristics like fruit infused, hop-accented or non-alcoholic beers (NAB). These beers are often distributed and consumed country- or even worldwide, making flavor stability a growing concern for their producers. To date, various studies have investigated flavor stability of alcoholic lager beer or beer model solutions and their chemical markers (e.g. SO2, aldehydes, or esters) are well established. Unfortunately, the chemical drivers of flavor changes in hop accentuated or NABs are largely unknown and it is questionable if they can be transferred to these products. In order to get insights into flavor changes of hoppy ales and NABs multiple studies investigating different Pale Ales, IPAs and double IPAs as well as different Pilsner style NABs were performed. It can be suggested that changes in hoppy ales are linked to chemical or physical modification in the hop aroma itself which is influenced by different hopping regimes (e.g., variety used, late- or dry hopping). Whereas aroma changes in NABs might be related to the different production techniques applied (e.g., stopped fermentation, thermal de-alcoholization, or mixed procedures). The beers analyzed in the different studies were subjected in any case to a storage period at 4 °C and 20 °C in the dark. Besides basic beer parameters (e.g. ABV, bitterness, degree of fermentation) different aroma relevant compounds like higher alcohols, fermentation related esters, hop related esters, hop mono- and sesquiterpenes, or staling aldehydes were analyzed over up to 12 months of storage. To enhance the significance of the results, in parallel a descriptive sensory with trained panelists was also carried out during the storage period to strengthen the analytical results with sensory data. The results are showing on the one hand that marker substance like staling aldehydes known to impact the flavor stability in (alcoholic) Lager styles are less relevant in these products. While on the other hand changes in compounds of interest in these styles (like decreasing concentrations in hop related esters) can highly influence the flavor after storage. These studies are demonstrating the high complexity in flavor changes of hoppy ales and NABs. Furthermore, it can also be seen that a one by one transfer of knowledge based in alcohol containing beer can lead to a misinterpretation of impact factors influencing these products stability.

Quantifying flavor: Characterization of a craft brewery experience using HS-GC-MS and LC-QTOF Ronald A. Quinlan1, ronald.quinlan@cnu.edu, David Mitchell1, Bryan McBride1, Dmitry Liskin1, Andrew Higgs1, Abigail Brehm2, Kevin Kingsbury2. (1) Molecular Biology and Chemistry, Christopher Newport Univ., Newport News, Virginia (2) Tradition Brewing Company, Newport News, Virginia Breweries use instrumental techniques such as gas chromatography, liquid chromatography, and spectrophotometry to monitor brewing processes and to ensure quality standards. For large breweries, these steps are essential for batch-to-batch consistency and brand development. For smaller, craft breweries, the goals for each beer are often more unique. Brewers are frequently seeking creative variants of classic styles to create a full experience for their patrons. Therefore, the ability to predict the phenotype of combinations of ingredients and environment is of great interest to the community. Here we present our characterization of three craft brewery beers using headspace gas chromatography (HS-GCMS) and liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QTOF) along with sensory analysis from untrained panelists. Sensory analysis was performed before and after exposure to environmental factors such as food, ambient lighting, and crowds.

Effect of copper complexation on polyfunctional thiol stability in beer Morgan Vincent1, m.vincent@setonhill.edu, Magdalena Naziemiec2, Alexey Silakov1, Ryan Elias2. (1) Chemistry, The Pennsylvania State Univ., Univ. Park (2) Food Science, The Pennsylvania State Univ., Univ. Park Beer is a deceptively complex and dynamic chemical system that is intrinsically unstable in its finished form. This chemical instability is generally attributed to deleterious oxidation reactions catalyzed by trace levels of transition metals (e.g., Fe, Cu, Mn) in beer, originating from brewing ingredients and metal-leaching from brewing equipment and packaging. Reactive oxygen species (ROS) produced by these reactions are known to oxidize a host of organic species in beer, including polyfunctional thiols, and those reactions inevitably result in the generation of off-flavors or the destruction of desirable flavors. Although present in low concentrations (μg/L), hop-derived polyfunctional thiols (e.g., 3-mercaptohexan-1-ol, 3-mercaptohexyl acetate, and 4-mercapto-4-methylpentan-2-ol) are responsible for the desirable aromas in many modern beer styles (e.g., passionfruit, guava, etc.) in finished beer. Unfortunately, in addition to their

susceptibility to oxidation by ROS, wine researchers have recently unveiled another significant degradation mechanism for polyfunctional thiols, which involves reaction with Cu2+. More specifically, Cu2+ reacts directly with thiols (i.e., thiol oxidation) to form odorless sulfides, thus damaging intended aroma profiles. Thiol oxidation has yet to be studied thoroughly in beer, especially with respect to transition metals. In the present study, electron paramagnetic resonance (EPR) spectroscopy was used to probe the molecular environment of Cu2+ in both a model beer and a commercial pilsner and paired with liquid chromatography with tandem mass spectrometry to assess the reactivity of Cu2+ towards three important hop-related polyfunctional thiols, in the presence of various known metal-binding compounds found in beer.

Crafting the future of beer: Rapid and in-situ quality monitoring using portable IR spectroscopy Haona Bao, bao.172@osu.edu, Luis Rodriguez-Saona. Food Sci. & Tech., The Ohio State Univ., Columbus The art of brewing is a delicate balance of ingredients, yeast metabolism and processing conditions, that yields numerous flavor-active compounds that are critical to the beer's flavor and aroma, which influences consumer acceptance. The aim of this study was to explore the capability of a portable IR as an efficient in-situ production control tool, enabling seamless quality monitoring including marker aroma compounds and common quality parameters during beer production. Various styles of beer (n=100) were provided by a local brewing company (Columbus, OH, USA). SPME-GC-MS method in combination with soft independent modeling of class analogy (SIMCA) was used for non-targeted metabolomics analysis to identify volatile fingerprints compounds of different beer styles. Targeted compounds were quantified using GC-MS headspace method. Then, a portable FT-IR with a triple-reflection diamond ATR was used for spectra collection to generate partial least squares regression (PLSR) models to predict quality parameters including bitterness, ethanol, real Extract P, key aroma compounds. Volatile compounds of interest were identified to contribute most significantly to classifying beers with different formulations and fermentation processes. Robust PLSR models were built from reference data and IR spectral patterns for predicting the alcohol, off-flavor compounds (2,3-butanedione and Dimethyl sulfide) levels, bitterness, real extract, and specific gravity of all samples with excellent correlation coefficients 0.95 and low standard errors of prediction. A portable FT-IR combined with the pattern recognition algorithm showed good predictions of beer quality parameters and volatile compounds, which could provide a rapid, non-destructive, and on-site routine screening tool for beer quality control. The infrared technology would allow brewers to have better control over the beer production process with more consistent quality.

Advancing non-alcoholic beer quality: Examining the impact of NAB chemical profiles on industrial professionals' perceptions and preferences Scott Lafontaine1, scott.r.lafontaine@gmail.com, Erich Leitner2. (1) Food Science, Univ. of Arkansas System, Fayetteville(2) Inst. of Analytical Chemistry and Food Chemistry, Technische Univ. Graz, Steiermark, Austria The surging demand for healthier beverage choices and the brewing industry's commitment to mitigate the adverse effects of alcohol have sparked a wave of interest in designing innovative non-alcoholic beer (NAB) brands. While health-conscious consumers drive this movement, flavor remains a critical factor. Nonetheless, substantial bias from industry professionals towards these products persists. In 2023, extensive evaluations of ten global NAB brands were performed at two international meetings in which industry professionals assessed the sensory profiles as well as their perceptions and preferences towards these brands. Comprehensive chemical profiling was then performed on the brands utilizing both non-volatile (e.g., bitterness units, alcohol by volume, residual extract) and volatile analysis techniques (including GC-MS and GC-SCD). Overall both volatile and non-volatile compounds played pivotal roles in shaping specific flavor profiles, which in turn influenced the preferences and perceptions of the industry experts. Furthermore, the perception of how 'Beer-like' these products were varied among the products. Notably, production techniques emerged as a significant determinant of the chemical and flavor profiles of NAB. This insight empowers the industry to design NABs with more desirable and stable flavor profiles which can better align with evolving consumer preferences.

Next-generation strategies for non-alcoholic lager beer production: A focus on both ethanol removal and flavor preservation Zhengyong Zhou, zz18@illinois.edu, Yong-Su Jin, Keith R. Cadwallader. Food Science and Human Nutrition, Univ. of Illinois Urbana-Champaign The increasing trend of reduced ethanol consumption among young generations, coupled with growing awareness of the health risks associated with alcohol, has led to a remarkable surge in the non-alcoholic beer market in recent years. In the current landscape of non-alcoholic beer production, a traditional and still common approach is to remove ethanol from finished beer products via physical methods such as vacuum distillation and membrane separation. Some manufacturers also choose to prevent ethanol accumulation through biological efforts like pausing the fermentation at the early stage or introducing some non-conventional yeast strains that barely ferment sugars in the wort. Current biological methods may result in high carbohydrate levels in the final product, while the physical techniques may remove considerable amounts of aroma/flavor molecules, and the equipment can be cost-prohibitive. This presentation aims to provide an overview of the current state-of-the-art techniques employed in the production of non-alcoholic beer, with a particular focus on addressing flavor-related challenges. We will also introduce a novel technique involving precision fermentation to remove ethanol from the finished beer with minimal flavor impact. We initiated the study with secondary aerobic fermentation using wild-type yeast strains. Guided by GC-MS and GCO techniques, we identified potential off-flavor compounds formed during the secondary fermentation. We subsequently selected a yeast platform to conduct CRISPR/Cas-9-based genome editing to suppress the formation of off-flavor compounds, mainly esters and phenyl ethanol. To conclude, this study provides a proof of concept of next-generation strategies for non-alcoholic lager beer production with precision fermentation.

MONDAY AFTERNOON

Chemistry of Alcoholic Beverages

1H-NMR-based metabolomics for profiling the chemistry of alcoholic beverages Nicole Kruse1, nicole.kruse@bruker-biospin.com, Clemens Anklin1, Thomas Spengler2. (1) Bruker BioSpin, Billerica, Massachusetts (2) Bruker BioSpin GmbH, Rheinstetten, Baden-Württemberg, Germany Alcoholic beverages have a complex chemistry that can be influenced for example by the alcoholic content, production process, additives or adulterants.1 H-NMR as an intrinsically quantitative method can directly observe, identify and quantify many components present in alcoholic beverages. This can include main components such as ethanol and water but also components present at much lower concentrations. These measurements are used for quality control and the development for example of the nutrition label. The principles behind the methodology are presented using the example of wine. Besides the direct quantification of over 50 compounds, the metabolic "fingerprints" can be established in combination with statistics to evaluate origin, varietals and quality.

From the chemistry of raw materials and fermentation on to the shelf-life stability of beer and distilled spirits Gary Spedding, gspedding@alcbevtesting.com. BDAS, LLC, Lexington, Kentucky, Production of beer and distilled spirits involves much exciting and intricate chemistry, biochemistry, and microbiology. A brief outline of the components derived from raw materials, or produced during fermentation, and then carried through to end products will be presented in a series of diagrams. How several of these key volatiles (flavor) and non-volatile flavor components are then manipulated during processing or in shelf-life-stability will be noted. Beer shelf-life stability has been extensively researched, but such is not the case for distilled spirits. For this presentation, the discussion will end with commentary upon a well-accepted, though little proven, volatiles "fixative effect" for gin. An area of rich terpene chemistry (as for hops in beer production). Speculations as to how a gin-fixative effect could apply will rely upon an understanding of perfume engineering and chemistry. Further illustrating the interdisciplinary nature of today's chemical research challenges.

Effect of proof on the headspace concentrations of methoxyphenols found in whiskey Leonard Demoranville, leonard.demoranville@centre.edu, Sol Y. Cabrera, Michael Curran, Mehak Mittal, Kevin Williams, Sunny Yusufji. Chemistry, Centre College, Danville, Kentucky The proof of whiskey is known to have effects on flavor. The solvent structure of ethanol-water mixtures varies with ethanol/water concentration. This difference in solvent structure leads to different interactions with congener molecules in whiskey. Existing computational literature demonstrated guaiacol partitions preferentially into ethanol-rich surface layers at low ethanol concentrations, suggesting there would be a higher concentration in the headspace above the solution. A headspace gas chromatography method was developed to study the effects of ethanol-water concentration on the relative headspace concentrations of whiskey congeners. Guaiacol and other methoxyphenols found in whiskey were studied and found to be present at higher levels in the headspace when ethanol concentrations were lower.

Application of spectroscopy technology in identification and quality screening of Pisco distillates Yalan Wu, wu.5671@buckeyemail.osu.edu, Luis Rodriguez-Saona. Food Science & Technology, 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. Distillation allows to separate 3 fractions with marked aroma differences, the head has high alcohol content and undesirable levels of volatile aldehydes and esters, the body becomes Pisco after a settling period, and the tail that contains high content of water, fusel alcohols and unwanted by-products. The head and tail fractions are discarded, and these cuts are done by sensory tasting analytical methods for determining the fractions are time-consuming and labor-intensive. We aimed to provide the Pisco industry with a rapid and field-deployable solution for monitoring the quality of Pisco during distillation by using a portable spectroscopy (FTIR-ATR) sensor and pattern recognition analysis. A total of 102 different fractions of distillates were donated by Bodega San Nicolas (Ica, Peru). Gas Chromatography-Mass Spectrometry (GC-MS) was used to verify the fractions of distillates and critical compound contents, and titratable acidity levels were assessed by an automated titrator. Soft Independent Modeling by Class Analogy (SIMCA) classification algorithm clustered the distillation fractions (head, body, and tail) identifying signature bands associated with alcohols (916–855 cm−1) that were related to the class grouping giving with an interclass distance (ICD) over 3. Partial least squares regression combined with variable selection techniques predicted the levels of ethanol (Rcv = 1.0 and SEP = 0.43 %), methanol (Rcv = 0.94 and SEP = 2.95 mg/100 mL), acetaldehyde (Rcv = 0.95 and SEP = 1.6 mg/L), and titratable acidity (Rcv = 0.99 and SEP = 1.12 mg/100ml) contents in Pisco fractions. Portable FTIR-ATR spectroscopy is a promising tool to classify and predict quality in spirits distillations. These methods could provide reliable rapid and non-destructive assessments for alcoholic beverage quality control purposes with minimal personnel training.

Evolution of chemical profiles in rice: From milling to malting and its influence on beverage/ beer quality Bernardo P. Guimaraes, bpg002@uark.edu, Rahul Sen, Scott Lafontaine. Dept. of Food Science, Univ. of Arkansas, Fayetteville Barley has been bred for malting and used in brewing for millennia for its optimal starch/protein ratio, enzymatic activity, and filterability. In brewing, rice has been primarily used only as milled rice serving as a neutral flavor adjunct (another source of starch) to be used in addition to barley malt, while rice hulls have been used as a filtration aid. However, recent studies have found that malted rice opens opportunities for new aromas, flavors, colors, which could lead to the development of novel gluten-free products. Rice has an enormous diversity of physiochemical characteristics (i.e., color ranging from white to black, zero to high apparent amylose content, gelatinization temperatures, aromatic or non-aromatic, etc.). Aromatic rice has 2-acetyl-1-pyrroline (2-AP) as the major odor active compound. This study aimed to analyze how milling and malting alter the volatiles when compared to paddy rice. To evaluate the impact of rice cultivar on the resulting aromatic profile of rice, 20 samples (19 cultivars from all over the world with one rice cultivar being procured from two different growing locations and years) were analyzed with SPME-GC-MS/MS as well as with other nonvolatile techniques. Generally, the volatile/ nonvolatile profile of the rice changed significantly over malting and there were differences observed between the cultivars. The resulting aroma of an all-rice-malt non-alcoholic beer of the three most promising cultivars from a brewing perspective was then evaluated against an all-malt product. This data shows that rice malt can be used to produce beverages with unique characteristics and could serve as a more climate-resilient and locally produced gluten-free source of starch for brewers and beverage/ food producers as compared to malted barley.

Quality and acceptability of wines processed using underutilized African edible indigenous fruits Omujal Francis2, fomujal@gmail.com, Sheilla Natukunda1, William Olupot3. (1) Food Technology, Nutrition and Bioengineering, Makerere Univ. College of Agricultural and Envir. Sci., Kampala, Uganda(2) Natural Chemotherapeutics Research Inst., Kampala, Uganda(3) Nature and Livelihoods, Kampala, Uganda Edible indigenous fruits (EIF) ripen within a short time generating surplus production that get wasted during their peak seasons. However, wines made from EIF have of recent dramatically attracted attention of scientists, given their range of health promoting properties and consumer preference. This study evaluated the quality and consumer sensory acceptability of wines made from three underutilized African EIF; Carissa edulis (Apocynaceae family) Flacourtia indica (Salicaceae family) and Vitex doniana (Lamiaceae family) of Uganda. The fruits were harvested during their peak seasons, depulped, pasteurized, blended with sugar to a brix of 24oB and fermented for 28 days. The respective formulated wines were tested for quality and consumer acceptability with a trained panel using a 9-point hedonic scale (9= like extremely and 1=dislike extremely). Data analysis was performed using analysis of variance. The pH, brix, titratable acidity (TA) and alcohol content (AC) of the wines ranged from 3.27±0.00-3.47±0.00, 12.00±0.00-19.00±0.00oB, 0.43±0.01-0.60±0.01% and 5.14±1.44- 13.30±2.27%. The bioactive compounds including; total

flavonoids (TF), total phenolic compounds (TPC), total anthocyanins and total antioxidant activity (TAA) ranged from 2.13±0.17-11.31±0.59mg/100g Quercetin Equivalent (QE), 4.33±0.03- 10.93±.13 mg/100g Garlic Acid Equivalent (GAE), 0.11±0.10-3.36±0.16 mg/g, 3.46±0.05-4.14±0.00mg/100g QE respectively. The sensory characteristics; appearance, colour, flavour, clarity, aroma, taste, mouth feel, and general acceptability had the scores ranging from 6.7±1.28-7.3±1.35, 6.5±1.48-7.3±1.39, 6.8±1.57-7.2±1.09, 6.4±1.53-6.8±1.64, 6.5±1.66- 6.8±1.65, 6.9±1.88-7.5±1.38, 6.8±1.75-7.3±1.27 and 6.8±1.67-7.6±0.92 respectively. Further data analysis showed no significant differences ($p \leq 0.05$) in AC, brix, TPC and TA of C. edulis and F. indica wines; and also total anthocyanins between F. indica and V. doniana. However, there were significant differences ($p \leq 0.05$) in TF and most sensory attributes in the three wines. In conclusion, wines made with F. indica and C. edulis fruits did not only have considerable bioactive contents with health promoting properties, but also received significant acceptability in taste, flavour, mouth feel and general acceptability. There is need to promote the production and commercialization of wines processed using F. indica and C. edulis fruits.

Sensory Beyond Earth: The Relevance of Flavor Chemistry in Space Exploration

Consequences of olfactory loss Thomas Hummel, thomas.hummel@tu-dresden.de. Dept. of Otorhinolaryngology, Technical Univ. of Dresden, Germany The sense of smell is important – many of us noticed its importance during the SARS-CoV2 pandemic where olfactory loss is one of the major symptoms of the infection. We respond to body odors of our fellow human beings - the nose modulates our preferences. To many of us the perception of odors and flavors are synonymous to quality of life! And smells also influence our working life: For example, perfumers, bakers or chefs are dependent on the sense of smell! And the sense of smell is important for the perception of fires / smoke or spoiled foods. Without smelling, life is poorer, it lacks one dimension! The lecture will show how olfactory disorders affect people, what types of olfactory disorders there are, and also touch upon aspects of how olfactory disorders can be diagnosed and treated.

The effects of a One-Year Antarctic Sojourn at the Concordia Research Station on olfactory and gustatory functions Isabelle Mack1, Isabelle.mack@uni-tuebingen.de, Bea Klos1, Sophia Wolf1, Stijn Thoolen2,3, Hannes Hagson2, Andrea Meyer1, Paul Enck1. (1) Dept. of Psychosomatic Medicine and Psychotherapy, Univ. Hospital Tuebingen, Baden-Württemberg, Germany(2) Institut Polaire Francais Paul Emile Victor, Plouzane, Bretagne, France(3) Dept. of Psychiatry, Massachusetts General Hospital, Boston, Massachusetts In isolated confined extreme (ICE) environments, it's crucial to maintain a healthy body weight. Sensory functions, specifically the senses of smell and taste, are of significant importance in the context of dietary intake, representing key factors in maintaining appropriate energy intake and body weight. In a hypoxic ICE environment, such as the Concordia Station in the mainland of Antarctica, it is believed that there may be potential changes in these sensory functions. However, existing data are scarce. We investigated olfactory function (threshold, identification, discrimination) using ODOFIN Sniffin' Sticks and gustatory function using ODOFIN Taste Strips (taste identification test for the taste qualities sour, salty, sweet and bitter) as part of the 'Immune and Microbiome Changes in Environments with Limited ANtigen Diversity' project (ICELAND). The 19 participants of the winter-over periods 2019/2020 and 2021/2022 (39.2±10.9 years, 3/19 female) were examined upon baseline (T0) and three times during the Antarctic sojourn (T1-T3) by trained staff. Taste was also tested six months post Antarctica (T4). At T0, 3 out of 19 participants exhibited hypogeusia. This proportion increased to 6 out of 19 participants 2-month post-arrival at the Concordia Station (T1) and subsequently stabilized at 4 out of 19 participants (T2-T4). The sweet taste quality consistently yielded the highest identification rates over all times. Notably, a significant decrease in cumulative salty taste scores was observed over the course of the Antarctic stay, returning to baseline levels at T4. At both T0 and T1, 4 out of 19 individuals experienced hyposmia. This prevalence increased to 5 out of 19 participants during the Antarctic winter, remaining stable until the end of the Antarctic stay. Overall, olfaction sum scores exhibited a downward trend from baseline throughout the duration of their time in Antarctica. Living one year in an extreme and hypoxic environment as Concordia Station in Antarctica affects olfactory and gustatory function individually to different extents. Some individuals may temporarily exhibit extreme reduced taste and/or olfactory function.

HABSIM – Unique R&D Infrastructure for closed-loop food production in space and on Earth Tor Blomqvist, tor.blomqvist@dlr.de, Daniel Schubert. Planetary Infrastructures, Deutsches Zentrum fur Luft- und Raumfahrt DLR Standort Bremen, Germany There is a reinvigoration of human space travel and the goal is to establish a lunar base with a continuous human presence by 2030, a vital step towards reaching Mars. However, a formidable challenge emerges: while technology can transport humans to the Moon, a self-sustaining food system is lacking, making food a limiting factor for extended space travel. Logistical and economic constraints, coupled with food acceptability challenges, render Earth-dependent resupply missions impractical for future lunar habitats. Consequently, in situ food production becomes imperative for sustained human space travel. Research has explored methods like insect farming, cultivated meat, and Controlled Environmental Agriculture (CEA), yet critical aspects like nutrient-rich crop production and post-harvest management remain overlooked. Addressing these gaps is crucial for establishing independent, variable, and nutritionally adequate food production on the Moon. Food processing enhances shelf life, nutritional quality, introduces new crop varieties, and facilitates the creation of novel products. It enables the processing, preparation, and storage of staple foods and alternative protein sources, contributing to a diverse and sustainable diet over extended missions. In the current fragmented landscape of space food research, the lack of a cohesive, integrated approach hinders progress. A holistic strategy is essential to systematically test synergies between innovations and human involvement. The proposed solution is a centralized research facility integrating post-harvest management and CEA, augmented by cutting-edge laboratory infrastructure. This facility acts as a versatile closed-loop food production system tailored for lunar habitats, fostering collaboration, accelerating research, and addressing critical gaps in the space food production ecosystem.The urgency of this initiative aligns with the plans of international space agencies to establish a constant human presence on the Moon within the decade. The research facility not only addresses the immediate need for advanced food production capabilities for prolonged lunar missions but also lays the groundwork for sustainable food systems in extraterrestrial and terrestrial environments. This comprehensive platform catalyzes collaboration, bridges gaps, and expedites research in space food production, propelling the realization of sustainable food systems for future space missions and on Earth.

Microwave processed ready-to-eat meals as a palatable and nutritional option for space missions Maria L. Montero, maria.montero@wsu.edu, Carolyn F. Ross. School of Food Science, Washington State Univ., Pullman In long duration space missions, prepared foods are often the only source of energy and nutrients

supporting human activities. Due to the challenges faced in space travel, it is critical that these foods are safe and free of pathogens, nutritionally dense, and tasty, while also having adequate shelf-life. To address these meal requirements, microwave assisted thermal sterilization (MATS) and pasteurization (MAPS) systems have been developed. These are novel technologies used to process multicomponent meals. To assess the application of MAPS and MATS for the production of ready-to-eat meals with possible extension to space missions, several studies were conducted. In evaluating the influence on the sensory quality of the MAPS processed meals, one study evaluated consumer (n=50) acceptance of ready-to-eat jambalaya meals processed with MAPS and stored over 12 weeks at 2°C. While noting some changes in meat texture over time, this study suggested that the shelf- life of microwave-processed meals could be extended up to 12 weeks without affecting overall liking. In addition to considering meal palatability, nutritional content of meals for space travelers is important. One study examined salt reduction, alongside MATS processing, in ready-to-eat chicken pasta meals. These meals were prepared at varying levels of salt reduction (25 – 100%) and herb addition, processed with MATS, and tested with consumers (n=165) at different storage times. After one-year of storage, no changes in acceptance of sensory properties or liking were noted. The addition of herbs also allowed for a 50% salt reduction while maintaining the overall liking of the meal. A follow up study examined the influence of combined strategies, flavor addition and MATS processing, to achieve salt reduction in mashed potatoes. Results showed that the salt level could be reduced by 50% while still maintaining flavor and overall acceptance in freshly prepared samples. As evaluated by consumers (n=100), the saltiness intensity of this 50% reduced salt sample was not different from the freshly prepared samples when processed via MATS. This body of research shows how MAPS and MATS processing of ready-to-eat meals produces a safe meal with extended shelf like, while maintaining palatability and providing an avenue for salt reduction. This technology shows great promise as an important element for diversifying the sources of energy and nutrition for space travelers

Development of a virtual reality tool ('food in space') for collecting sensory data during immersion for space ground-based strategy Grace Loke1, Ian Peake2, Anne Besnard3, Kevin Kantono3, Gail Iles1, Lisa Newman1, Julia Low1, julia.low2@rmit.edu.au. (1) School of Science, RMIT Univ., Melbourne, Victoria, Australia(2) RMIT Univ. STEM College, Melbourne, Victoria, Australia(3) International Flavors and Fragrances Nederland BV, Hilversum, North Holland, Netherlands The present study aimed to address the limitations of ground-based food and sensory research in representing the isolated and confined environment of spacecraft. Virtual Reality (VR) technology was employed to simulate the experience of isolation and confinement within space. The VR simulation emulates the International Space Station in low Earth orbit, comprising interconnected space modules equipped with integrated sensory analysis tools for evaluating food odour cues within the VR environment. Participants were asked to rate the intensity of 8 food odours (vanilla, lemon, almond, eucalyptus, peppermint, lemon myrtle, lemongrass, vinegar) and a control on a 5-point Likert scale, in the neutral sitting posture context, a NASA-Neutral sitting posture (mimicking a 'microgravity' posture using a commercial 'Zero-gravity' outdoor chair set at 122-124°) and within the VR simulation. To account for individual scale usage, we applied individual scale factors for response standardisation. The study involved 44 adults between the ages of 18 – 39 years, with no history of motion sickness and/or vertigo. Odour evaluation within the VR context demonstrated significantly higher intensity ratings for the vanilla (P=0.002) and almond (P=<0.001) odours, as compared to when evaluated in the neutral context. However, the intensity of lemon odour was not found significantly different between the two contexts. Interestingly, the perception of nasal trigeminal stimuli such as eucalyptus, peppermint, vinegar was also perceived as significantly more intense in the VR simulation environment in comparison to when evaluated in the neutral context (all P<0.05). The perception of nasal trigeminal stimuli requires further investigation as they may influence food palatability within the outer space/ simulated isolated context eating environments. These results suggest that environmental context may manipulate odour perception of select odours and such manipulation is achievable using VR technology. Personal variation of odour perception should also be taken into consideration, especially in creating personalised meal plans for space applications.

Correlations between food odour perception during space simulated analogs and their volatile profiles Jayani Chandrapala1, jayani.chandrapala@rmit.edu.au, Grace Loke1, s3732147@student.rmit.edu.au, Ian Peake2, Gail Iles1, Julia Low1 (1) School of Science, RMIT Univ., Melbourne, Victoria, Australia(2) RMIT Univ. STEM College, Melbourne, Victoria, Australia The constraints of Earth-based studies limit our comprehension of sensory perception in the unique conditions of confinement and isolation characteristic of extended spaceflights. In prior experiments, our team assessed the odour intensity perception of eight commercial odours (vanilla, lemon, almond, eucalyptus, peppermint, lemon myrtle, lemongrass, vinegar). These were evaluated in three distinct contexts: a neutral sitting posture, a NASA-neutral sitting posture (emulating a microgravity posture with a commercial 'Zero-gravity' outdoor chair set at 122-124°), and a virtual reality (VR) simulation, all using 5-point intensity scales. Within the VR context, trigeminal stimuli like eucalyptus, peppermint, and vinegar were rated significantly higher intensity ratings in the VR space-simulated environment in comparison to the NASA-Neutral posture, although there were no significant differences observed for all the citrus odours evaluated. However, it is of utmost importance to establish a connection between volatile compounds and trigeminal sensory responses. To achieve this, HS-SPME GCMS experiments were carried out. The unique profiles of individual volatile compounds were compared with the trigeminal sensory stimuli and correlations were deduced through PCA.

Exploring effective tasting delivery modalities for tasting sensory studies in simulated space analogs Thejani Prabodha1, S3969476@student.rmit.edu.au, Lauren Ong1, Chloe Gilden1, Ian Peake1, Charles Brennan1, Lukas Danner2, Gail Iles1, Julia Low1. (1) RMIT Univ. STEM College, Melbourne, Victoria, Australia(2) CSIRO Sensory and Consumer Science, CSIRO Agriculture and Food Business Unit, Werribee, Victoria, Australia Assessing sensory responses in simulated space conditions is essential to understand astronaut eating behaviors and perceptions in challenging environments. This project seeks to identify optimal feeding methods for ground-based space simulations, enhancing our comprehension of human food perception in space. We are examining various feeding modalities, including pouches alone and pouches with straws for liquid tasting, as well as pouches/bags paired with spoons or direct cup consumption for solid and semi-solid foods. Our study includes an array of liquid beverages, varying from different textural thicknesses to semi-solids, and solid foods, specifically messy and sticky foods like rice with diverse textures. We evaluate sensory aspects such as smell and taste intensity, the appeal of smell and taste, and participants' preferences regarding the feeding methods. Our research is set in three distinct contexts: a traditional sensory booth (where participants sit in a neutral posture), a NASA-Neutral setting (mimicking a 'microgravity' posture using a commercial 'Zero-gravity' outdoor chair set at 122-124°), and a 4K virtual reality (VR) environment replicating the

confined and cluttered dining conditions of the International Space Station. The study will involve 30 participants and is currently ongoing. The results from this research will provide crucial insights to improve methods for conducting ground-based food studies in space-simulated settings. Additionally, they will help comprehend how the mode of food presentation in these contexts affects sensory perceptions, guiding the development of an ecologically valid approach.

Influence of immersion in a space-like environment on taste and odour perception Alicia Tran1, Julia Low2, Lisa Duizer1, lduizer@uoguelph.ca. (1) Dept. of Food Science, Univ. of Guelph, Ontario, Canada(2) School of Science, RMIT Univ., Melbourne, Victoria, Australia Existing literature suggests that environmental factors (i.e., sound and smell) may contribute to a change in sensory perception of food eaten in space, however, this has yet to be fully investigated. To explore the effects of environmental space-like conditions on taste and odour perception, two studies were conducted. The first study involved 60 participants with no hearing impairments, investigated the effect of environmental International Space Station (ISS) sounds played through headphones on intensity of the five basic taste (aqueous solutions, model foods using chocolate pudding). This study revealed that the ISS-like sounds at 70 dB had no impact on taste. A second study investigated the effects of immersion in a space-like environment on odour perception (food grade vanilla, almond and citrus scents), hunger ratings and emotional responses. Two separate audio clips were used and edited together [Audio from the STS-134 final launch of the Space Shuttle Endeavour (NASA, 2011)] and was played on a 7.7m (length) x 3.2m (height) immersive screen angled in the centre at 126° to create an immersive effect. This experiment involved 29 participants watching a 20 min video whilst completing sensory evaluation at 1.5, 5, 10, and 15 min timepoints. Findings suggested that odour perception and emotional responses varied based on the specific odours presented and light conditions (light versus dark immersion environments). This research, while foundational, emphasizes the need for more refined studies in settings closely replicating space to understand the relationship between space environments and sensory perceptions better. Interestingly, the utilization of immersive screens resulted in more positive emotional ratings towards the end of the evaluation while decreases negative emotional ratings such as boredom, suggesting that the experimental setup might have been reminiscent of a cinematic experience rather than inducing the stress of actual space-like eating conditions. Further studies must be performed under more representative conditions and with more dynamic food systems to fully characterize the effect of environmental factors on perception of taste and odour in space.

VIRTUAL SESSION

AGFD General Poster Session and Undergraduate Poster Competition

Exploring Taiwan citrus extract's potential in inhibiting colorectal cancer growth Zheng-Yuan Su1, zysu@cycu.edu.tw, Chia-En Chiang1, Guor-Jien Wei2. (1) Chung Yuan Christian Univ., Taoyuan City, Taiwan(2) National Yang Ming Chiao Tung Univ., Taipei, Taiwan The health challenge of colorectal cancer rates worldwide has remained high in recent years. Flavonoids, which are found in citrus fruits and are abundant in vegetables and fruits, have been studied for their potential anticancer, anti-inflammatory, and antioxidant properties. This study examines the inhibition effects of Citrus depressa (CD) and Citrus microcarpa (CM) extracts on the growth of HCT116 colorectal cancer cells. Various solvents were used to extract pomace from CD and CM fruits at first. The active compounds in each extract were quantified using high-performance liquid chromatography (HPLC). Ethyl acetate extract of CD (CD-EAE) exhibited the highest concentration of polymethoxylated flavones (PMFs), including nobiletin and tangeretin, at 73.0 ± 7.5 and 35.80 ± 3.7 mg/g dried extract, respectively. CD-EAE was found to have the strongest inhibition of HCT116 cell growth among these extracts, with an IC50 of 41.8 g/mL. CD-EAE induced an increase in mRNA expression of tumor suppressor genes p21 and DLEC1, while inhibiting epigenetic regulatory enzymes (DNMTs and HDACs). Additionally, CD-EAE increased the expression of pro-apoptotic proteins, including caspase 3, caspase 9, and Bax. In conclusion, CD-EAE exhibits substantial potential as an herbal medicine for inhibiting growth of colorectal cancer, representing a promising avenue for further research and development.

General overview of intoxications by wild toxic mushrooms, case study: Algeria Mimoune Souna, mimoun.souna@univ-tlemcen.dz. Univ. Abou Bekr Belkaid Tlemcen, Algeria The incidence of wild mushroom poisoning varies from country to country, depending on the consumption rate. Although poisoning by wild mushrooms or mycetism (mycetismus) is rare, but sometimes fatal, we thought it would be useful to take a brief look at the poisoning caused by toxic higher fungi. A retrospective descriptive study of cases of accidental intoxication by ingestion of mushrooms recorded by the national Inst. of public health and a bibliographical study of intoxication syndromes. A preface on the different approaches by clinical syndrome and the interpretation of the epidemiological data for 2008, as well as a preamble on the protocol to be followed. The most dramatic case of mycetism in Algerian history occurred in 2008, a series of cases of poisoning was recorded, 195 cases including 16 deaths. It is difficult to identify the species of fungi consumed, so diagnosis is based on the clinical signs and the time taken for them to appear. According to the 6-hour rule, short-latency syndromes (Resinoidian, Sudorian, Pantherinian, Narcotinian, Coprinian and Paxillian syndromes) have a favourable prognosis, with rare serious cases, while long-latency syndromes (Phalloidian, Gyromitrian, Orellanian, Proximian, Acromelalgian and Rhabdomyolysis syndromes) are potentially serious and require hospitalisation. A distinction was made between 3 situations: ingestion less than six hours ago with no clinical signs, mild forms and severe forms. This rule can go awry when multiple species are consumed during the same meal, or when a type is consumed consecutively.

Phytochemical properties, processing, and applications of juvenile Ginger (Zingiber officinale) Bokary Sylla, bsylla@umes.edu, Victoria Volkis. Natural Sciences, Univ. of Maryland Eastern Shore, Princess Anne, Maryland, USZingiber Officinale, commonly known as ginger, has a long-standing history as a natural remedy for ailments and disease. Adult rhizomes are used in medicine, food, and beverages. It has been shown that juvenile ginger harvested at 9-11 weeks has strong anti-obesity properties, while the mature ginger typically found on the shelves of food markets, does not possess the same qualities. This project aims to explore the capabilities of young ginger rhizomes, with the intent of determining whether or not young ginger is more phytochemically potent than its adult form. Young ginger has the advantage of being easier to grow in a variety of conditions, and easier to use in culinary applications. We have studied the ripeness process of ginger supported by phytochemical analysis of samples and found that behind its tender flesh, young ginger is a host to many bioactive compounds such as gingerol, shogaol, and zingerone essential oils. Moreover, we have found that phenolics, and flavonoids have much higher concentration in young ginger as compared to the mature one. Quantitative analysis of ginger extracts created from high-tunnel cultivars reported an increase of up to 60%

(mg GAE/g) in total phenolics, 87% (mg QE/g) in flavonoid content, and 67% (mg TAE/g) in tannin content difference between ginger grown within the first nine weeks of maturity and ginger older than eleven weeks. We will also report the comparison of fresh-frozen and freeze dried ginger, the influence of bread on phytochemical process, and the influence of thermal processing on antioxidants capacity.

Photocatalytic visible light active Co doped ZnO/cellulose acetate nanofiber membranes for functional food packaging Sachini Deshapriya, sachinideshapriya4@gmail.com, Imalka Munaweera. Dept. of Chemistry, Univ. of Sri Jayewardenepura, Nugegoda, Western , Sri Lanka As a food packaging material, an electrospun nanofiber (NF) membrane of cellulose acetate (CA) with visible light (VL) active cobalt-doped ZnO (Co-ZnO) nanohybrids was developed, utilizing the photocatalytic mechanism of Co-ZnO to degrade microbes available in fruits and to slow down the ripening process by degrading ethylene. ZnO photocatalyst is typically active in the ultraviolet range; therefore, it was fine-tuned by doping Co to operate in the visible-light spectrum. Undoped ZnO nanoparticles (NPs) and Co-ZnO nanorods with Co: Zn atomic ratios of 5%, 10%, 15%, and 20% were synthesized, using co-precipitation method. Crystallization of the NPs occurred in a hexagonal wurtzite structure, as evidenced by the PXRD and Raman spectra. The inclusion of Co ions into the ZnO lattice was confirmed by X-ray photoelectron spectroscopy, energy dispersive X-ray spectroscopy, and PXRD patterns. According to scanning electron microscopy (SEM) analysis, doping ZnO NPs with Co causes them to transform from their original spherical shape into a rod-like one. Doping with Co caused a red shift in band gap energy, from 3.26 to 3.01 eV, close to the VL region. The breakdown of methylene blue dye molecules under VL was used in the photocatalytic research of NPs. The most efficient photocatalyst was 15% Co-ZnO, with a degradation rate of 40% when exposed to sunshine. The NF membrane was created using an electrospinning process that included 15% Co-ZnO in the CA polymer matrix. The successful incorporation of Co-ZnO into the polymer matrix was measured by PXRD patterns and peak shifts in Fourier-transform infrared spectroscopy. The prepared NF mat with CA+ Co-ZnO provided the model crop with the longest shelf life, strawberries, compared to the control mats. The optimized Co-ZnO NF mat increased shelf life by up to 18 days while reducing weight loss, hardness, and titratable acidity and increasing pH less than control mats.

Comparison of phytochemical and antimicrobial activity of leaf, stem and root of Terminalia avicennoides Oluwayemi O. Onawumi1, estherdr@rocketmail.com, Abiodun Sodamade1,2, sodamade1@gmail.com, Dupe L. Abiona1,3, Olufisayo A. Onawumi4. (1) Pure and Applied Chemistry, Ladoke Akintola Univ. of Technology, Ogbomoso, Oyo, Nigeria(2) Dept. of Chemistry, Emmanuel Alayande Univ. of Education, Oyo, Nigeria(3) Dept. of Chemistry, The Polytechnic, Ibadan, Oyo, Nigeria(4) Dept. of Bioscience, Federal Research Inst. of Nigeria, Ibadan, Oyo Plants have proved useful to man in many forms over the years. They have been good sources of food, medicine, shelter and various form of raw materials of immense value. Terminalia avicennoides is an important medicinal plant in which leaf, stem and root are used to treat many pathological conditions. The phytochemical and the antimicrobial activities of the leaf, stem and root were determined so as to compare the most active part of the plant. The leaves, stem and roots of Terminalia avicennoides were selected and processed to analyze their phytochemical constituents and its antimicrobial activity using standard methods. The results of the qualitative analysis showed the presence of alkaloids, tannin, saponin, steroids, phlobatannin, terpenoids, and cardiac glycerides. The results of the quantitative analysis show the presence of tannin; 3.65±0.36mg/100g, 2.41±0.78 and 11.30±0.93 in the leaf, stem and root respectively. Total phenols are 2.96±0.88, 1.34±0.46 and 6.79±0.58, and showed that phytate and oxalate in the root are greater than the content in the leaf and stem. Alkaloids present in the leaf, stem and leaf respectively are 5.65±0.41, 2.08±0.71, 10.47±0.86, while in saponin 2.47±0.031, 1.45±0.73 and 3.63±0.62respectively. The Flavonoid content was greater in the leaf compared to other parts. The ethanolic extracts of the leaf, stem and root of the plant sample showed strong antimicrobial activities against Staphylococcus aureus, Neisseria gonorrhea, Streptococcus pyogenes Streptococcus faecalis, Pseudomonas aeruginosa, Klebsiella pneumonia and Proteus mirabilis. All the plant parts contain phytochemicals which are useful as medicine with the root part to be most potent with high concentration of the phytochemicals. Pharmaceuticals are therefore encouraged to take advantage of Terminalia avicennoides root.

Novel approaches of microscopes application on the development of comparison of fruit flies Edward J. Parish1, Hiroshi Honda1, chrishonda@yahoo.com, Yu-Chen Lo2, Gui Ren4, Huey-Lih Shyu3, Tsao-Yi Wei1. (1) Chemistry, Auburn Univ., Auburn(2) Chemistry, Univ. of California Los Angeles(3) Medical Technology, Central Taiwan Univ. of Science and Technology, Taichung, Taiwan(4) Economics, Shanghai Univ., China This paper reports novel application of the development of scanning electron microscopes comparison of fruit flies.

Untargeted and targeted metabolomics reveal the chemical characteristic of pu-erh tea (Camellia assamica) during pile-fermentation Piaopiao Long, piaopiao-long@outlook.com. Anhui Agricultural Univ., Hefei, Anhui, China Pile-fermentation is the most important process of producing ripened pu-erh tea. To study the chemical changes of tea leaves during pile-fermentation (PF), liquid chromatography coupled with tandem mass spectrometry (LC-MS) was used. Untargeted metabolomics analysis revealed that the first stage of PF is crucial in transforming the original secondary metabolites, whereas the contents of flavan-3-ols and gallic acid were decreased after long-term PF. Targeted metabolomics analysis indicated that the levels of puerins (N-ethyl-2-pyrrolidinone substituted gallocatechin and catechin) were significant increased after the first stage of PF, but after long-term PF the levels of flavonol glycosides, procyanidins and galloylated flavan-3-ols were significantly decreased. Accordingly, long-term PF also decreased the inhibition of α-amylase and α-glucosidase activities of the extracts. As a conclusion, pile-fermentation is an important step of changing the polyphenols and bioactivities of pu-erh tea.

Enhancing potato storage efficiency: A blend of essential oils Hanin Almutairi1, hanin.almutairi@oregonstate.edu, Valtcho Jeliazkov1, Charles L. Cantrell2. (1) Dept. of Crop and Soil Science, Oregon State Univ., Corvallis(2) Natural Products Utilization Research, USDA Agricultural Research Service, Univ., Mississippi Managing potato sprouting during storage presents a significant challenge, leading to food wastage and economic losses. Essential oils (EOs) have shown promise as sprout suppressants, yet their effectiveness varies based on EO type, concentration, and storage conditions. Based on our previous study, this study aimed to identify the optimal blend of three EOs; Pelargonium graveolens, Cinnamomum camphora, and Origanum majorana for effectively inhibiting potato sprouting during room temperature storage. The experiment involved three potato cultivars; Ranger, La Ratte, and Norkotah mini tubers. These potatoes were exposed to different EO blends and stored for 90 days, with regular measurements of sprout weight, length, and quantity. Results indicated that Origanum majorana EO displayed significant sprout suppression when used alone for 60 days. Notably, blending two or more EOs exhibited

enhanced efficacy. An optimal EO blend for suppressing potato sprouting at room temperature storage was identified that most effectively restrained both sprout length and number throughout the entire 90-day storage period. These findings highlight the potential of EO blends as efficient sprout suppressants for potatoes stored at room temperature. Further research is imperative to validate this blend's efficacy under diverse storage conditions and across various potato cultivars, paving the way for sustainable and eco-friendly solutions to the potato sprouting challenge.

MONDAY EVENING

AGFD Sci-Mix

See first 23 abstracts listed under the Sunday Evening AGFD Poster Session

TUESDAY MORNING March 19

Toward Precision Nutrition - Holistic View of Relationship Between Food, Food Components Contribute to Taste, Aroma, Color, and The Gut Microbiome in Health Promotion

Chronic dietary zinc deficiency alters gut microbiota composition and function Elad Tako, et79@cornell.edu. Dept. of Food Science, Cornell Univ., Ithaca, New York Zinc (Zn) deficiency is a prevalent micronutrient insufficiency. Although the gut is a vital organ for Zn utilization, and Zn deficiency is associated with impaired intestinal permeability and a global decrease in gastrointestinal health, alterations in the gut microbial ecology of the host under conditions of Zn deficiency have yet to be studied. By conducting a series of long term in vivo (Gallus gallus) feeding trials, we aimed to characterize distinct cecal microbiota shifts induced by chronic dietary Zn depletion, and in the context of complete diets are based on Zn biofortified food crops that are relevant to target populations, and in geographical regions where dietary Zn deficiency in a major health concern. We demonstrate that Zn deficiency induces significant taxonomic alterations and decreases overall species richness and diversity, establishing a microbial profile resembling that of various other pathological states. Through metagenomic analysis, we show that predicted Kyoto Encyclopedia of Genes and Genomes (KEGG) pathways responsible for macro- and micronutrient uptake are significantly depleted under Zn deficiency; along with concomitant decreases in beneficial short chain fatty acids, such depletions may further preclude optimal host Zn availability. We also identify several candidate microbes that may play a significant role in modulating the bioavailability and utilization of dietary Zn during prolonged deficiency. Our results are the first to characterize a unique and dysbiotic cecal microbiota during Zn deficiency, and provide evidence for such microbial perturbations as potential effectors of the Zn deficient phenotype.

Dietary carbohydrates, gut microbes, satiety, and health Mary Kable1,2, mary.kable@usda.gov, Danielle Lemay1,2, Nancy Keim3,2. (1) Immunity and Disease Prevention, US Dept. of Agriculture, Agricultural Research Service, Davis(2) Nutrition, Univ. of California Davis(3) Obesity and Metabolism Unit, US Dept. of Agriculture, Agricultural Research Service, Davis, California Increased consumption of dietary fiber is frequently advocated as way to improve diet quality and potentially, health. However, the amount of dietary fiber consumed in the US remains well below the amount recommended in the dietary guidelines. Researchers at the USDA are working to understand the composition of carbohydrates that are already being consumed by Americans, and how various food types affect satiety, postprandial glucose response, and gut microbiome composition. Work from Kable, Lemay and Keim Labs at the USDA-ARS, Western Human Nutrition Research Center will be presented.

Comparative analysis of western diet and chronic alcohol consumption shows dramatic alterations in the gut and plasma metabolome using non-human primate model Courtney Christopher1, cleathe3@vols.utk.edu, Hector F. Castro1, Shawn R. Campagna1, Liz Simon2,3,4, Robert Siggins2,3,4, Patricia Molina2,3,4, David Welsh2,3,4. (1) Chemistry, Univ. of Tennessee Knoxville (2) Comprehensive Alcohol-HIV/AIDS Research Center, LSU Health New Orleans, Louisiana, (3) Dept. of Physiology, School of Graduate Studies, LSU Health New Orleans, Louisiana (4) Dept. of Biostatistics, School of Public Health, Louisiana State Univ., Baton Rouge Western diet (WD) and chronic binge alcohol (CBA) consumption are common confounding factors in human gut microbiome (GM) studies and are known to alter the composition and function of the GM. In an era harnessing the GM in precision medicine, it's not only crucial to understand the individual impact of WD and CBA on the GM, but it's equally important to study the complex interaction of WD+CBA on the GM to increase the translational value of the conclusions to humans. The work herein used a non-human primate model (NHP) to identify the fecal and plasma metabolic alterations induced by WD, CBA, and interaction of WD+CBA. To analyze the impact of WD and CBA on the fecal and plasma metabolome, an ultra-high performance liquid chromatography high resolution mass spectrometry approach was used. Fecal and plasma samples were collected at the following times: baseline, 3-month fed WD, 7-month fed WD and 4-month CBA, and 7-month fed WD and 4-month vehicle control. Statistical analysis revealed 24, 45, and 72 microbial related fecal metabolites that were and significantly altered by CBA, WD, and WD-by-CBA, respectively. In the plasma metabolome, there were 18, 33, and 64 metabolites significantly altered by CBA, WD, and WD-by-CBA, respectively. Metabolites unique to CBA in both the fecal and plasma metabolomes included aromatic amino acids, sulfur, purine, pyrimidine, and NAD metabolism. Also, metabolites involved in methionine metabolism, which are markers of oxidative stress, were significantly increased by CBA. Metabolites unique to WD were primarily involved in arginine biosynthesis, starch and sucrose metabolism, and amino acid degradation. While metabolites altered in a WD by CBA manner were associated with taurine, hypotaurine, inositol phosphate, sulfur, and methionine metabolism, TCA, and tryptophan biosynthesis. Combined, this demonstrates the complex interaction of WD+CBA on the fecal and plasma metabolome.

Advances in neuroimaging to explore the microbiota-gut-brain axis Sally Eldeghaidy, sally.eldeghaidy@nottingham.ac.uk. Univ. of Nottingham, Nottingham, United Kingdom An increasing amount of evidence suggests a bidirectional communication between the gut microbiome and the brain. Alteration in these interactions showed to affect brain structure and function. For example, alterations of the gut microbiota have shown to be associated with neurodevelopmental, neurodegenerative, and psychiatric disorders. Over the past two decades, neuroimaging techniques, particularly MRI (MRI), have revolutionised our understanding to brain function and structure. This talk will provide an overview of what can structural and functional MRI offer to improve our understanding to the microbiota-gut-brain axis in healthy and clinical populations.

Effect of Allyl Isothiocyanate on the gut microbiota of different age groups Karley Mahalak1, karley.mahalak@usda.gov, Adrienne Narrowe1, Lin Liu1, Pieter Van den Abbeele2, Aurelian Baudot2, Jenni Firrman1, Johanna M. Lemons1. (1) Dairy and Function Foods RU, USDA Agricultural Research Service, Wyndmoor, Pennsylvania (2) Cryptobiotix SA, Ghent, Belgium Allyl

isothiocyanate (AITC) is the pungent compound commonly found in wasabi and mustard that is also produced by certain members of the gut microbiota in vivo via the catabolism of sinigrin, found in vegetables of the Brassica family. AITC has reported anti-bacterial and anti-carcinogenic activity. It has also been shown to reduce inflammation-induced colitis in mouse models and regulate tight junctions within the gut. However, it is unknown whether these effects are the result of changes in the gut microbial community caused by AITC. In this study, an ex vivo model was used to test the response of the gut microbiota of four different age groups, ranging from infants to older adults, to AITC treatment. Genomic and metabolic analyses were performed to determine what changes occur in the gut microbiota in response to AITC. Preliminary analysis of the results suggests that there were surprisingly few metabolic changes compared with control, however, the addition of AITC did lower the pH of the cultures, and increase butyrate production in the older age groups.

Analysis of fenugreek supplementation reveals significant alterations in large intestinal metabolome and microbiome of Western Diet fed mice Katarina Jones1,3, jones.katarinaa@gmail.com, Allison J. Richard2, J. M. Salbaum2, Susan Newman2, Richard Carmouche2, Sara Webb2, Annadora J. Bruce-Keller2, Jacqueline M. Stephens2, Shawn R. Campagna1,3. (1) Chemistry, The Univ. of Tennessee Knoxville College of Arts and Sciences(2) Pennington Biomedical Research Center, Baton Rouge, Louisiana(3) Biological Small Molecule Mass Spectrometry Core, The Univ. of Tennessee Knoxville College of Arts and Sciences In recent years, herbal supplements have been gaining popularity and increased usage as a potential therapy for a variety of health challenges. One such supplement is fenugreek seeds (Trigonella foenum-graecum), which have been traditionally used to treat Type 2 Diabetes and hyperlipidemia. Fenugreek seeds are known to impact the gut microbiome and contain several bioactive compounds including phytochemicals such as trigonelline and diosgenin, and the fiber galactomannan. Despite this knowledge, the cause of the benefits of fenugreek supplementation, and if there is a link to the gut microbiome is not well understood. This study aimed to investigate the link between fenugreek supplementation and the gut microbiome using a multi-omics approach utilizing metabolomics and 16S sequencing of the intestinal contents of C57BL/6J mice. Specifically, forty male mice were divided into four dietary groups for 14 weeks: Western diet (WD), WD with fenugreek (WDFG), low fat diet (LF), and LF diet with FG (LFFG). Diets were supplemented with 2% w/w ground fenugreek seeds. Samples were collected at euthanasia for both metabolomic and 16S analyses. Metabolomic samples were prepared using an acidic acetonitrile extraction protocol and analyzed via ultra-high performance liquid chromatography high resolution mass spectrometry. While the biological matrix had the greatest impact, fenugreek did have a noticeable impact on the metabolome. Specifically, fenugreek showed the greatest influence on the large intestinal contents. In these regions, several metabolites, including myo-inositol, gluconolactone, and glucose phosphate which are related to sugar metabolism were decreased by WD relative to LF, but partially restored by FG supplementation. These metabolites also showed strong correlations ($p<0.01$) to two OTUs from the genus Blautia, which has previously been described to provide anti-inflammatory benefits to the mammalian host. Together these data support the hypothesis that the gut microbiome may play an important role in the benefits of fenugreek supplementation.

Hydrogen sulfide modulates gastrointestinal metabolome, an ex vivo study Lin Liu1, linshu.liu@usda.gov, Karley Mahalak1, Jenni Firrman1, Adrienne Narrowe1, Johanna M. Lemons1, Aurelian Baudot2, Stef Deyaert2, Pieter Van den Abbeele2. (1) Dairy and Functional Foods RU, USDA Agricultural Research Service, Wyndmoor, Pennsylvania (2) Cryptobiotix SA, Ghent, Belgium Microbial fermentation of dietary nutrients can generate hydrogen sulfide (H2S) gas in the gastrointestinal tract which is generally considered harmful to human health. A research study was conducted to assess the impact of H2S on the gut microbial community of individuals from across a large age spectrum, including breastfed infants, toddlers, adults (25-40) to senior adults (60+ years old), using Systemic Intestinal Fermentation Research (SIFR®) technology. Analysis of fermentation end products showed that H2S lowered the production of total short-chain fatty acids (SCFA) and branched-chain fatty acids (BCFA). Conversely, H2S increased the butyrate content, suggesting that H2S may selectively favor specific beneficial butyrate-producing gut microbes. Alternatively, available H2S may serve as an electron donor, potentially replacing fermentative metabolic activity by facultatively respiring gut bacteria which may explain the observed reductions in SCFA production. Donor age was a clear driver of differences in metabolite production, with adult samples producing more SCFA than infant or toddler samples. The main exception to this was the production of lactate. Measured lactate concentrations were low, but for adults this metabolite decreased significantly with H2S, while increasing in toddlers with lactate in infant samples unchanged, indicating that H2S may have a particular effect on lactic acid bacteria such as members of the genus Bifidobacterium which are typically associated with infants and children.

Mycotoxins: Challenges and Future Perspectives

Quantitative biomarkers for exposure and risk from aflatoxins in high-risk regions of the world John D. Groopman, jgroopma@jhsph.edu. Johns Hopkins Univ. Bloomberg School of Public Health, Baltimore, Maryland Liver cancer is the third leading cause of cancer deaths worldwide and has risen rapidly over the past 20 years in the US and Central America. In the US, immigrants, and persons with ancestry from Central American countries account for the 2nd highest numbers of liver cancer deaths. In contrast to most of the world where liver cancer is much higher in men, in Central American countries, where liver cancer rates are the highest in the Western Hemisphere, the incidence in men and women is almost equivalent (gco.iarc.fr). An epidemiologic transition underpinning etiology of liver cancer is underway impacting concepts of cancer prevention and control interventions for this nearly always fatal disease. The proportional contributions of traditional etiological factors in HCC - hepatitis B virus (HBV), hepatitis C virus (HCV), alcohol, aflatoxin and smoking - are changing with the emergence of metabolic syndrome, obesity, non-alcoholic fatty liver disease (NAFLD), air pollution, and diabetes. In our continuing work in Central America where liver cancer is high and HBV and HCV infections are low, aflatoxin continues to be a major risk factor for HCC. These findings are grounded by quantitative measurements using mass spectrometry and synthesized internal standards. In summary, despite the recent successes in the prevention and treatment of HBV and HCV through vaccination and chemotherapy, the incidence of liver cancer continues to rise across many different populations. To affect future success in liver cancer prevention and control the identification of new underlying and modifiable risk factors are required. Well annotated epidemiologic studies and concomitant biorepositories will provide the foundational resource for this research.

Aflatoxin and growth: A complex relationship between exposure intervention and measures of infant growth Paul C. Turner1, pturner3@umd.edu, Erica Phillips2, Neema Kassim5, Edna Makule5, Laura Smith3, Francis Ngure5, Nyabasi Makori5, Rebecca Nelson2, Rebecca Stoltzfus4. (1) Univ. of Maryland, College Park

(2) Cornell Univ., Ithaca, New York (4) Goshen College, Indiana (5) Nelson Mandela African Inst. of Science and Technology, Arusha, Tanzania, United Republic of Several studies in developing parts of the world report strong associations with aflatoxin and growth, while others find no, limited or suggested opposite effects. I will report a longitudinal trial we conducted in Tanzania to try to better understand a causal role for aflatoxin and early infant stunting. The study recruited infants at 6 months of age over a 1-year time period, and followed all until they were 18 months, thus we captured seasonal variation in recruitment and followed through a significant time frame where growth faltering is common. In addition, half of the study group received 365 days of maize and or ground nut flours that were prepared as aflatoxin "safe", i.e. below regulatory levels, using food locally grown. I will report anthropometry between control and intervention groups, and discuss with respect to biomarkers of aflatoxin exposure.

Aflatoxin exposure is a potential risk factor for mortality in acutely ill children in the CHAIN network cohort Yunyun Gong1, medyg@leeds.ac.uk, Lei Xia1, Hang Wu1, Ali Faisal Saleem6, Syed Asad Ali6, Ezekiel Mupere7, Christina Lancioni8, Abdoulaye Diallo9, Isabel Potani10, Weiger Voskuijl11, Mohammod Chisti12, Abu Sayeem12, Molline Timbwa2, Shalton Mwaringa2, Caroline Tigoi2, Moses Ngari2, Benson Singa13, Robert Bandsma10, Tahmeed Ahmed12, James Njunge2, Kirk Tickell5, Judd Walson5, James A. Berkley2,3, Michael N. Routledge4. (1) Food Science and Nutrition, Univ. of Leeds Faculty of Engineering and Physical Sciences, West Yorkshire, UK (2) KEMRI, Kilifi, Kenya(3) Centre for Global Health & Tropical Medicine, Univ. of Oxford, Oxfordshire, UK (4) School of Medicine, Univ. of Leicester College of Life Sciences, UK (5) Global Health, Univ. of Washington, Seattle (6) Paediatrics and Child Health, Aga Khan Univ., Karachi, Sindh, Pakistan(7) Paediatrics and Child Health, Makerere Univ., Kampala, Uganda(8) Pediatrics, Oregon Health & Science Univ., Portland (9) Public Health, Univ. Joseph Ki-Zerbo, Ougadougou, Burkina Faso(10) The Hospital for Sick Children, Toronto, Ontario, Canada(11) Global Health, Amsterdam UMC Locatie AMC, Noord-Holland, Netherlands(12) Nutrition Research Div., International Centre for Diarrhoeal Disease Research Bangladesh, Dhaka (13) KEMRI Centre for Clinical Research, Nairobi, Kenya Background: Aflatoxins are food borne fungal toxins contaminating various grains including maize and groundnuts. Chronic exposure to aflatoxins is associated with liver cancer, slowed child growth, and compromised immune function. The Childhood Acute Illness and Nutrition (CHAIN) cohort was established to identify risk factors for mortality in acutely ill children admitted to nine hospitals in four African and two Asian countries. A nested case cohort study was undertaken to understand the role of aflatoxin exposure in the inpatient and post-discharge mortality of acutely ill children. Methods: A nested case-cohort was developed from the CHAIN cohort whereby children who died or survived between admission and up to 180-days post-discharge were compared, together with community participants (CP). Serum samples collected at admission (N=755) and discharge (N=586) from hospitals and from CPs (N=222), were analysed for aflatoxin exposure using the biomarker aflatoxin-albumin adducts (AF-alb) using an in-house ELISA method. Findings: 56% and 55% of the hospitalised participants tested positive for AF-alb with geometric mean (GM) and 95% confidence interval (CI) of 4.7 (4.2 – 5.1) and 3.7 (3.3-4.1) pg/mg albumin at admission and discharge, respectively. AF-alb levels were not statistically different between the children being hospitalised and those of the CP groups. Children at discharge had significantly lowered AF-alb concentrations than at admission ($p<0.001$). African children had higher AF-alb levels than Asian children with GM and 95% CI of 7.4 (6.5 – 8.5) vs 1.9 (1.8 – 2.1) pg/mg at admission. AF-alb levels were lower in children being breastfed, compared to those with family food or complementary food ($p < 0.001$). After adjusting for age, hospital site, socioeconomic status and gender, AF-alb concentrations were positively associated with mortality overall, although only significantly in the subset of hospital sites of highest exposure. The highest AF exposure quartile group had an 84% higher mortality rate than the lowest quartile group ($p=0.043$). Interpretation: Aflatoxin exposure level was influenced by the child's age, diet, and geographical location. Higher exposure levels were observed in children of African sites than Asian. In children with the highest level of aflatoxins exposure were found to have an increased risk of mortality.

Metabolomic changes associated with aflatoxin exposure in children from the CHAIN cohort Hang Wu2, Celine Bourdon3,14, Lei Xia12, Rupasri Mandal20, Ali Faisal Saleem4,14, Ezekiel Mupere5,14,15, Christina Lancioni6,14, Abdoulaye Diallo7,14,16, Isabel Potani3,17, Weiger Voskuijl8,14,17, Mohammod Chisti9,14, Abu Sayeem9,14, Molline Timbwa13,14, Shalton Mwaringa13,14, Caroline Tigoi13,14, Moses Ngari13,14, Benson Singa13,14, Kirk Tickell10,14,18, Judd Walson10,18,14, David Wishart21, Robert Bandsma3,14,17, James Njunge13, James A. Berkley11,13, Yunyun Gong12, Michael N. Routledge1,19, mnr9@le.ac.uk. (1) School of Medicine, Univ. of Leicester College of Social Sciences Arts and Humanities, Leicester, UK (2) Univ. of Leeds Faculty of Medicine and Health, Leeds, West Yorkshire, UK (3) Translational Medicine, The Hospital for Sick Children, Toronto, Ontario, Canada (4) Paediatrics and Child Health, The Aga Khan Univ., Karachi, Sindh, Pakistan(5) Paediatrics and Child Health, Makerere Univ., Kampala, Uganda(6) Pediatrics, Oregon Health & Science Univ., Portland (7) Public Health, Centre MURAZ, Bobo-Dioulasso, Hauts-Bassins, Burkina Faso (8) Child Global Health, Amsterdam UMC Locatie AMC, Noord-Holland, Netherlands (9) Nutritional Research Division, International Centre for Diarrhoeal Disease Research Bangladesh, Dhaka, Bangladesh (10) Univ. of Washington, Seattle (11) Tropical Medicine and Global Health, Univ. of Oxford, Oxfordshire, UK (12) School of Food Science & Nutrition, Univ. of Leeds Faculty of Engineering and Physical Sciences, West Yorkshire, UK (13) KEMRI/Wellcome Trust Research Programme, Kilifi, Kenya (14) The Childhood Acute Illness and Nutrition Network, Nairobi, Kenya (15) Uganda Case-Western Reserve Univ. Research Collaboration, Kampala, Kenya (16) Univ. Joseph Ki-Zerbo, Ougadougou, Burkina Faso (17) Univ. of Malawi College of Medicine, Blantyre, Southern Region (18) Johns Hopkins Univ., Baltimore, Maryland (19) Jiangsu Univ., Zhenjiang, China(20) Metabolomics Innovation Centre, Univ. of Alberta, Edmonton, Canada(21) Biological Sciences, Univ. of Alberta, Edmonton, Canada Aflatoxin exposure is associated with child growth impairment in sub-Saharan Africa. Serum (n=883) from children in the Childhood Acute Illness and Nutrition Network (CHAIN) was analysed for aflatoxin albumin as a marker of exposure and by targeted metabolomics using a combination of direct injection mass spectrometry with a reverse-phase liquid chromatography tandem mass spectrometry (LC−MS/MS) custom assay. Boruta modelling utilizing a Negative Binomial Generalised Linear Mixed Model (NB GLMM) was used to identify candidate metabolites associated with aflatoxin exposure. Several amino acids were identified and exploration through KEGG enrichment analysis revealed 14 pathways associated with aflatoxin exposure, including many amino acid metabolism pathways such as arginine and proline metabolism, glutamate metabolism, phenylalanine, tyrosine and tryptophan biosynthesis, and glutathione metabolism. These pathways are integral to protein synthesis and growth. Existing literature indicates that the first three pathways can impact intestinal function, with disruption of these pathways potentially leading to reduced nutrient absorption, which may contribute to negative impacts on growth.

Additionally, disruption of glutamate metabolism can inhibit glutathione metabolism, potentially intensifying oxidative stress leading to inflammation, liver disease, cancer, and ultimately death. Therefore, the disruption of those pathways caused by aflatoxin exposure may explain novel mechanisms of aflatoxin altered child growth and disease.

Human mycotoxin exposure: From biomonitoring towards exposomics Sarah De Saeger, sarah.desaeger@ugent.be, Roger Pero-Gascon, Marthe De Boevre. Faculty of Pharmaceutical Sciences, Dept. of Bioanalysis, Universiteit Gent, Ghent, East-Flanders, Belgium The assessment of human mycotoxin exposure can be conducted through two approaches: an indirect method, which relies on combining food chemical analysis with food consumption data, and a direct method that involves analyzing mycotoxin biomarkers of exposure in biological fluids like urine, blood, feces, or breast milk. In recent years, many efforts have been put in the development of fast and robust (micro)sampling techniques as well as ultra-sensitive targeted and untargeted multi-mycotoxin LC-MS/MS methods for the analysis of mycotoxin biomarkers of exposure. Nevertheless, still many gaps in our understanding of the human mycotoxin metabolism exist. Therefore, human toxicokinetics studies are invaluable to further optimize the human biomonitoring approach. Examples of ongoing human mycotoxin biomonitoring studies will be discussed during the presentation. Moreover, mycotoxins are only one group of dietary and environmental contaminants humans are exposed to. The exposome concept attempts to measure all non-genetic exposures from conception throughout the life course. As an example, FLEXiGUT -the Flemish exposome project- is the first large-scale exposomics study focused on chronic low-grade gut inflammation. The project aims to characterize human life course environmental exposure to assess and validate its impact on gut inflammation and related biological processes and diseases. The main research question of FLEXIGUT is "What is the importance of the exposome in the development and progression of low-grade gut inflammation and related diseases?". However, sub-questions such as "What is the role of chronic low-dose multiple mycotoxin exposure on the gut microbiome-inflammation axis?" are being investigated as well. To answer these questions, we combine exposure science and high-throughput -omics technologies with epidemiological studies. The integration and analysis of various -omics datasets, such as the metabolome, metagenome, and DNA adductome, using a multi-omics approach, present the potential for identifying relationships between these features. This approach enables the creation of classifiers and predictive models, facilitates the discovery of biomarkers associated with exposure and disease risk, and sheds light on the early molecular events within pathways leading to the development of diseases.

Estimating aflatoxin exposure by use of LC-MS/MS: Twenty years of CDC laboratory innovations and investigations Nicholas Zitomer, nzitomer@cdc.gov, Michael E. Rybak. National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, Georgia Aflatoxins are mycotoxins produced by species of Aspergillus and other fungi. They are teratogenic, carcinogenic, and acutely toxic. In 2023 our laboratory established an LC-MS/MS method for estimating aflatoxin exposure by measuring aflatoxin B1 adducts with serum albumin. Over the past twenty years we used this measurement capacity in support of a variety of observational and interventional studies aimed mainly at areas of the world challenged by endemic aflatoxin exposure and food insecurity. We have reported thousands of patient sample results ranging from single-patient inquiries to country-wide surveillance studies, investigated aflatoxicosis outbreaks in Ethiopia, Kenya, and Tanzania by use of case-control sampling, and have generated cross-sectional estimates of aflatoxin exposure in Kenya, Uganda, and the US. Parallel to our support of epidemiological studies and investigations, we have conducted in-house research and development activities resulting in iterative improvements to our laboratory methodology by leveraging advanced instrumentation and automation. We have also investigated the impacts of preanalytical factors related to sample collection, processing, storage, and transportation challenges that are frequently encountered in aflatoxin exposure study settings. These efforts have led to our current LC-MS/MS method that maximizes analyte detection and analysis throughput while minimizing sample volume requirements, and has yielded a better understanding of the impacts of hemolysis, elevated storage temperatures, and the substitution of plasma for serum on overall biomarker measurement quality. In this presentation we will reflect on our past accomplishments in developing and implementing our LC-MS/MS methodology and discuss challenges in estimating aflatoxin exposure by use of LC-MS/MS. Disclaimer: The findings and conclusions in this presentation are those of the authors and do not necessarily represent the views of the Centers for Disease Control and Prevention.

Optimization of aflatoxin B1-lysine analysis for public health exposure studies Justin Renaud, justin.renaud@agr.gc.ca. Agriculture and Agri-Food Canada, London Research and Development Centre, London, Ontario, Canada Human exposure to aflatoxin can be estimated by analysis of the diet, however, determination of the serum albumin aflatoxin adduct, a validated biomarker, provides the best health-relevant exposure measure. Although measuring serum albumin aflatoxin is critically important, its analysis is difficult owing to multiple analytical challenges, which limits the ability of different laboratories to perform this work in a cohesive and comparable manner. Firstly, the necessary analytical standard, AFB1-lysine is not currently commercially available. Additionally, there is no reference serum with a well characterized level of aflatoxin-albumin adduct available to allow different laboratories to assess the performance of their respective methods. Sampling still predominately involves obtaining a serum sample on-site, and carefully shipping it to a laboratory capable of performing the analysis. In this work, we describe efforts to produce a well-defined human serum sample synthetically fortified with the aflatoxin adduct. Finally, we use this material to carefully assess the suitability of alternative sample collection methods including volumetric absorptive microsampling (VAMS), dried bloodspots (DBS), quantitative dried blood spot (qDBS) sampling.

TUESDAY AFTERNOON
General Papers

Biochemical changes during spoilage of milk with different fat content Prashanti Iyer, rxi119@psu.edu, Christopher J. Blowers, Francelys Medina, Arshad Khan. Chemistry, Pennsylvania State Univ., DuBois Our study aims to compare the bacterial growth profile on milk with differing fat content. This includes pasteurized fat-free, 2% reduced fat and whole milk samples, obtained from the same vendor and produced by the same brand. Milk samples were incubated at 4°C (temperature in fridge), 25°C (room temperature), and 37°C (body temperature) and growth parameters in the form of turbidity, color changes, precipitation and pH variations were recorded at regular time intervals. In course of the incubation, the fat-free milk displayed more remarkable changes in the form of marked precipitation and lowering of pH, which is the indication of fermentation of lactose to lactic acid. Upon plating these milk samples, the fat free milk samples again displayed a larger colony count. Thus, our preliminary results show that the bacterial growth was initiated more rapidly on the fat-free milk followed by 2% and whole milk samples. Further studies, including the FTIR analysis,

are currently underway to identify the bacterial species that contaminate the milk samples.

Chemical characterization of bioactive compounds of Uva caimarona(Pourouma cecropiifolia) fruit by LC-MS non-targeted analysis Camilo Andres A. Correa Lozano1, camacorrealoz@unal.edu.co, Coralia Osorio Roa1, Timo D. Stark2, Corinna Dawid2, Gina M. Méndez Callejas3. (1) Univ. Nacional de Colombia, Bogota, Colombia(2) Technische Univ. Munchen, Bayern, Germany(3) Universidad de Ciencias Aplicadas y Ambientales, Bogota, Colombia After the burning of the Amazon Forest in 2019, seven presidents of the region signed the "Leticia Pact" in which sustainable development based on Amazonian biodiversity is promoted. Nonetheless, the lack of knowledge of the properties of Amazonian endemic species has delayed this development. Therefore, it is necessary to strengthen the knowledge of the attributes of these species. Uva caimarona (Pourouma cecropiifolia), an Amazonian fruit tree, possesses a great adaptability and capacity to restore the biome. Additionally, this plant has shown promising activity in three cancer cell lines, associated with the presence of proanthocyanins, which was the cause of nearly 10 million deaths in 2020. Considering the vulnerability of cancer patients during the COVID-19 pandemic, related to the almost 10 billion deaths worldwide by 2020, identifying compounds with antiproliferative activity present in the fruit not only represents a potential benefit to human health but would also contribute to the sustainable development of the Amazon Forest. The MTT assay was used to determine the cytotoxic activity (in vitro) against three different carcinomas of polar fractions obtained from three organs of Uva caimarona, whose chemical characterization was analyzed by UPLC-TOF-MS and NMR. The fractions that exhibited selective systemic cytotoxic activity against colon carcinoma cell lines, were mainly composed of flavonoids, triterpenoids, and fatty acid esters. The chemical characterization of the active fractions will be presented.

Foliar Nanoparticles Application Alleviate Cadmium Toxicity in Wheat (Triticum aestivum L.) via Long Distance of “Leaf-Root-Microorganism” Regulation Min Wang, dg21250045@smail.nju.edu.cn, Dongmei Zhou. Nanjing Univ., Jiangsu, China Foliar use of beneficial nanoparticles (NPs) shows potential in alleviating cadmium (Cd) toxicity in crops, while systematic understanding their leaf-root-microorganism process is needed for sustainable development of efficient nano-enabled agrochemicals. Herein, different rates of four commonly used NPs including nano-selenium (SeNPs), nano-silica (SiO2NPs), nano-zinc oxide (ZnONPs), and nano-manganese dioxide (MnO2NPs) were sprayed in wheat plants grown in a Cd-contaminated soil. Results showed that SeNPs and SiO2NPs most effectively reduced Cd concentration in wheat grain. After 240 days of cultivation, compared to control, Cd concentration in wheat grains was significantly ($p < 0.05$) decreased by 35.0% and 33.3% by applying 40 mg/L SeNPs and 100 mg/L SiO2NPs, respectively, and the grain yield was significantly ($p < 0.05$) increased by 33.9% with SeNPs. Down-regulated gene expression of Cd transport proteins (TaNramp5 and TaLCT1) and up-regulated gene expression of vacuolar fixation protein of Cd (TaHMA3 and TaTM20) were observed with foliar SeNPs and SiO2NPs use. On the other hand, SeNPs spraying increased leaf antioxidant metabolites such as ferulic acid, trehalose, ketohexose, and galactinol, promoted rhizosphere secretions, and increased carbon and nitrogen sources for growth of soil microorganisms (Solirubrobacter and Pedomicrobium). This process subsequently affected rhizosphere organic acid metabolism, resulting in lower abundances of rhizosphere organic acids and reducing Cd bioavailability in rhizosphere soil. Our overall findings demonstrate that foliar application of SeNPs and SiO2NPs could offer a plant and rhizosphere soil metabolism-regulating approach to reduce Cd accumulation in wheat grains.

Preparation and characterization of sodium alginate- carboxymethyl cellulose based essential nutrient slow release nanohybrids Koshila R. Maduwanthi1, koshilarm@gmail.com, Imalka Munaweera1, Pamoda T. Perera2. (1) Dept. of Chemistry, Univ. of Sri Jayewardenepura, Nugegoda, Colombo, Sri Lanka(2) Dept. of Research and Development, Panam Biotech Pvt (Ltd), Homagama, Colombo, Sri Lanka The synergistic properties of nano-hybrids created by integrating several nanomaterials inside can boost the fertilizer’s potency. The nano-hybrid was established with the goal of maximizing the synergistic effect of three nanoparticles: CuO, ZnO, and MgO. The nanoparticles' slow-release behavior was achieved by infusing them with a sodium alginate-carboxymethyl cellulose (SA-CMC) combination. To create nano-hybrid hydrogel beads, oxide nanoparticles produced by the sol-gel technique were sonicated with SA-CMC composite before being crosslinked by Ca2+. Powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), Raman spectroscopy, and Fourier Transform Infrared (FTIR) spectroscopy were used to characterize nanoparticles. The average particle sizes of CuO, ZnO, and MgO nanoparticles were determined to be 220 nm, 285 nm, and 110 nm, respectively. FTIR analysis was used to determine crosslink formation, whereas SEM analysis was used to analyze nutrient particle distribution across the matrix. The nutritional percentages of the nano-hybrid Cu, Zn, and Mg after digestion were determined as 0.15+0.00016%, 0.90+0.00060%, and 1.17+0.0036% using data from flame atomic absorption spectroscopy (FAAS). FAAS research done in a water medium with a pH of 7.2 revealed that 3.03+0.08% of Cu, 11.23+0.05% of Zn, and 22.73+0.09% of Mg were released over 6, 11, and 6 day time periods, revealing the slow release nature of the nutrients. Statistics confirmed a statistically significant variation in harvest from mung bean plants when analyzed over a period of 42 days.

Electrospun nanofiber membranes infused with essential oils for extending the shelf life of perishable produce like grapes and tomatoes Maheshika C. Sethunga1, maheshichathuranganee@gmail.com, Imalka Munaweera2, Ranaweera K.K.D.S.1, Prasanna Gunathilake3. (1) Dept. of Food Sci. & Tech., Univ. of Sri Jayewardenepura, Nugegoda, Sri Lanka(2) Dept. of chemistry, Univ. of Sri Jayewardenepura, Nugegoda, Sri Lanka(3) Dept. of Food Sci. & Tech., Wayamba Univ. of Sri Lanka, Kuliyapitiya, Sri Lanka The increasing demand for fresh produce is being driven by a worldwide environment characterised by rapid population growth and changing nutritional habits. Active food packaging methods have arisen in an effort to address this issue and extend the shelf life of perishable fruits and vegetables. This work focuses on the use of extremely volatile essential oils, notably cinnamon bark oil (CNO) and clove bud oil (CBO), in electrospun nanofibers made of cellulose acetate at 10%, 30%, and 50% loadings. The electro-spun membranes were characterised using Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FT-IR), and Gas Chromatography Mass Spectrometry (GC-MS) and used to preserve fresh grapes and tomatoes for up to 45 days at 4 oC using physiochemical attributes, sensory profiles, and microbial counts.The results of this study demonstrated a uniform distribution of volatile compounds with average diameters ranging from 46 nm to 600 nm and controlled release kinetics of bioactive compounds, ensuring their sustained efficacy over a 60-day storage period at 4 oC and significantly outperforming control samples. Nanofibers loaded with 50% CNO and CBO demonstrated the pinnacle of in-vitro antioxidant and antimicrobial properties, tangibly extending the shelf life of both

fresh tomatoes and grapes and confirming microbiological safety for up to 40 days of storage compared to 15 days of storage in control samples. Nonetheless, sensory evaluation and specific physiochemical aspects suggested that fresh grapes and tomatoes might be stored for up to 30 days. The study's findings highlight the effectiveness of an electrospun nanofiber membrane loaded with CNO and CBO in significantly extending the shelf life of fresh tomatoes and grapes, and this approach offers a promising solution to address the challenge of preserving perishable produce in an environmentally friendly manner.

Electrochemical quantification of capsaicin levels: A novel approach to assessing chili heat consistency in culinary applications Austeja Rudokaite1, austeja.rudokaite@gmc.stud.vu.lt, Ausra Baradoke1, Nemira Zilinskaite2. (1) Vilniaus Univ. Lithuania (2) Univ. of Oxford, Oxfordshire, UK Chilli peppers' spiciness, originating from capsaicin, has traditionally been assessed by the subjective Scoville Test, prone to human variability and time inefficiencies. Our study introduces a real-time electrochemical technology for capsaicin measurement, merging electrochemical biosensing with molecular recognition. Utilizing Scanning Electron Microscopy (SEM) for morphological analysis of screen printed electrodes (SPEs), alongside electroanalytical techniques like Cyclic Voltammetry (CV) and Square Wave Voltammetry (SWV) for redox behavior investigation, our system ensures cost-effective, portable capsaicin detection suitable for culinary settings. Chronoamperometry (CA) and Electrochemical Impedance Spectroscopy (EIS) further enable time-resolved and impedance-based analyses respectively, enhancing sensor sensitivity and selectivity even in complex food matrices. This facilitates immediate capsaicin evaluation, beneficial for food makers and chefs aiming for consistent flavors. The configuration, involving customized recognition components with strong capsaicin affinity, guarantees accurate measurements, revolutionizing spiciness assessment and aligning with the evolving precision and reliability demands of the food sector.

Pesticide-induced biochemical changes in tomatoes by FTIR spectroscopy: Implications for Food Safety and Agriculture Pavani Yerra1, paavaneyerra11@gmail.com, Janaki P2, Karthikeyan S3, Jagadeeswaran R4, Sankari A5, Murali A. P6, Ramalakshmi A7. (1) Soil Science and Agricultural Chemistry, Tamil Nadu Agricultural Univ., Coimbatore, India(2) Nammazhavr Organic Farming Research Centre, Tamil Nadu Agricultural Univ., Coimbatore, India(3) Physics, Dr Ambedkar Government Arts College, Chennai, Tamil Nadu, India(4) Remote Sensing & GIS, Tamil Nadu Agricultural Univ., Coimbatore, India(5) Vegetable Science, Tamil Nadu Agricultural Univ., Coimbatore, India(6) Agronomy, Tamil Nadu Agricultural Univ., Coimbatore, India(7) Food process engineering, Tamil Nadu Agricultural Univ., Coimbatore, India Pesticide residue analysis is vital to assess environmental contamination and ensure food safety. Various methods like GC, HPLC, thin layer chromatography, and capillary electrophoresis exist for pesticide residue detection, but their extensive use is limited by time and cost constraints, making it impractical for comprehensive product monitoring. Hence the screening, development and validation of non-destructive and in situ methods for residue detection in a wide range of matrices are researched area all the time across the world to meet the food safety standards requirement. Employing Fourier-Transform Infrared (FTIR) spectroscopy for non-destructive detection in fresh tomatoes has been the focus of present research. Tomatoes in the pot experiment were exposed to varied concentrations of carbendazim and mancozeb pesticides as per the recommendation suggested for their application. Later fruit surface samples were collected at different intervals (0, 1, 3, 7, and 10 days after spraying of pesticides) and changes in spectral pattern were monitored to assess the intricate biochemical alterations in fruit resulting from pesticide application. The shift and intensity changes in key components such as polysaccharides, cellulose, lipids, amides, pectin, and cutin in tomato samples were observed. Results showed complex interactions between pesticides and biochemical constituents in tomato. Polysaccharides and cellulose displayed subtle responses to pesticides and their concentrations, suggesting a delicate balance between applied dose and structural integrity. Lipid content exhibited concentration-dependent effects, while amides demonstrated intriguing changes, possibly indicating alterations in protein composition. Pectin and cutin absorption revealed temporal effects, emphasizing the dynamic nature of pesticide-induced modifications. Understanding functional groups and their spectral signatures helps in interpreting intricate pesticide-tomato interactions, providing valuable insights into agricultural practices and food safety.

Paring Flavors with Health and Wellness Food Products

Role of flavor in health and wellness food products: An overview Xiaofen Du, xdu@twu.edu, Daniel Salta. Nutrition and Food Sciences, Texas Woman's Univ., Denton Health and wellness food products deliver improved nutrition and other health benefits compared to conventional foods, and some also provide a reduced environmental footprint. The health and wellness of foods and beverages is a broad subject, and the current market includes natural, organic foods and ingredients (clean label), nutrient-dense foods (nutrient fortified or reduction in excessive sugar, salt, fat, alcohol, and animal protein), and free-from specific offending compositions (gluten, lactose, and artificial food additives). Consumers are also paying attention to plant-based proteins, a growing niche within health and wellness foods. Consumer interest in the health and wellness market is driving dramatic growth in the food and flavor industries. This presentation will focus on the role of flavor and flavor modulates in health and wellness food products, their major challenges, and future perspectives. Flavor (aroma, taste, and mouth sensation) is an important sensory attribute in determining consumer food intake and continued consumption. Flavor has many vital roles in the health and wellness arena, including improving the palatability of reduced-sugar, -salt, -fat, and -alcohol food and beverage products and nutrient fortified foods, along with masking off-flavors and bitter tastes in plant-based protein products. Additionally, the transition from conventional to clean-label and free-from flavors provides added value to ready-to-eat products. These new trends, knowledge, and technologies are closely related to product development and ingredient innovations. Flavor, as one important ingredient for food production, is an area with great growth potential.

Physicochemical factors that affect baked sweetpotato textures and sweetness Matthew Allan1, matthew.allan@usda.gov, Suzanne Johanningsmeier1, Mariam Nakitto2, Osvalda Guambe3, Modesta Abugu4, Kenneth Pecota4, Craig Yencho4. (1) Food Science and Market Quality and Handling Research Unit, USDA Agricultural Research Service, Raleigh, North Carolina, US(2) International Potato Center, Kampala, Uganda(3) International Potato Center, Maputo, Mozambique(4) NC State Univ. College of Agriculture and Life Sciences, Raleigh, North Carolina, US Sweet potato varieties vary greatly in perceived textures and sweetness along with diverse consumer preferences around the world. Our objective was to identify physicochemical factors that impact the textures and sweetness of baked sweet potatoes. Fifteen sweet potato genotypes with diverse sensory attributes were selected and grown in three plots. Sweet potatoes were harvested and stored using standard commercial practices, baked, then evaluated by a trained descriptive

sensory panel for 13 textural attributes and sweetness. Textures were also mechanically measured by texture profile analysis (TPA). Sweet potato composition (starch, cell wall material, sugar contents), starch properties (thermal, granule type ratios, granule sizes), and amylase activities were characterized. Linear correlations and random forest modeling were used to identify factors related to sensory textures, while structural equation modeling was used to test the hypothesis sweetness perception is affected by sugar concentrations and texture. TPA predicted fracturability and firmness well but was limited to these textures. Adhesiveness, cohesiveness, firmness, mealiness, moisture, particle size, and rate of breakdown textures were multifaceted and affected largely by starch and cell wall material contents; B-type starch granule ratio and gelatinization temperature; plus α- and β-amylase activities. Sweetness perception was impacted by the perceived particle size and sugar contents, particularly sucrose and maltose, and maltose generation during baking was highly correlated with starch content. These relationships between physicochemical sweet potato properties and the perceived textures and sweetness of baked roots could aid breeders, processors, and food scientists develop sweet potatoes and products thereof that meet varying consumer preferences.

Multi-omics discovery of aroma-active compounds formation in three different mango cultivars Xin Liu, xin.liu@ufl.edu, Yu Wang. Citrus Research and Education Center, Univ. of Florida, Lake Alfred Mango (Mangifera indica L.) is one of the most economically important fruits in the world. Understanding aroma active compounds formation is critical for enhancing flavor quality of mangoes. Here, multi-omics strategy (volatolomics, metabolomics, and proteomics) along with sensory test was used to investigate the key pathways involved in the formation of volatile compounds in three different mango cultivars (Ah Ping, Rosa, and Rosigold). A total of 87 volatile compounds were semi-quantified using GC-MS. Further, untargeted metabolomics and proteomics were employed to elucidate the potential molecular mechanisms of aroma compounds formation, then, 508 metabolites and 4481 proteins were identified, respectively. Integrative analysis of multi-omics data indicated that fatty acid, amino acid, and sugar metabolism had a global impact on the aroma compounds formation in three different mangoes, ultimately resulting in distinct flavor characteristics among the three mango cultivars examined. Notably, the expression of LOX, HPL, and ADL were responsible for the accumulation of C6 and C9 aldehydes, alcohols and acids in linoleic acid and α-linolenic acid metabolisms. The different expression levels of ACSL, AOX, ACAD, ECH, HADH, and AACT influenced the conversion of oleic acid to straight chain volatile compounds. Glutamate, valine, and phenylalanine, serving as precursors, are involved in the production of butyl esters under the actions of aminotransferase and decarboxylase. Additionally, the formation of furan and pyran aroma active compounds was significantly influenced by pentose and hexose. These findings provide new insights into understanding the characteristic flavor of mango.

Detection of smoke-derived volatile phenols in grapes using a portable easy to use biomimetic sensor Aqsa Khan1, aqkhan@clarkson.edu, Arran Rumbaugh2, Silvana Andreescu1. (1) Chemistry & Biomolecular Science, Clarkson Univ., Potsdam, New York(2) Dept. of Viticulture and Enology, Univ. of California Davis Smoke exposure poses a significant challenge to the wine industry, leading to the presence of volatile phenolics (VPs) in grapes, which can result in undesirable sensory attributes in wine. Traditional methods to detect volatile phenols involve complex laboratory-based chromatography and mass spectrometry instrumentation that are expensive and cannot be deployed in the field. Despite their high reliability and accuracy, these laboratory-based techniques can only analyze a limited number of samples, hindering their broad applicability for quantifying grape quality in the field. A simple, portable, user-friendly, and cost-effective detection method capable of reliably measuring VPs in field grapevines would provide a decision-support measurement tool to rapidly assess the quality of grapes and minimize the economic losses faced by wine grape growers due to smoke. This presentation introduces a portable easy-to-use sensor that functions as a colorimetric probe and catalysis amplifier for real-time monitoring of total VPs in grapes prior to the winemaking process. The sensor's performance was evaluated by monitoring the color change and relating it to the composition and concentration of these volatiles. These sensors were able to achieve detection limits below established thresholds, using the optimized procedure. The method has been successfully implemented on a paper substrate, serving as a compact portable label to identify phenolic targets through surface chemistry reactions. Current efforts involve testing within a controlled smoke chamber to validate the suitability of this technology for real-time in situ monitoring of exogenous, spanning from minimal to substantial smoke exposure. The simplicity and portability of the system provide a practical monitoring tool for winemakers and grape growers, facilitating real-time quality assessment in the vineyards.

Chemical composition and bioactive compounds of γ-irradiated stable chamomile accessions (chamomilla recutita (L.) Rauschert.) Yatish Pant1, yogipantt19@gmail.com, Kamlesh Yadav1, Raj K. Lal2, Chandan S. Chanotiya1. (1) Phytochemistry, CSIR - Central Inst. of Medicinal and Aromatic Plants, Lucknow, Uttar Pradesh, India(2) Plant Breeding, CSIR - Central Inst. of Medicinal and Aromatic Plants, Lucknow, Uttar Pradesh, India Chamomile is a dainty flowering plant belonging to the Asteraceae family. With its soothing aroma and a history that spans centuries, chamomile is one of the world's most beloved and well-known medicinal herbs for its therapeutic properties, particularly in traditional and alternative medicine systems. Chamomile's versatility, mild flavour, and well-documented health benefits have made it a popular enjoyed as a calming tea, incorporated into skincare products, or used for its anti-inflammatory properties, chamomile continues to play a prominent role in herbal medicine and holistic wellness practices. The main components of German chamomile essential oil are as α-bisabolol, α-bisabolone and its α-bisabolol oxide A and B, and chamazulene, which is responsible for the blue colouration of the essential oil. In the present study, we have worked on some γ-irradiated stable chamomile accession of German chamomile to explore the diverse chemical composition of chamomile and its potential health benefits, emphasizing the importance of continued research into this valuable botanical resource for the development of new therapeutic interventions and natural remedies. In the present study, about 20 different, γ-irradiated accessions were studied for two consecutive years and their further chemical investigation shows that some γ-irradiated accessions were enriched in α bisabolol oxide A while some in α-bisabolol oxide B, a few in α-bisabolone and α-bisabolol. A detailed chemical investigation has been carried out, including morphological parameters, oil yield, oil colour, and physiochemical parameters, along with the antimicrobial activity of the selected accessions. The detailed results will be shown during the presentation.

Advancing stem in agriculture with active experiential learning engagement for high school and college students focused on creation of health product from super-fruits and medical herbs William Weaver1, Sasha Grebenyuk2, Andrew G. Ristvey3, Victoria Volkis1, chvolkis2013@gmail.com. (1) Natural Sciences, Univ. of Maryland Eastern Shore, Princess Anne (2) WOM communications LLC, Framingham, Massachusetts (3) Wye Research & Education Center, Univ. of Maryland Extension, College Park Modern

agriculture and food science is a highly technical field of science and technology that often requires an interdisciplinary approach involving professionals with specializations in chemistry, biology, Envir. Sci., and engineering, along with traditional agriculture and food science specialists. However, students majoring in these science disciplines often do not correlate their professional training with careers within food and agriculture. Since 2020, PI and collaborators run successfully AFRI-EWD-REEU program bringing college students for summer internships to work as interdisciplinary teams in active experiential learning projects focused on super-fruit aronia (Aronia mitschurinii), medical herbs, and creating, phytochemically analyzing, and planning production of health products: power aid drinks, and vitamin gummies. Active experiential learning, along with extensive training in STEM in agriculture and professional and leadership developing, prepare them to apply their majors in agriculture. In 2023, authors have expanded the pipeline of training to include high school students and their educators with the help of AFRI-EWD-FANE grant. The program covers STEM in agriculture topics in genomics, biotechnology, interdisciplinary horticulture and phytochemistry, precise irrigation, instrumental chemical analysis, and more, while active experiential learning during the summer places students into interdisciplinary teams, led and mentored by experienced undergraduate and graduate students and a group of faculty-mentors to work on phytochemical analysis of specialty crops, such as aronia, holy basil and young ginger, and creation and planning production of healthy products from these crops – power aid drinks, and vitamin gummies. External evaluation from WOM Communications LLC allows us to optimize the activities and estimate the effectiveness of training and active experiential learning. Here we present a short description of program activities, and focus in particularly on currently being patented all-organic, colorants-free, sugar-free, natural power aid drinks that claim high content of phenolic antioxidants, including anthocyanins, essential minerals and microelements projects, developed during the summer active experiential learning teams activities, and healthy gummies with similar properties as drinks.

Mycotoxins: Challenges and Future Perspectives

From AflaZ to SoLFOOD and beyond: German-Kenyan World Nutrition Projects aimed at reducing food losses due to mycotoxin contamination in sub-Saharan Africa Christian Roder, Markus Schmidt-Heydt, markus.schmidt-heydt@mri.bund.de. Dept. for Safety and Quality of Fruit and Vegetables, Workgroup for Mycotoxin--producing and pathogenic Fungi and Yeast, Max Rubner-Institut Bundesforschungsinstitut fur Ernahrung und Lebensmittel, Karlsruhe, Baden-Württemberg, Germany Maize, as the most widely consumed staple food in sub-Saharan Africa, is frequently and highly contaminated with fungal mycotoxins such as aflatoxins, which regularly leads to fatal outbreaks of aflatoxicosis. Especially in Kenya, a model region with high-risk for aflatoxin contamination in Africa, the situation is worsening due to climatic changes. Heavily contaminated maize cannot be safely used for human and animal consumption, resulting in economic and nutritional losses. An interdisciplinary German-Kenyan research consortium consisting of the Max Rubner-Institut (MRI, coordinator of both projects), the Julius-Kühn Inst. (JKI), the Univ. of Landau (RPTU), the Eastern Africa Farmers Federation (EAFF) and the Kenya Agricultural and Livestock Research Organisation (KALRO) is focusing within the AflaZ project on deciphering the genetics of different aflatoxin chemotypes of selected Aspergillus species found in Kenya, the influence of insects and the soil microbiome on plant health and susceptibility to fungal infection, and the carry-over from aflatoxin B1 in feed to aflatoxin M1 in cow milk. In addition, the SoLFOOD project goes one step further and, based on the research results of the AflaZ project, aims to improve the smallholder maize production chain in Kenya, with a focus on reducing food losses due to fungal infection and aflatoxin contamination, and to develop alternative usage strategies for mycotoxin-contaminated maize, starting in the soil and ending with the utilization and detoxification of harvested products for subsistence and commercial use. Corr.Auth.,Project coordinator: Markus.Schmidt-Heydt@mri.bund.de AflaZ FKZ.: 2816PROC12; SoLFOOD FZK:2822NIPS04; funded by the Federal Ministry of Food and Agriculture (BMEL) https://www.mri.bund.de/en/Inst.s/safety-and-quality-of-fruit-and-vegetables/research-projects/afla-z/

Dynamic geospatial modeling of mycotoxin contamination of corn in Illinois: Unveiling critical factors and predictive insights with machine learning Lina Castano-Duque1, Lina.Castano.Duque@usda.gov, Edwin Winzeler2, Joshua Blackstock2, Cheng Liu3, Noemi Vergopolan4, Marlous Focker3, Kristin Barnett5, Phillip Owens2, H.J. van der Fels-Klerx3, Martha M. Vaughan6, Kanniah Rajasekaran1. (1) USDA-ARS Southern Regional Research Center, New Orleans, Louisiana (2) USDA-ARS Dale Bumpers Small Farms Research Center, Booneville, Arkansas (3) Wageningen Food Safety Research, Gelderland, Netherlands(4) Atmospheric and Ocean Science Program, Princeton Univ., New Jersey (5) Illinois Dept. of Agriculture, Springfield (6) USDA-ARS National Center for Agricultural Utilization Research, Peoria, Illinois Mycotoxin contamination of corn is a pervasive problem that negatively impacts human and animal health and causes economic losses to the agricultural industry worldwide. Historical aflatoxin (AFL) and fumonisin (FUM) mycotoxin contamination data of corn, daily weather data, satellite data, dynamic geospatial soil properties and land usage parameters were modeled to identify factors significantly contributing to outbreaks of mycotoxin contamination of corn grown in Illinois (IL), AFL >20 ppb and FUM >5 ppm. Two methods were used: a gradient boosting machine (GBM) and a neural network (NN). Both GBM and NN models were dynamic at a state-county geospatial level because they used GPS coordinates of the counties linked with soil properties. GBM identified temperature and precipitation prior to sowing as significant influential factors contributing to high AFL and FUM contamination. AFL-GBM showed that a higher aflatoxin risk index (ARI) in January, March, July, and November led to higher AFL contamination in the southern regions of IL. Higher values of corn-specific normalized difference vegetation index (NDVI) in July led to lower AFL contamination in central and southern IL, while higher wheat specific NDVI values in February led to higher AFL. FUM-GBM showed that temperature in July and October, precipitation in February, and NDVI values in March are positively correlated with high contamination throughout IL. Furthermore, the dynamic geospatial models showed that soil characteristics were correlated with AFL and FUM contamination. Greater calcium carbonate content in soil was negatively correlated with AFL contamination, which was noticeable in southern IL. Greater soil moisture and available water holding capacity throughout southern IL were positively correlated with high FUM contamination. Higher clay percentage in the northeast areas of IL negatively correlated with FUM contamination. NN models showed high class-specific performance for one-year predictive validation for AFL (73%) and FUM (85%), highlighting its accuracy for annual mycotoxin prediction. Our models revealed soil, NDVI, year-specific weekly average precipitation and temperature were the most important factors correlated with mycotoxin contamination. These findings serve as reliable guidelines for future modeling efforts to identify novel data inputs for prediction of AFL and FUM outbreaks and potential farm-level management practices.

Peptide natural products from the fungus Aspergillus flavus: Potential virulence factors? Matthew Lebar1, matthew.lebar@ars.usda.gov, Jeffrey Cary1, Brian Mack1, Carol Carter-Wientjes1, Mallika Kumarihamy1, Qijian Wei1, Raj Majumdar2, Valdet Uka3, Sarah De Saeger3, José Diana Di Mavungu3. (1) Food and Feed Safety Research Unit, USDA Agricultural Research Service, New Orleans, Louisiana (2) Northwest Irrigation and Soils Research, USDA Agricultural Research Service, Kimberly, Idaho (3) Univ. Gent, Belgium Aspergillus flavus can colonize corn and contaminate food and feed with aflatoxins, a group of toxic and carcinogenic secondary metabolites. The genome of A. flavus contains the potential to produce many other secondary metabolites. Bioinformatic analysis of the A. flavus genome has revealed at least 70 putative secondary metabolite biosynthetic gene clusters. The metabolic products of most of these clusters have not been characterized and their biological role is not known. Secondary metabolites that enhance the ability of the fungus to survive and infect crops are of particular interest. Transcriptomic data has revealed that several biosynthetic gene clusters are expressed during A. flavus infection of corn seed. We focused on identifying the products of two of these upregulated clusters: one cluster contains a nonribosomal peptide synthetase (NRPS)-like core gene and the other a putative ribosomally synthesized post-translationally modified peptide (RiPP) encoding gene. We found that the biosynthetic gene cluster containing the NRPS-like core gene produced aspergillic acid, a hydroxamic acid containing pyrazinone that binds iron. We subsequently found that an A. flavus mutant with the NRPS-like core gene knocked out was less virulent on corn seeds, suggesting that aspergillic acid is a virulence factor. We also have generated A. flavus strains harboring deletions of the RiPP encoding gene. Chemical extracts of these mutants and their wild type counterparts were analyzed using comparative metabolomics revealing some gene-dependent features. Investigations targeting the RiPP products and their effects on virulence are ongoing.

Innovative research on mycotoxins in grains from Costa Rica to guarantee quality for human consumption: Research Center for Seeds and Grains of Univ. of Costa Rica Andrea Irias-Mata, andrea.iriasmata@ucr.ac.cr, María Viñas-Meneses. Research Center for Seeds and Grains, Universidad de Costa Rica, San Jose Costa Rica is a nation where the daily diet includes the consumption of grains. Nowadays, 80% of the grains are imported, attempting to the food sovereignty and food security of the Country, since local producers are incapable of meet the local demand. From the academy, through the Research Center for Seeds and Grains of Univ. of Costa Rica, we perform research on grains postharvest quality to guarantee quality of the most consumed grains, rice, beans, and maize. Grains quality is evaluated by physical traits, absent of microorganism and nutritional value. One of the critical points that threat grains in postharvest are the fungi grown and mycotoxins development. In a tropical country as Costa Rica, the climate conditions of humidity and temperature are suitable for their development, mostly if the storage techniques are not adequate. Mycotoxins are secondary fungi metabolites with proven negative effects in animal a human health, including carcinogenic effects. In terms of nutritional quality, there is a lack of information regarding the most abundant nutrients in the Costa Rican rice and beans varieties, which is necessary for the promotion and utilization of this grains and its possible association with reduction of mycotoxins incidence. Our research aims, by one side, to identify toxigenic fungi and mycotoxins in grains from Costa Rica and study strategies for reduce their incidence by the application of innovative bio-fungicides, as extracts of fruits rich in polyphenols. On the other hand, we aimed to develop and validate analytical methods for the identification and quantification of nutrients and bioactive compounds in these grains to assess its association with reduction of mycotoxins incidence. And finally, with the research results we aimed to perform outreach activities among local producers of grains.

Management of aflatoxins and fumonisins in corn using biocontrol with non-toxigenic strains of Aspergillus flavus, bioplastic, and biochar Hamed K. Abbas1, Hamed.Abbas@ars.usda.gov, Ryan Paulk1,2,3, ryan.paulk@usda.gov, Cesare Accinelli4, Nathan Little3, Nacer Bellaloui5, Wayne Shier6. (1) BCPRU, USDA Agricultural Research Service, Stoneville, Mississippi(2) Biochemistry, Molecular Biology, Entomology, and Plant Pathology, Mississippi State Univ.(3) SIMRU, USDA Agricultural Research Service, Stoneville, Mississippi(4) Universita degli Studi di Bologna, Emilia-Romagna, Italy(5) CGPSRU, USDA Agricultural Research Service, Stoneville, Mississippi(6) College of Pharmacy, Univ. of Minnesota Twin Cities School of Medicine, Minneapolis Mycotoxins, including aflatoxins and fumonisins, are produced by fungi that commonly infest corn (maize), especially in the Mississippi Delta and the rest of southern US. Aflatoxins are potent carcinogens that cause liver damage and liver cancer. Fumonisins cause health problems in animals in the Mississippi Delta, including leukoencephalomalacia in horses, and have been implicated in causing Spina bifida and other neural tube defects in humans. We have developed improved biocontrol methods that use non-toxigenic strains of Aspergillus flavus to out-complete toxin-producing A. flavus. Included are improved delivery systems, which use starch-based biodegradable bioplastics in seed coatings and in sprayable formulations. Biochar has also been added to bioplastic-based seed coatings to improve seedling nutrition and germination frequency. Recent work has focused on optimizing biocontrol agent delivery strategies in order to help farmers minimize the effects of fungi and their toxins on maize crops and as a strategy to improve safety and quantity of feed and food supplies. In the last three years from 2021 to 2023 a series of experiments have been conducted to evaluate the feasibility of using these agents for coating corn seeds. Results and strategies going forward will be discussed.

Evaluating Acheta domesticus for the reduction of fumonisin B1 in livestock feed Hamed K. Abbas1, Ryan Paulk1,2, ryan.paulk@usda.gov, Guadalupe Rojas1, Juan Morales-Ramos1, Mark Busman3, Nathan Little4, Wayne Shier5. (1) BCPRU, USDA Agricultural Research Service, Stoneville, Mississippi(2) Biochemistry, Molecular Biology, Entomology, and Plant Pathology, Mississippi State Univ., (3) NCAUR, USDA Agricultural Research Service, Peoria, Illinois(4) SIMRU, USDA Agricultural Research Service, Stoneville, Mississippi(5) College of Pharmacy, Regents of the Univ. of Minnesota, Minneapolis Mycotoxin contaminated grain is a major issue in agriculture systems worldwide. Finding alternatives to the destruction and waste of contaminated grain is needed for a sustainable future. Re-introduction into the farm food web through a consumable intermediary such as insects may be possible. The domestic cricket, Acheta domesticus (L., 1758), is a polyphagous insect that has come under consideration as an alternative protein source in domestic animal feed. Fumonisin is a commonly found mycotoxin in corn produced by Fusarium verticillioides that has significant impact on livestock by causing various diseases such as leukoencephalomalacia in horses, pulmonary edema in swine, and is possibly carcinogenic in humans and other animals. Small colonies (n=25) of 2nd instar A. domesticus were reared to 5th instar and beyond on nutrient-optimized corn-based diets spiked with zero, low (1 ppm), and medium (5 ppm), and high (20ppm) levels of fumonisin B1. At the time of harvest, we were able to show in A. domesticus that: 1) there is no feeding aversion to fumonisin B1, 2)

increasing levels of fumonsin B1 have no effect on survivorship, 3) increasing levels of fumonisin B1 have no effect on growth and development. Determined by HPLC, the concentrations of fumonisin B1 in A. domesticus after eight hours of pre-harvest starvation were found to be significantly lower ($p < 0.001$) than that of the diet that they fed upon by 95 to 97%. The reduced fumonisin B1 concentration in A. domesticus and their successful rearing to adulthood supports the idea that less wasteful agricultural practices can be developed through remediation of contaminated corn and other grains by insects suitable for livestock feed.

Bioinformatically informed evaluation of Sarocladium zeae biocontrol agent viability Sydney M. Schoellhorn, sydneyschoellhorn@my.unt.edu, Timothy H. Lim, Tram Nguyen, Ian G. Sartor, Elizabeth Skellam. Chemistry / BioDiscovery Inst., Univ. of North Texas, Denton One third of the global corn supply is produced in the US, making maize the largest American agricultural product. Any biocontrol agents that protect maize against exogenous threats must be safe for consumption. The fungal pathogens Aspergillus flavus and Fusarium verticillioides, which respectively produce aflatoxins and fumonisins, are major exogenous mycological threats to maize. Pyrrocidines A and B, which have been found to selectively protect against these mycotoxins, have been isolated from Sarocladium zeae, piquing interest in using S. zeae as a biocontrol agent. A research group at UCLA sequenced S. zeae and elucidated the biosynthesis of pyrrocidines but left remaining biosynthetic gene clusters (BGCs) unexplored. Hence, it is necessary to screen all secondary metabolites produced by remaining BGCs to determine its viability for use as a biocontrol agent. To do so, genes from these BGCs will be expressed in a fungal host to isolate and identify associated natural products, prioritized by bioinformatic analyses. Once identified, the product metabolites will be evaluated for potential toxicity.

X-ray irradiation of Aspergillus flavus and Aflatoxin B1 contaminated maize Hannah Glesener, glesener@asu.edu. School of Engineering of Matter, Transport and Energy, Arizona State Univ., Tempe Food crops around the world are commonly contaminated with Aspergillus flavus, which can produce the carcinogenic mycotoxin Aflatoxin B1 (AFB1). The objective of this study is to establish a sterilization method for studying toxins in food products in the laboratory using AFB1 on maize as a case study. The aims are to (1) remove all viable A. flavus from the maize and (2) maintain a constant concentration of AFB1. A batch of ground maize was inoculated with an aflatoxigenic A. flavus strain. X-ray irradiation was used to dose the maize with 0.0, 1.0, 1.5, 2.0, 2.5, and 3.0 kGy. AFB1 was quantified in the dosed maize by HPLC and by ELISA. A. flavus was quantified by dilution plating on potato dextrose agar and modified rose bengal media for viability and qPCR for gene presence. AFB1 concentration did not significantly change with increasing doses of radiation. HPLC data showed a mean AFB1 concentration of 240.22 ± 17.66ppb. ELISA data showed a mean AFB1 of 286.63 ± 56.57ppb. A. flavus viability, but not gene copies, changed significantly by increasing doses of radiation. Dilution plating showed log CFU decreased 4.5 fold from 0.0 to 2.5kGy; the organism was not viable beyond a 2.5kGy radiation exposure. qPCR showed consistent A. flavus presence across doses with a mean of 7.04 ± 0.34 log gene copies of MDR1 gene. These results imply that x-ray irradiation is an effective means of rendering A. flavus non-viable in maize materials without affecting AFB1 concentrations. These findings are important because they show the effective sterilization of a food product using the non-radioactive, non-thermal, and non-chemical X-ray irradiation, which has rarely been done in food and can be tested more broadly using other food matrices.

Stable, sustainable, and edible Chitinase formulation for biocontrol of fungal rot Farah Deeba1, farahdeeba777@gmail.com, David W. Wood1, Davita L. Watkins2, Chad Rappleye3. (1) Chemical and Biomolecular Engineering, The Ohio State Univ., Columbus(2) Chemistry and Biochemistry, The Ohio State Univ., Columbus(3) Microbiology, The Ohio State Univ., Columbus Emerging resistance to chemical fungicides and negative environmental impacts have compelled researchers to evaluate alternative methods to control disease-causing fungi. Among various food safety methods, chitinolytic enzymes provide a safe and cost-competitive natural (biological) approach to controlling fungi as compared to chemical fungicides, but the main disadvantage of enzymes relies on their instability, which decreases their half-life in the case of temperature and pH fluctuations. Enzyme immobilization can offer an opportunity to enhance enzyme stability and reusability. In this scenario, waste-derived nanoparticles (NPs) are considered ideal for synthesizing sustainable, green, highly stable fungicides. Enzyme immobilization using biopolymer strategies is considered efficient in enhancing chemical and physical properties, high surface specificity, and stability of enzyme formulation. In this study, we are synthesizing low-cost, nontoxic, environmentally friendly chitinase immobilized (NPs) based on (1) Poly (ethylene glycol)-poly(caprolactone) (PEG-PCL) and (2) Agro-waste-derived polymers (Pullulan). Once synthesized, the chitinase NPs are tested for their stability and ability to control two relevant species of Aspergillus using in vitro mycelial growth inhibition and colorimetric growth assays. The most active and highly stable nano-chitinase formulations are applied as a crosslinked film both directly and indirectly on post-harvest strawberries and onions. Our results indicate nano-chitinase formulation as a promising, effective, and sustainable food packing material against fungal rot.

WEDNESDAY MORNING March 20

Michael Granvogl Memorial Symposium

Spotlight on Michael Granvogl: Science and Socializing Timo D. Stark, timo.stark@tum.de. Food Chemistry and Molecular Sensory Science, Technische Univ. Munchen, Bayern, Germany Michael Granvogl started to study food chemistry at Technical Univ. of Munich (TUM) two years before me. I remember very well and with a smile on my face that we had the first intensive contact on the soccer field where Michael and his food chemistry Ph.D. team played soccer against our student's food chemistry team. Afterwards, we joined several years together as Ph.D students at the German Research Center of Food Chemistry, now known as Leibniz Inst. for Food Systems Biology at the Technical Univ. of Munich (Leibniz-LSB@TUM), where he investigated the flavor of cooked onions. After my post-doc time, we meet us again at TUM, he was doing his habilitation and exploring the field of food born toxicants. Till his leaving for the Association of the German Confectionary Industry and, afterwards, in 2019 his Professorship for Food Chemistry at the Univ. of Hohenheim, we spent many years together as colleagues under the same proverbial "big roof" food chemistry. In this talk, his greatest scientific achievements were highlighted in sociable embedded atmosphere, where he also and courageous significantly contributed.

Formation of furan and furan derivatives in model systems and food products Alena Schoepf, alena.schoepf@uni-hohenheim.de, Claudia Oellig, Michael Granvogl. Inst. of Food Chemistry, Univ. Hohenheim, Stuttgart, Baden-Württemberg, Germany Furan and furan derivatives are processing contaminants that are known to exhibit adverse effects and occur in a wide range of different heat-

treated food products, like canned and jarred food, cereals, and coffee products. Furan was classified as a possible human carcinogen (Group 2B) in 1995. Therefore, human exposure to these contaminants should be minimized. The formation pathways are diverse and not fully known so far. The data on furan derivatives, which have recently been highly interesting because of their potential health risk, is limited. A systematic study on the formation of furan and its derivatives is crucial to consider these findings as a basis for predicting the formation of these processing contaminants in food and finding minimization strategies to enhance food safety. Therefore, different precursors were heat processed in model studies and the presence of food matrix, e.g., vegetable puree, to clarify the contribution of these food ingredients to the formation of furan and its derivatives. Already known precursors leading to furan formation due to oxidation and thermal degradation are ascorbic acid, polyunsaturated fatty acids (PUFA), saccharides, amino acids, and carotenoids. As infants and young children form a vulnerable group, baby food is highly interesting and was, therefore, investigated regarding furan formation. Due to their chemical properties (boiling point of furan 31.5 °C), the analysis was performed by headspace-solid phase micro-extraction gas chromatography (HS-SPME-GC) coupled to tandem quadrupole mass spectrometry (MS/MS), and quantification was based on stable isotope dilution analysis (SIDA). With the developed HS-SPME-GC–MS/MS method furan, alkylated furans (2-methylfuran, 3-methylfuran, 2-ethylfuran, 2,5-dimethylfuran, and 2-pentylfuran), oxygenated furans (furfural, 3-furaldehyde, furfuryl alcohol, and 3-furanmethanol), and the acetylated furan 2-acetylfuran were determined.

Enhancing sensory quality of Golden Delicious apple brandies: Identification of key aroma compounds for distillation parameter optimization Sarah Kramp, sarahann.kramp@uni-hohenheim.de, Claudia Oellig, Michael Granvogl. Inst. of Food Chemistry, Univ. Hohenheim, Stuttgart, Baden-Württemberg, Germany The sensory quality of food products influences the purchasing behavior of consumers. An increase in quality can also lead to increased profits for the producer. An evaluation of brandies from regional associations of small-scale and fruit distillers in North and South Württemberg (Germany) revealed that approximately 30% of the spirits fell into categories described as 'noticeable quality deviations' and 'significant defects' when combined. Therefore, enhancing sensory quality through adjustments in production parameters is crucial. In distillates, the aroma compounds present in the raw material and those generated during fermentation, distillation, or maturation processes may be present. Yeast and other microorganisms during fermentation contribute to forming compounds that influence a fruit brandy's aroma. Additionally, distillation is a step in which the distillate is separated into the head-, heart-, and tail-fraction, and the quality depends on the extent to which aroma compounds are separated from the heart-fraction. To improve this process, it is necessary to identify the aroma compounds that contribute to the good quality of the brandy. Therefore, screening for odor-active substances, including aroma extract dilution analysis using gas chromatography-olfactometry and identification, quantification with stable isotope dilution analysis, and assessing the relevance with odor activity value have been performed. This research project focuses on golden-delicious apple brandies. Thus, various Golden Delicious apple brandies were purchased and rated using sensory evaluation. Using the data, we identified key aroma compounds in both 'high-quality' and 'low-quality' brandies. This step serves as the fundamental prerequisite for optimizing distillation parameters.

Exploring edible halophytes: Polyphenols extraction, characterization, and antioxidant activity of endemic sea asparagus (Salicornia europaea L.) from the Apulian region of Italy Roberta Tardugno1, roberta.tardugno@gmail.com, Francesco Limongelli1, Marilena Muraglia1, Pasquale Crupi2, Maria Lisa Clodoveo2, Filomena Corbo1. (1) Pharmacy - Drug Science, Univ. degli Studi di Bari Aldo Moro, Bari, Puglia, Italy(2) Interdisciplinary Dept. of Medicine, Univ. degli Studi di Bari Aldo Moro, Bari, Puglia, Italy Halophytes constitute a highly specialized flora adapted to hypersaline environments. The stress of the alkaline environment induces the synthesis of metabolites that can be useful to humans for their bioactivities. Salicornia europaea L., commonly known as sea asparagus or glasswort, is an endemic halophyte growing in the coastal area of the Apulian region of Italy and used for centuries in local food recipes due to its nutritional and beneficial effects. In this study, response surface experimental design methodology applied to ultrasound-assisted extraction (UAE) optimized the recovery of polyphenolic constituents. The chemical analysis was performed by RP-HPLC coupled with MS and UV/DAD detection. The phytochemical analysis of S. europaea extracts revealed the presence of polyphenolic compounds belonging to different classes, mainly flavonols such as isorhamnetin O-glycosides. The total phenolic content and the antioxidant profiles of S. europaea extracts have been evaluated by Folin-Ciocalteau, DPPH, ABTS and FRAP assays. The most interesting antioxidant profile was detected using the combination of 50% ethanol solution, 10 min, and a molar ratio matrix: solvent of 1:10 (w:v). The design of experiment approach for mixture composition optimization turned out to be a useful and effective method for S. europaea polyphenol extraction conditions.

Different wood – different smell? Elucidation of wood odors of different species Adina Baum1, Helene M. Loos1,2, Andrea Buettner1,2, andrea.buettner@fau.de. (1) Dept. of Chemistry & Pharmacy, Friedrich-Alexander-Univ. Erlangen-Nurnberg, Bayern, Germany(2) Fraunhofer-Institut fur Verfahrenstechnik und Verpackung IVV, Freising, Bayern, Germany Wood is an important raw material. Due to its versatility in indoor and outdoor use, humans often come into contact with the smell of wood, which can influence their well-being and health. Therefore, it is relevant to investigate the odorants which create the wood scent. Furthermore, a wide range of applications is possible with the knowledge of the molecular odorous composition of woods. Previous research mainly focused on specific wood species like oak wood, which is utilized to develop the aroma of wine and spirits through storage in wooden barrels. The odorous composition of other wood species has been rarely investigated to this extent. To close this gap and increase the knowledge of which odor-active compounds are present in which wood species, odors of various hardwood and softwood species have been investigated. The elucidation of the odors was achieved via sensory analysis and sensory-instrumental analysis methods like (two-dimensional) gas chromatography-mass spectrometry/olfactometry. A variety of chemical substance classes which contribute to the wood odors were detected and differences and similarities in the odorous composition of different wood species were observed.

Linking the dynamics of aroma release and flavor perception via in vivo analytics and time-resolved sensory assessments Jonathan Beauchamp1, jonathan.beauchamp@ivv.fraunhofer.de, Nina Cleve1,2, Maria Izaber1,2. (1) Sensory Analytics and Technologies, Fraunhofer-Institut fur Verfahrenstechnik und Verpackung IVV, Freising, Bayern, Germany(2) Dept. of Chemistry and Pharmacy, Friedrich-Alexander-Univ. Erlangen-Nurnberg, Erlangen, Bayern, Germany The perception and enjoyment of flavor during food consumption is driven by a complex interplay of physics, chemistry and biology. When the food enters the mouth, it encounters physical breakdown via mastication and chemical alteration through interactions with saliva that lead to the release of tastants and aroma compounds, which ultimately interact with the respective biological

receptors on the tongue and in the nasal cavity to elicit sensory signals interpreted by the brain. This multifaceted sequence of events is invariably given little regard by consumers in their busy daily lives, with flavor perception often taken for granted, especially when simultaneously assaulted with a battery of external sensory stimuli. When consumers are mindful to take the time to focus on their sensory perceptions during food consumption, they will become aware that flavor is not a static stimulus but rather changes dynamically from the first impression to the lingering flavor after the food has been swallowed. This shifting flavor is almost universal across all foods and beverages. Shedding light on this phenomenon requires tools that cater for time-resolved assessments, ideally combining both sensorial and analytical means of data acquisition. One such approach is to utilize dynamic sensory methods, for instance temporal dominance of sensations (TDS) or time-resolved check-all-that-apply (TCATA) in combination with in vivo (nosespace) analysis of aroma release via direct injection mass spectrometry, such as proton transfer reaction-mass spectrometry (PTR-MS). This presentation will introduce this complementary approach of combining objective analytical with subjective sensory assessments to explore the link between the dynamics of aroma release and flavor perception, focusing on technical challenges, key discoveries, and insights garnered from contemporary studies. This contribution is dedicated to the memory of Michael Granvogl, who was cognizant of the complexity of flavor and was passionate at unraveling its individual elements.

Odorants identified in Chinese dry-cured ham contribute to salty taste enhancement Yanping Chen, catherinechenyp@sjtu.edu.cn. Shanghai Jiao Tong Univ., China Jinhua dry-cured ham (JDH) is a traditional fermented Chinese meat product. We studied the dynamic sensory and emotional profiles of JDHs obtained by five preparation methods and the corresponding release of sodium, potassium, and volatile organic compounds (VOCs) during oral processing. The VOCs with salty taste enhancement abilities were screened based on the correlations of VOCs with salty flavor and concentration of sodium, potassium, and ammonium ions with salty flavor. A trained sensory panel evaluated the saltiness enhancements of selected VOCs using static and dynamic sensory methods. The results revealed that sodium (Na^+), potassium (K^+), and selected VOCs were mainly released during 0-10 s of the chewing process. The release of Na^+ and K^+ ions in JDH residue samples exhibited consistently decreasing trends while in saliva their concentrations increased. The VOCs showing a high correlation with Na^+ and K^+ ions and salty flavor have saltiness enhancement abilities both in NaCl solutions and NaCl +MSG mixtures. Odor-induced saltiness was pronounced at low salt concentrations (0.2% NaCl). The investigation demonstrated 16 VOCs exhibiting saltiness enhancement abilities, including 4 pyrazines, 5 acids, 4 sulfur-containing compounds, and 3 other compounds. The sensory evaluation suggested pyrazines and sulfur-containing compounds as good saltiness enhancers. 2- Furfuryl mercaptan significantly enhanced the salty sensation in the NaCl + MSG solutions when compared with MSG alone ($p<0.05$). This research provides evidence that certain odorants identified in JDHs exhibit salty-enhancing properties, indicating their potential for salt reduction at the industrial level.

Mining and rapid screening model and database construction of umami peptide taste patterns based on amino acid sequences Cui Zhiyong, Wenli Wang, Yuan Liu, y_liu@sjtu.edu.cn. Shanghai Jiao Tong Univ., China Umami taste is one of the five basic tastes that make food palatable. Umami peptides, which have dual characteristics of nutrition and delicious taste, have been a hot topic in recent years. To discover umami peptides from umami base materials (fermented fish, etc.), there is little information on the taste patterns of umami peptides. Furthermore, the identification of taste peptides in traditional method is laborious, expensive and time consuming, due to the complicated experiment process including pretreatment, separation, synthesis, and sensory evaluation. Therefore, developing a more accurate and effective method is urgent for judging the tastes of peptides. TastePeptides-Meta was proposed, which includes the taste peptide database TastepeptidesDB (Figure 1, http://tastepeptides-meta.com/TastePeptidesDB) the umami/bitter peptide judgment model (TastePeptidesDM, Umami_YYDS), and umami substance EEG data Analysis program (TastePeptides-EEG). TPDB is a bioinformatics database and focuses on collecting taste related information of taste peptides, including taste peptide sequences, identification thresholds, and related corresponding authors etc. Based on the taste peptide data collected in TPDB, our team established two umami peptide screening models: (1) Umami_YYDS (http://tastepeptides-meta.com/YYDS), (2) TastePeptidesDM (http://tastepeptides

Formation of volatile heterocyclic compounds and open-chain amides of theanine in model systems with glucose, tea leaves, and tea extract under tea roasting conditions Mengru Li, Xiaochun Wan, xcwan@ahau.edu.cn, Xiaoting Zhai, zhai189@outlook.com. Anhui Agricultural Univ., Hefei, China Theanine is a non-proteinogenic amino acid found in the tea plant Camellia sinensis, the thermal reactions of theanine and its interaction with sugars and the matrix of tea leaves remain unclear. Therefore, the objective of the present study was to investigate the volatile products formed from the thermal degradation of theanine and the Maillard reaction of theanine/glucose under tea roasting conditions. The thermal reactions were also conducted in crude tea leaves and their aqueous extract to study the interactions with the tea matrix. We found that at elevated temperature (>90 °C), theanine released two major volatile compounds 1-ethyl-1,5-dihydro-2H-pyrrol-2-one and N-ethylsuccinimide. Other products were identified including 10 pyrroles and 10 amides/imides. In the presence of glucose, the formation of the theanine volatiles was accelerated and further Maillard reactions occurred. A total of 56 compounds were identified in the model system of theanine and glucose, including 12 amides/imides, 16 pyrazines, 16 pyrroles, and other N-heterocycles, as well as 12 furans and other O-heterocycles. Although most of the reaction products were detected in tea leaves and in their aqueous extract with or without the addition of theanine under the same experiment conditions, amides and imides were considerably suppressed, left only minute amounts or even no longer detectable. Pyrazines and pyrroles were also shown at reduced concentrations due to interaction with tea components but to a lesser extent. A total of 16 and 12 pyrazines were identified in the theanine/glucose reaction system and tea leaves/aqueous extract after roasting, respectively. The results indicated that pyrazines and other main volatiles in roasted tea leaves were formed from the Maillard reactions of the aqueous fraction of tea leaves. Theanine participated in the formation of pyrazines in tea leaves under roasting conditions.

Consumer mushroom quality expectation and the impact of thermal process on mushroom desired flavor creation and nutrient retention Xiaofen Du2, xdu@twu.edu, Yixiang Xu1. (1) Healthy Processed Foods Research Unit, USDA ARS Western Regional Research Unit, Albany, California (2) Nutrition and Food Sciences, Texas Woman's Univ., Denton Mushroom has high nutritional value, low energy density, and distinctive sensory qualities, making it an ideal food. However, mushroom consumption varies worldwide. The U.S. has a relatively low amount of 4 lbs per capita. Currently, the research regarding consumer viewpoints on mushroom products and the effect of thermal processing on mushroom flavor and nutrition quality are very limited. The current

study aimed to 1) conduct a survey with the subject sample size of 4,050 with the intent to investigate mushroom consumption behavior, quality expectation, and perceived market gap, and 2) investigate the effect of thermal processing on mushroom flavor and nutrients. The survey results showed that shiitake, porcini, and white mushrooms were the major varieties that were mainly consumed cooked (49.3%) or in a canned soup (43.0%). Enjoying its flavor or health benefits shared same ratio (48.1%) as the major reasons for consumers to choose eating mushroom. The ideal mushroom sensory traits included fresh (50.9%) with a typical mushroom flavor (41.6%), while ideal nutritional compositions were minerals (49.9%) and vitamins (49.0%). Slimy/sticky texture and wrinkles along with a dry appearance were undesirable. Consumer perceived market gap for mushroom included limited variety, lack of freshness upon purchase, short shelf-life, and high price. Since flavor and nutritional quality were the self-stated consumption motivators, the effect of thermal processing on mushroom quality was further investigated using instrumental analysis. The results showed cooking significantly increased desired flavors such as meat-like aroma and savory notes; as well as other relevant volatile and non-volatile compositions. However, cooking significantly reduced nutritional composition, especially amino acids for both free and those bound in protein. These findings elucidate consumer expectation, increase knowledge/insight with regards to potential flavor creation approaches, and minimize nutrient loss, consequently increasing the recognition and consumption of mushrooms.

Influence of thermal treatment on the formation of dry jujube flavor: A new insight into pyrazines production with important bakery-type aroma compounds Qing Xiao, qingxiao619@gmail.com, Chi-Tang Ho. Food Science, Rutgers The State Univ. of New Jersey, New Brunswick Comparing with its natural fresh state, dry jujube (Ziziphus jujube Mill.) is supposed to have good potential to produce novel aromatic substances and special flavor quality. Proteins, amino acids and reducing sugars of itself are considered to undergo Maillard reaction during drying or thermal processing. Regarding this key reaction for flavor generation, our current study aimed to intensify natural dry jujube aromas via thermal treatment and identify key volatile compounds. GC-MS results showed that megastigmatrienone (1.27 ± 0.06 μg/kg), a carotenoid breakdown product as the heart of tobacco aroma was first identified in dry jujube fruit. Thermal treatment improved the formation of aromatic compounds with sweet, caramel and roasted odors. When treated at 120 °C for 1.5 h, furaneol was produced, meanwhile, pyrazines, furans and furaneol were all significantly enhanced. Proline-derived 2,3-dihydro-1H-pyrrolizines and cyclopent[b]azepine-8(1H)-ones with bready/cracker-like aroma were abundantly generated among nitrogen-containing compounds. We investigated the dominance of these two classes compounds formation using the model reaction of asparagine and proline with glucose. It suggested that with a secondary amino group attached a five-carbon pyrrolidine ring, proline showed its high reactivity to react with α-dicarbonyl intermediates, producing pyrrolizines and azepines in large amounts in a competing Maillard system with other amino acids.

Characterization of ethyl vanillin in nature and its potential impact on flavor industry Xuebo Song1, xuebosong@ufl.edu, Mark Porter2, Vance Whitaker2, Seonghee Lee2, Yu Wang1, yu.wang@ufl.edu. (1) Food Science and Human Nutrition, Univ. of Florida, Lake Alfred(2) Dept. of Horticultural Sciences, Univ. of Florida Inst. of Food and Agricultural Sciences, Wimauma Ethyl vanillin exhibits a characteristic vanilla-like odor and with three times more potency than vanillin. It is a very important artificial flavor compound in food production; however, its use is very limited due to its missing status and potential usability as a natural flavor compound. In this study, ethyl vanillin was identified for the first time in strawberry, as well as in nature, based on a targeted metabolomics strategy. To enhance the confirmation of qualitative precision, a polar column FFAP, a non-polar TG-5MS column and a chiral Rt-bDEXsm column were applied to conduct the identification analysis of ethyl vanillin utilizing the MRM mode in GC-MS/MS. Furthermore, Orbitrap LC-MS, and UPLC-MS/MS were used to confirm the identification of ethyl vanillin. In addition, the stable isotope dilution analysis method was applied to quantify ethyl vanillin in strawberry. The identification of ethyl vanillin in strawberry has important impact on it as "natural identical" status.

General Papers

Absorption, distribution, metabolism, and excretion (ADME) studies of [14C]-nitrofurazone residues in broiler chickens Anuradha Singh, anuradha.singh@usda.gov, David J. Smith. Animal metabolism-Agricultural Chemicals Research Unit, USDA Agricultural Research Service, Fargo, North Dakota Nitrofurazone (NF) is an antibiotic banned from use in food animals because of its potential carcinogenicity/mutagenicity. Regulatory agencies screen poultry for NF exposure by detecting the semicarbazide (SEM) moiety of NFZ which is released upon mild hydrolysis of tissue-bound NF metabolites. But SEM detection has proven to return false positive results in unexposed animals. Therefore, identification of a NF-specific alternative marker is a pressing need. To this end, ADME studies of 14C-NF in broiler chickens were performed. NFs containing 14C either at the furaldehyde carbon (NF-A) or the carbonyl carbon of SEM (NF-B) were synthesized and groups of 12 birds were provided feed containing 14C-NF-A or 14C-NF-B (5 mg/kg) for 7 consecutive days. Control birds (n=6) were fed with NF-free feed. Birds were euthanized on withdrawal days (WD) 0, 4, 7, and 14 and blood and tissues were harvested. Total radioactive residues in liver, kidney, muscle, and gizzard were determined by oxidation followed by liquid scintillation counting (LSC). At WD 0, kidney was the major depot for total radioactive residues followed by liver and muscle (about 636 ng/g to 180 ng/g, NFZ equiv). At WD 14, radioactive residues were detected in a range from about 67 ng/g to 17 ng/g (NFZ equiv) in the same tissues. Total radioactive residue depletion data in liver and muscle were fit to a one-phase exponential decay curve using least squared regression, which suggested no difference ($P > 0.20$) in the depletion rate between NF-A and NF-B. Extraction of liver or muscle tissues in organic solvents indicated that about >70% NF-related residues were bound to the tissues, regardless of withdrawal day. Total radioactive analysis in other tissues and metabolite identification studies are undergoing.

Determination of acrylamide content in common pelletized small animal food Steven McComis1, mccomis.s01@mymail.sxu.edu, Tatiana Tatum2, tatum@sxu.edu. (1) Chemistry, Saint Xavier Univ., Chicago, Illinois(2) Biological Sciences, Saint Xavier Univ., Chicago, Illinois Acrylamide is a carcinogenic chemical found in food products, especially fried and roasted foods. While much work has been done to determine acrylamide content in food for human consumption, less has been done on animal feedstuff. Numerous studies have examined dog, cat and dairy feed; however, little work exists reporting acrylamide content in small animal feed, such as pelletized bird and hedgehog food. As small animals become more prevalent in households, their care, husbandry and diet deserve increased attention. This work examines the acrylamide content in common pelletized small animal foods.

Exploring and understanding food emulsion systems with neutron scattering and spectroscopy Theresia Heiden-Hecht, t.heiden-hecht@fz-juelich.de, Henrich Frielinghaus, Maren Müller,

Olaf Holderer. JCNS, Forschungszentrum Julich GmbH, Garching, Bayern, Germany Food emulsions may be either stabilzed by amphiphilic milk-based and sustainable plant-based proteins. The protein is affecting the interfacial and emulsion stabilization mechanisms on a macro- and microscale of length and time. To understand these mechanisms in detail different length scales from interatomic to macroscopic distances as well as time dependent mechansims need to be investigated. Neutron scattering techniques provide insight into such emulsions on these length scales depending on the technique used. Combining structural information on molecular length scales from small angle x-ray and neutron scattering (SAXS and SANS) with time dependent neutron spin echo spectroscopy (NSE) allows to expand our understanding towards intermolecular interactions within the interface. These interactions are linked to the emulsion stability – the elastic properties of the protein or protein/phospholipid stabilized oil/water interface on molecular length scales. NSE provides in this combination the time dependent correlation function in reciprocal space, S(q,t), on molecular length scales and time scales in the nanosecond range relevant for thermally driven motion of mesoscopic systems such as the emulsion interfaces. This presentation introduces the neutron and x-ray scattering techniques which broadens the classical characterization of food emulsions. Results from emulsions stabilized with b-lactoglobulin as a representative milk protein, and different plant-based proteins, are presented and discussed. Contrast variation by deuteration of some components of the emulsions is applied to focus on the interfacial region, relying on the uniqueness of neutrons. Connecting these emerging results with classical characterizations such as interfacial tension or viscoelasticity helps understanding the complex mechanisms of interfacial stability and may contribute to a knowledge driven development of sustainable food emulsions.

Rekindling a cherished memory: The flavor of the American chestnut Wenxi Yang1, vince17@illinois.edu, Sara Fitzsimmons2, Keith R. Cadwallader1. (1) Food Science and Human Nutrition, Univ. of Illinois Urbana-Champaign(2) Ecosystem Science and Management, The Pennsylvania State Univ., Univ. Park Exploration of the flavor chemistry of the American chestnut, a tree species deeply entrenched in the memories of past generations, is enabled by the existence of surviving American chestnut specimens. We conducted comprehensive examination of the chemical composition, flavor chemistry, and sensory attributes inherent to the American chestnut. Chemical composition analysis was conducted on both American chestnut and other selected chestnut species cultivated within the US. In addition, our investigation employed cutting-edge flavor analysis techniques, including the identification and quantification of potent odorants through gas chromatography olfactory (GC-O), gas chromatography-mass spectrometry (GC-MS), and gas chromatography triple quadrupole mass spectrometry (GC-TQ-MS), complemented by sensory evaluation. The relationship among chestnut species with respect to chemical composition (moisture, water activity, sugar, protein, lipid, and ash), flavor profiles, and sensory attributes was established through multivariate statistical analysis. The results of this research identified various distinctive qualities inherent to the American chestnut and highlights the potential for reintroducing this legacy nut tree for future generations.

Chitosan films made from food and agricultural waste as replacements for petroleum-based plastics Kaydren Orcutt1, kaydren.orcutt@gmail.com, Zach McCaffrey1, Jong H. Kim2, William Hart-Cooper1. (1) Bioproducts Research Unit, USDA-ARS Pacific West Area, Albany, California (2) Foodborne Toxin Detection and Prevention Research, USDA-ARS Pacific West Area, Albany, California Chitosan films made from shellfish waste can be used for a wide array of applications – textiles, packaging, agriculture, food safety – as a green alternative to petroleum-based plastics. The properties of these films can be tuned via chemical modification or through the addition of bio-based fillers or actives. Type and composition of fillers can lead to stronger films and novel ways of incorporating actives. We will present the effects of using these additives on the tensile, antimicrobial, solubility, and biodegradation properties of chitosan films as they relate to their potential applications.

Micro-thermography reveals new insights into ice nucleation and growth inside frozen food products Martin Zalazar, Ran Drori, rdrori@yu.edu. Chemistry and Biochemistry, Yeshiva Univ., New York Controlling ice nucleation (the formation of ice from liquid water) and growth during the freezing process of food products will improve the quality of such products and minimize food waste. Imaging the kinetics of ice growth and nucleation inside solid materials is challenging since they are not transparent, thus, light microscopy cannot be used. Instead, indirect methods are currently used to measure ice crystal size and structural damage to the sample tissue at different time intervals. Some more direct methods are used for ice growth imaging; however, the cost of these methods is exorbitant. Using micro-thermography and temperature-controlled stages, we have measured ice growth and nucleation rates inside food products as well as in ultra-pure water and in sucrose solutions at various concentrations. First, the melting point of ice inside each food product was measured. Next, ice growth rates measurements in various food products were obtained, including broccoli, potato, zucchini, apple, chicken, beef and dough. The ice growth rates inside these food products increased with the increase of the supercooling degree (the difference between the measured temperature and the melting temperature of the sample). However, at higher supercooling degrees (~8 ○C), the velocity of the ice reached a maximum after which it remained constant up to a supercooling of 16 ○C. Our hypothesis is that at higher supercooling degrees tested here (>10 ○C), the lower availability of water molecules in the biological tissue and the limited ability of the growing ice crystal to move through tissues are slowing down the measured velocity. Ice nucleation rates are currently being measured using a dedicated system named INANM (Ice Nucleation Assay inside Non-transparent Materials). The combination of the ice nucleation rates with the ice growth rates have immediate implications on the manufacturing procedures of frozen products, especially on the initial cooling process of the product.

Developing humidity-sensitive pectin-based triboelectric devices for monitoring relative humidity as a food-quality indicator Zhenhui Jin, jinzh6@gmail.com, Yang Fu, Longwen Li, Yi-Cheng Wang. Food Science and Human Nutrition, Univ. of Illinois Urbana-Champaign Relative humidity (RH) can critically affect food quality, with high RH facilitating the growth of molds, for example. Thus, it is imperative to monitor the RH of food-storage environments. This study developed a proof-of-concept pectin-film-based triboelectric device (P-TENG) to serve this purpose. This P-TENG mainly comprises two triboelectric materials – one piece of biodegradable pectin film, and one of polytetrafluoroethylene (PTFE) film – that are respectively attached to two conductive layers. When these two triboelectric layers come into contact via external mechanical force (e.g., finger tapping), contact electrification occurs: i.e., the PTFE becomes negatively charged owing to its electron-withdrawing nature, and the pectin, positively charged due to its electron-donating nature. When the external force ceases (e.g., finger pressure is removed), electrons flow through the two conductive layers attached to the two oppositely charged triboelectric layers to balance the build-up of electrical potential between them. Such electron flow generates electrical signals that

can serve as sensor signals. We placed the P-TENG in five different RH conditions – 16%, 30%, 55%, 75% and 99% – and studied its output performance: specifically, open-circuit voltage (Voc). Initially, i.e., from 16% to 75%, the device's Voc increased in line with RH; but when RH reached 99% it dropped drastically. The orderly rise in Voc could have been related to interactions between the pectin film and moisture, which we characterized using Fourier-transform infrared spectroscopy. The signal drop at RH 99%, on the other hand, might have been due to excessive hydration of the pectin film affecting contact electrification. Due to the flexibility of both its triboelectric layers, the P-TENG can potentially be integrated into food packaging to monitor real-time food-storage conditions.

Thermogravimetric kinetics analysis of synthesized bio-lubricants from naturally derived oleic acid Kalidas Mainali, Kalidas.Mainali@usda.gov, Majher I. Sarker, Brajendra Sharma, Madhav P. Yadav, Helen Ngo, Richard Ashby. Biobased and Other Animal Co-products Research Unit, USDA, Agricultural Research Service, Eastern Regional Research Center, Wyndmoor, Pennsylvania This research demonstrates the evaluation and comparison of bio-lubricants synthesized from oleic acid. The oxidative degradability of the vegetable oil-based bio-lubricants affects their storage stability, reusability. Five different types of bio-lubricants were synthesized from Oleic acid. The thermogravimetric analysis was conducted in the presence of air and N2. Comparative studies of the kinetic parameters of each synthesized product showed that these bio-lubricants are thermally stable. The calculated activation energy showed that trimethylolpropane iso-oleic acid ester (TMP-IOA) is thermally stable with (Ea)=188.37 kJ/mol. In the oxidative environment, trimethylolpropane iso-stearic acid (TMP-ISA) ester exhibited the most stable bio-lubricant with average activation energy (Ea)= 109.8 kJ/mol. The lubricant Glyceride-iso-stearic acid (GLY-IOA) showed a high range frequency factor indicating complex behavior in an air environment. Among these lubricants, the GLY-IOA exhibited superior cold flow properties as measured using cryogenic DSC. Overall, these comparative studies confirmed that the monosaturated oleic acid could synthesize thermally and oxidative stable bio-lubricants.

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

Mycotoxins: Challenges and Future Perspectives

Portable mass spectrometry as a tool for monitoring mycotoxin contamination Chris M. Maragos, chris.maragos@usda.gov. Mycotoxin Prevention & Applied Microbiology, USDA-ARS Midwest Area, Peoria, Illinois Preventing exposure to mycotoxins begins, and ends, with toxin detection. It begins with the use of detection methods to facilitate the development of other methods of control, such as host resistance, biocontrol, and remediation. It ends with the use of detection methods to monitor commodities to divert contaminated material. Because of the variety of circumstances in which testing is conducted, analytical methods for mycotoxins are diverse. They range from rapid, ease-to-use, immunoassays to complex laboratory-bound procedures. Cost, speed, accuracy, and the skill level of the personnel conducting the testing are important factors in selecting a method. For regulatory purposes, where accuracy is of utmost importance, liquid chromatography with tandem mass spectrometry (LC-MSn) is often used. Because of their requirements for high vacuums and large volumes of inert gases, such methods are typically confined to well- supported analytical laboratories with highly trained personnel. In an ideal situation the speed, cost, and portability of immunoassays would be combined with the selectivity and accuracy of mass spectrometry. Portable MS instruments have recently become commercially available, which has created the opportunity to take MS out of the laboratory. We have developed methods for testing fumonisins (B1, B2, B3) in maize, and T-2 toxin in wheat and maize using a portable linear ion trap instrument. Two challenges have become apparent: instrument sensitivity and the elimination of matrix effects. Eliminating the large vacuum pumps and tanks of inert gases inherent to laboratory-based instruments is not without cost, as the portable instruments do not attain the same levels of selectivity and sensitivity as good laboratory-based instruments. The challenges associated with portable MS instruments include the development of rapid, field portable, cleanup methods. Despite the challenges, portable MS instruments can be used to develop methods that are as rapid as many immunoassays.

Thermal degradation of the mycotoxin citrinin Lea Brückner, Benedikt Cramer, cramerb@uni-muenster.de, Hans-Ulrich Humpf. Inst. of Food Chemistry, Westfalische Wilhelms-Univ. Munster, Nordrhein-Westfalen, Germany Citrinin is a secondary microfungal metabolite and is attracting worldwide attention due to its toxic effects (nephrotoxic, teratogenic and embryotoxic). Typical citrinin producers are fungi of the genera Penicillium, Aspergillus and Monascus. Among the most affected foods are cereals, red mold rice and spices. A study funded by the European Food Safety Authority (EFSA) found that citrinin levels in processed cereals were significantly lower than those in unprocessed cereals. Overall, citrinin was detected in only 8% of the cereal samples tested. In contrast, when human samples such as blood or urine are analyzed for citrinin, they usually show comparably high levels of exposure. The discrepancy of citrinin levels in processed and non-processed foods suggests that food processing and especially thermal processing has a decisive influence on the citrinin concentration in food. It is conceivable that citrinin reacts with components of the food matrix during food processing and is thus unavailable for conventional analytical techniques. Therefore, in the course of this project model experiments were conducted to investigate which food components can react with citrinin upon heating. Important cereal components such as sugar, starch and functional groups in proteins were mimicked by model components. The resulting reaction products were then analyzed using high-resolution UHPLC-DAD-ESI-QTOF methods and the data statistically evaluated using volcano-plot analyses, among other methods. Reaction products were isolated and further characterized with the aim to use them as standards for investigations in real food samples after structure elucidation. Based on these references, food processes such as baking and extrusion cooking were performed using cereals fortified with citrinin in order to understand the formation of the citrinin

reaction and degradation products during classical cereal manufacturing processes.

Fluorescent DNA aptamer sensor platforms for ochratoxin A detection Richard A. Manderville, rmanderv@uoguelph.ca. Chemistry, Univ. of Guelph, Ontario, Canada Ochratoxin A (OTA) is a naturally occurring chlorophenolic mycotoxin that contaminants a wide range of food products and poses a threat to animal and human health. A 36 nucleobase long OTA binding DNA aptamer (OTABA) has been developed, which binds OTA with high affinity and specificity and provides the opportunity to develop biosensor-based platforms to eliminate the need for complex instrumentation to deliver rapid, on-site detection of OTA in food products. The OTABA is a guanine (G)-rich DNA sequence that folds into an antiparallel G-quadruplex (GQ) in the absence and presence of OTA. The GQ motif is a common aptamer structure and is stabilized by intraquartet hydrogen bonds, p-stacking interactions between G-tetrads and cation coordination within the central cavity. In this presentation, different fluorescent aptasensor strategies for OTA detection in red wine samples will be discussed and include label-free platforms that use extrinsic light-up fluorescent probes, internal fluorescent probes that are covalently attached to the aptamer and finally use of the natural OTA fluorescence to create a 'turn-on' fluorescence self-signaling platform in which the emission of the aptamer-target complex is enhanced in comparison to the emission of the free toxin. The utility of fluorescent probes to afford insight into the GQ structure produced by OTABA and the site of OTA binding within the DNA aptamer will also be presented.

Novel aptasensor for the ultrasensitive mycotoxin detection Muhammad Shoaib1,2, shoaib_ju@hotmail.com, HuanHuan Li1, Quansheng Chen1,3. (1) School of Food & Biological Sciences, Jiangsu Univ., Zhenjiang, Jiangsu, China(2) International Joint Laboratory on Food Safety, Jiangnan Univ., Wuxi, Jiangsu, China(3) College of Food and Biological Engineering, Jimei Univ., Xiamen, Fujian, China Aptamers are an emerging class of nucleotides, also known as "synthetic antibodies" and novel replacement of antibodies in the field of diagnostics. Aptamers with preferential binding, recognition, and specificity towards the small to big targets making them an ideal recognition probs for future. Functional nanomaterials and aptamers are a vital combination to design different chemical, electrochemical, optical, and mass sensitive for small to big molecules. Gold nanoparticles, which play a key role in enhancing the detection sensitivity and specificity for various biomolecules. A fluorescence labelled silica shelled with AuNPs as a metal core nanocomposite was prepared and a gold nanostar grafted graphene nanocomposite was reported to enhance the metal enhanced fluorescence (MEF) material and Raman signals (SERS), respectively. The designed dual-mode fluorescence and surface-enhanced Raman scattering nanoprobe was successfully applied for the detection of mycotoxin (T-2). On the exposure of target molecules, the dye dopped silica shelled AUNPs move away from the surface of rGO-AuNS, resulting in the restoration of FL and reduction of the SERS signal. The results were very promising and showed a lower limit of detection compared to the previous methods, respectively. The developed FL and SERS aptasensor presented excellent recovery ratio and RSD in wheat and maize, respectively, as compared with the standard ELISA method. The complementary performances of the developed stratagem revealed a high correlation between the FL and SERS sensing modes with exquisite detection properties.

Emerging mycotoxins in the food chain: Challenges and perspectives Doris Marko, doris.marko@univie.ac.at. Food Chemistry and Toxicology, Univ. Wien, Wien, Wien, Austria Since the discovery of aflatoxins in the 1960s, more than 300 fungal metabolites have been characterized as "mycotoxins". The respective structures are as diverse as the modes of action, comprising cytotoxic, genotoxic, immunomodulatory as well as endocrine disruptive compounds. In addition to the few regulated mycotoxins such as aflatoxins or ochratoxin A, nowadays numerous additional secondary metabolites can be detected. For most of these potentially "emerging" mycotoxins data on occurrence and/or toxicity are not sufficient yet for comprehensive risk assessment. Prominent representatives are Alternaria toxin, formed by black molds of the genus Alternaria, which occur ubiquitously, growing under varying temperature and moisture condition as well as on a large diversity of substrates. Reports on the occurrence of Alternaria toxins comprise a broad spectrum of plant-based food commodities including grain and grain-based products, apples, oilseeds, sun flower oil and tomato products. Although Alternaria species are known to generate a spectrum of secondary metabolites, toxicological studies have focused so far predominantly on the commercially available toxins e.g. alternariol (AOH), its monomethyl ether AME, tenuazonic acid (TeA) and tentoxin (TEN). In 2011, EFSA performed the first risk assessment on Alternaria toxins, but could only evaluate these four toxins due to the limited amount of data. In April 2022, the European Commission published a recommendation of indicative values for AOH, AME and TeA in certain food commodities. However, Alternaria alternata is able to generate a broad spectrum of secondary metabolites with different activity profile. Thus, in native toxin mixtures, a complex overlay of biological activities might occur including immunosuppressive, endocrine disruptive and genotoxic properties. Besides TeA , TEN and the two major dibenzo-α-pyrones AOH and AME, Alternaria spp. may produce significant amounts of perylene quinone derivatives, potent DNA-damaging components with high mutagenic potential. So far, data on the occurrence of perylene quinones in food and the fate of these compounds during food processing are still limited. Taken together, Alternaria toxins comprise a spectrum of mycotoxins with different molecular targets. Data are accumulating, underlining the toxicological relevance of these potential food contaminants thus arguing for a regulation of contamination levels and the development of mitigation strategies.

Realistic follicular fluid concentrations of Fusarium toxins trigger apoptosis and activate NLRP3 inflammasome in bovine primary theca cells Imourana Alassane-Kpembi1, imourana.alassane-kpembi@umontreal.ca, Guodong Cai2, Isabelle P. Oswald3, Christopher Price1. (1) Veterinary Biomedicine, Univ. de Montreal, Quebec, Canada(2) College of Veterinary Medicine, Yangzhou Univ., Jiangsu, China(3) TOXALIM, Institut National de Recherche pour l'agriculture l'alimentation et l'environnement, Toulouse, Occitanie, France Cattle are deemed less susceptible to mycotoxins due to the limited internal exposure resulting from rumen microbiota activity. However, the significant amounts of Fusarium mycotoxins deoxynivalenol (DON) and zearalenone (ZEN) frequently detected in bovine follicular fluid samples suggest that they could affect ovarian function. Both mycotoxins trigger several patterns of cell death and activate the NLRP3 inflammasome in the intestine. In vitro studies have reported a number of adverse effects on bovine oocytes. However, the biological relevance of such findings with regard to realistic concentrations of DON and ZEN in bovine follicular fluid is still not clear. Hence, it is important to better characterize the effects of dietary exposure to DON and ZEN on the bovine ovary. Using bovine primary theca cells, this study investigated the effects of real-life patterns for bovine ovary exposure to DON and ZEN, but also DON metabolite DOM-1, on cell death and NLRP3 inflammasome activation. Exposure to DON starting from 0.1µM significantly decreased theca cell viability. The kinetics of phosphatidylserine translocation and loss of membrane integrity showed that ZEN and DON, but not DOM-1, induce an

apoptotic phenotype. qPCR analysis of the expression of NLRP3, PYCARD, IL-1β, IL-18, and GSDMD in primary theca cells at concentrations of mycotoxin previously reported in cow follicular fluid clearly indicated that DON and DOM-1 individually and in mixture, but not ZEN, activate NLRP3 inflammasome. Altogether, these results suggest that real-life dietary exposure of cattle to DON may induce inflammatory disorders in the ovary.

Aflatoxin B1 metabolism in vitro and in vivo: New insights by HPLC-MS/MS analysis in combination with intravital imaging Andrea Gerdemann1, Benedikt Cramer1, Matthias Behrens1, Ahmed Ghallab2,3, Reham Hassan2,3, Gisela Degen2, Jan Hengstler2, Melanie Esselen1, Hans-Ulrich Humpf1, humpf@uni-muenster.de. (1) Inst. of Food Chemistry, Univ. Münster, Muenster, Germany(2) Leibniz-Institut fur Arbeitsforschung an der TU Dortmund, Nordrhein-Westfalen, Germany(3) Dept. of Forensic Medicine and Toxicology, Faculty of Veterinary Medicine, South Valley Univ., Qena, Egypt Aflatoxin B1 (AFB1) is known to exert species-dependent toxicity and carcinogenicity that may be related to its metabolism and formation of DNA adducts in the respective species [1].The first part the study focused on the kinetics of AFB1 metabolism in primary hepatocytes of mouse, rat and human origin by HPLC-MS/MS analysis. Selective and sensitive quantification of AFB1 and its metabolites such as aflatoxin P1 (AFP1), aflatoxin M1 (AFM1), aflatoxin Q1 (AFQ1), aflatoxicol (AFL), AFB1-N-acetylcysteine, AFB1-glutathione (AFB1-GSH), AFB1-guanine and AFB1-lysine in cells and cell medium. Upon treatment of cells with AFB1, samples were collected up to 24 h. In addition, the cellular DNA was analyzed for adducts (AFB1-guanine) which are linked to the carcinogenicity and mutagenicity of AFB1. Fast metabolization and comparably high levels of the far less toxic AFP1 as main metabolite were observed for mice hepatocytes. Furthermore, AFB1-GSH and AFM1 were formed quickly, and only low amounts of AFB1-DNA adducts were detected, which disappeared almost completely from the DNA up to 24 h. In contrast, rat hepatocytes metabolized AFB1 significantly slower and formed mainly AFM1 and AFB1-GSH. Compared to mouse hepatocytes higher amounts of AFB1-DNA adducts were detected, explaining the higher carcinogenic potency of AFB1 in rats in comparison to mice. The main human metabolites were AFM1 as well as AFQ1 and AFL, which had only a minor role in the other species. In the second part AFB1 was applied to mice and rats, and samples from plasma, urine and bile were collected for up to 24 h. The metabolite pattern of this in vivo time-course showed comparable results to the in vitro experiments with primary rodent hepatocytes. In order to analyse also the tissue distribution a two-photon microscopy-based technique for intravital imaging of AFB1 based on its blue fluorescence was applied [2]. The results show a very rapid uptake of AFB1 in hepatocytes of mice and enrichment in the nuclei with kinetic differences between mice and rats. In summary, the results demonstrate a strong correlation between the sensitivity of certain species towards AFB1 and their respective metabolism and distribution. [1] Schrenk et al. EFSA Journal 2020, 18(3):6040. DOI: 10.2903/j.efsa.2020.6040. [2] Ghallab et al. Arch Toxicol 2020, 95(6), 2163. DOI: 10.1007/s00204-021-03073-5. [3] Gerdemann et al. Arch Toxicol 2023, in press.

Data delivery from the US-EPA Center for Computational Toxicology and Exposure to support mycotoxin researchers Antony J. Williams1, tony27587@gmail.com, Gregory Janesch1, Erik T. Carr1, Valery Tkachenko2. (1) Center for Computational Toxicology and Exposure, Office of Research and Development, U.S. Environmental Protection Agency, ORAU Student Services Contractor, Research Triangle Park, North Carolina (2) ScienceDataExperts, Rockville, Maryland In recent years, the growth of scientific data and the increasing need for data sharing and collaboration in the field of environmental chemistry has led to the creation of various software and databases that facilitate research and development into the safety and toxicity of chemicals. The US-EPA Center for Computational Toxicology and Exposure has been developing software and databases that have served the chemistry community for many years. Several web-based software applications have been developed at the US-EPA and made available to the community to provide access to information regarding mycotoxins. This includes related structures, experimental and predicted properties, hazard data and mass spectrometry analytical data and methods. While the primary software application from the Center is the CompTox Chemicals Dashboard almost a dozen proof-of-concept applications have been built serving various capabilities. The publicly accessible Cheminformatics Modules (https://www.epa.gov/chemical-research/cheminformatics) provides access to modules to allow for hazard comparison for sets of chemicals, structure-substructure-similarity searching and batch QSAR prediction of both physicochemical and toxicity endpoints. This presentation will provide an overview of all tools in development that provide access to mycotoxin related data and the integrated nature of the applications based on the underlying chemistry data set. This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

WEDNESDAY AFTERNOON

General Papers

Fluorine-19 NMR analysis of polymers used in food packaging Clark Ridge1, clarkridge@gmail.com, Fu Chen2, Katherine Carlos1, Peter F. Scholl1. (1) Center for Food Safety and Applied Nutrition, US FDA, College Park, Maryland(2) Dept. of Chemistry and Biochemistry, Univ. of Maryland, College Park The presence and identification of fluorine-containing compounds in food contact materials has been of interest to the FDA for many years. Polymers containing fluorine have been applied to paper-based food packaging to impart grease and water resistance. Assessing the identity and structure of additives and coatings on papers and packaging can be challenging. NMR offers several promising advantages that can be leveraged to acquire useful information difficult to obtain by other techniques. Additionally, fluorine-19 NMR (19F-NMR) has been shown to be very useful for observing fluorine and fluorinated compounds due to the favorable NMR properties of the fluorine nucleus. In addition to being spin-1/2, 100% isotopically abundant, and possessing a high gyromagnetic ratio, the fluorine-19 nucleus also has a large and informative chemical shift range. It also provides relatively clean spectra in complex samples as there are often very few fluorine-containing compounds present. We have applied liquid-state 19F-NMR and solid-state, magic-angle-spinning, fluorine-19 NMR (19F-MAS-SSNMR) to several polymers and packaging materials to assess fluorine content and the structure of the fluorine therein. The quality and utility of the 19F-NMR spectra were highly dependent on how the sample was prepared. Solvent choice and sampling handling were shown to be particularly important in the liquid state samples. Several sample preparation techniques will be discussed for both the liquid-state and solid-state samples. Also, we will present steps and recommendations for quantification and the limitations of NMR with current preparation methods for the types of materials analyzed.

Microfibrillated cellulose (MFC) barrier coating for extending banana shelf life Junyong Zhu1, junyong.zhu@usda.gov, Jing Geng2, Nicole Stark1, Peter Kitin1, Xiao Zhang2. (1) USDA Forest Products Laboratory, Madison, Wisconsin(2) Washington State Univ., Pullman This study for the first time evaluated the feasibility of using 100% microfibrillated cellulose (MFC) for

barrier coating to preserve the shelf life of bananas. MFC was produced from a commercial bleached kraft hardwood pulp through mechanical milling and barrier coating was accomplished through dipping bananas in aqueous MFC suspensions. The performance of barrier coating on banana peel surface was evaluated from visual observations, banana weight loss, firmness, and dissolved soluble sugars content. The results indicate that coating MFC on banana peel surface delayed the banana browning, softening, and conversion of banana carbohydrates into soluble sugars. Furthermore, the extent of mechanical fibrillation in producing MFC affected MFC suspension wettability of banana peel surface, as well as the effectiveness of banana preservation. Casting-made MFC films were used to understand various factors on MFC barrier coating performance. The effects of the extent of MFC fibrillation was found to be more effective than increasing the amount of coating in reducing water vapor permeation for better fruit protection.

Dissipation of Pendimethalin and Clomazone in sugarcane soil in Louisiana Darcey Wayment1, darcey.wayment@nicholls.edu, Dallas Bergeron2,1, Alice A. Wright2, Gerald A. mccollam2, Paul White2. (1) Nicholls State Univ., Thibodaux, Louisiana(2) ARS, USDA Agricultural Research Service, Houma, Louisiana Some sugarcane (Saccharum sp.) growers in Louisiana report that the widely-used herbicide, pendimethalin, is less effective at controlling itchgrass (Rottboellia chochinchinensis), possibly through accelerated dissipation from repeated applications. Others have started to use another herbicide, clomazone, in conjunction with pendimethalin to increase the efficacy. However, little is known about the dissipation of these two herbicides, especially when applied together, in diverse sugarcane soils in Louisiana. Thus, the objective of the research was to measure the dissipation of pendimethalin and clomazone in soils having high itchgrass pressure. Soil samples from each field were fortified (4µg g-1) with clomazone and pendimethalin and monitored over the course of 163 days under laboratory conditions. Herbicide levels were determined by extracting the herbicides from soil with acetonitrile and performing analysis using high performance liquid chromatography (HPLC). The results confirm that clomazone is persistent in the soils studies, with a half-life of 79 d or higher. Pendimethalin dissipates more rapidly with bi-phasic kinetics, and a half-life ranging from 7d-59d, depending on the soil. When these soils were seeded with itchgrass, pendimethalin was more effective at controlling itchgrass than clomazone.

Comparative study of cannabis moisture techniques Kerri-Ann Blake, kerriann.blake@metrohmusa.com, Eduardo Simoes. Metrohm USA, Riverview, Florida Moisture in cannabis impacts potency and product quality. Karl Fischer (KF) titration is the only chemically specific test for moisture and can be used to accurately determine moisture in cannabis and cannabis products. Other techniques are not specific to moisture and the loss of any volatile components, such as terpenes, will be incorrectly classified as moisture. Attend this oral presentation to learn how Karl Fischer titration compares to other popular moisture techniques. In this study, over 100 cannabis samples were analyzed by Karl Fischer, loss on drying, vacuum oven and vacuum desiccation.

Waterpipe (shisha) tobacco packing density and product performance John H. Lauterbach, john@lauterbachandassociates.net. Chemistry & Toxicology, Lauterbach & Associates LLC, Deland, Florida, Waterpipe (shisha) tobacco is used smoked in a hookah pipe (also known as a waterpipe). Contemporary shisha tobaccos do not combust during use due to glycerol contents in excess of 30% of product weight, with the remainder being sugar syrups, tobacco, and flavors. The tobacco is placed in a bowl and heated from above by charcoal briquettes or electric heaters to release an aerosol composed mostly of glycerol and water when the pipe is puffed. Bowls are designed to hold between 10 and 30 g of tobacco, however, smokers can pack more or less depending on the type of shisha [either flue-cured (FC) or dark air-cured (DAC)] used. The FC shishas tend to have particles greater than 5 mm in size, while DAC shishas are most all under 5 mm in size. Experts on sensory properties of shisha smoke have developed mathematical relationships for how tightly or loosely a give brand of shisha should be packed, and have websites describing how major brands should be packed. The relationships are based on how much of a given shisha can be packed into the bowl. Once that amount of tobacco is known, suggested amounts vary from 90% of that weight down to less than 50%. However, this method is flawed for two reasons: 1) more DAC shisha can be packed than can FC shisha due to the much smaller particle size of the DAC product; and 2) it assumes that the thermal properties of both types of shisha are the same. To solve this problem, a DAC shisha was made from minimally processed (enough water to make the leaf pliable) DAC tobacco leaf, sold at retail under the Grabba Leaf brand. Samples of this leaf were cut into strips with dimensions similar to those found in FC shisha products. These strips were made into a surrogate DAC shisha product by adding 20 g of strips to a mixture of 50 g glycerol, 20 g liquid invert sugar, and 10 g propylene glycol (or commercial shisha flavor). A similar FC surrogate shisha was made using the same cut FC leaf that is used in commercial shisha products. When this was done, the differences in ideal packing weight between the DAC and FC products was minimized.

Spoilage kinetics of vegetable products: Making sense of fluorescence fingerprints to gain insights into stability and nutritional losses Maleeka Singh1,2, maleeka@uoguelph.ca, Xiaoli Liu1, Maia Zhang1, Hui Zou4, Xue Jun2, John Shi2, Maria Corradini1,3. (1) Dept. of Food Science, Univ. of Guelph, Guelph, Ontario, Canada(2) Agriculture and Agri-Food Canada Guelph Research and Development Centre, Guelph, Ontario, Canada(3) Arrell Food Inst., Guelph, Ontario, Canada 4) China Agricultural Univ. College of Food Science and Nutritional Engineering, Beijing Increased consumption of fresh vegetable products requires the development of methods to monitor their stability and quality. A food's fluorescence fingerprint, or excitation-emission matrix (EEM), provides a simple and comprehensive tool to scout progressive spoilage and quality losses in these highly perishable products. Organic spinach was blended with deionized water (1:1, w/w) to prepare juice-like products. Half of the homogenates were pasteurized (72°C for 15s), and the untreated and pasteurized samples were stored at 4, 15, and 23°C for two weeks. A Fluoromax-4 spectrophotometer was used to collect the EEMs (λex= 250-530nm, λem= 270-750nm, slits = 2 and 3, respectively) of the juices after 0, 2, 6, 9 and 13 days of storage. EEMs of spinach juices were examined using PARAFAC to identify distinctive features indicative of quality loss. The correspondence of the main EEMs features with known fluorophores was confirmed by LC-MS/MS. Similar EEMs were observed for untreated and themally processed products, with three regions showing most changes over time. LC-MS/MS confirmed the correspondence of these features with aromatic amino acids, polyphenols, and chlorophyll a, respectively. The degradation kinetics of these individual markers of spoilage was characterized using a Weibullian model, however they provided limited discrimination in treatment or degree of spoilage. A fluorescence index (FI) was developed based on the ratio of the aromatic amino acids' relative intensity and the combined relative intensity of the remaining fluorophores (λem350/(λem425+λem680)), which allow discrimination between processed and unprocessed samples and reported on spoilage more

accurately (after 2 days: 95 vs 50% change in unprocessed and processed samples). Therefore, EEMS may allow for identifying unique and distinctive features, which can be used to characterize spoilage in spinach products. This may improve supply chain transparency, ensure that consumers receive safe and high-quality/nutritious foods, improve shelf-life reporting, and reduce food waste.

Comparison of volatile aroma compounds between cricket (Acheta domesticus) powder and cricket protein isolate Edward -, Thanakorn Wongprasert, Inthawoot Suppavorasatit, inthawoot.s@chula.ac.th. Food Technology, Chulalongkorn Univ. Faculty of Science, Bangkok, Thailand The cricket insect is recognized as a promising alternative protein source. However, negative biases and off-flavors from lipid in the cricket have been obstacles impeding the incorporation of cricket insect into the food industry. Therefore, the objective of this study was to compare volatile aroma compounds between cricket powder and cricket protein isolate (CPI). The volatile aroma compounds of commercial cricket powder (~70% protein) and CPI (~94% protein) obtained through alkaline extraction process together with ammonium sulfate were analyzed using solvent-assisted flavor extraction (SAFE) coupled with gas chromatography-mass spectrometry (GC-MS) techniques. It was found that dominant compounds with positive attributes found in both samples were 2-acetyl-1-pyrroline (odor activity value; OAV~50), trimethylpyrazine (OAV~24), and 2-ethyl-3,5-dimethylpyrazine (OAV~86). These compounds contributed to roasty, nutty, buttery, and popcorn-like aromas. Conversely, several predominant compounds contributed off-aromas including hexanal (OAV, 10), 2-pentylfuran (OAV, 8), (E,E)-2,4-decadienal (OAV, 12), and 1-octen-3-ol (OAV, 25) were found in cricket powder sample, In addition, these compounds were also presented CPI, but in smaller quantities (hexanal, OAV of 5; 2-pentylfuran, OAV of 1; (E,E)-2,4-decadienal, OAV of 2; 1-octen-3-ol, OAV of 14). These findings could benefit manufacturers looking to offer alternative protein sources and can be used as a food supplement to increase the protein content and nutritional value in the foods.

Rapid analysis of sugarcane quality parameters by Near-Infrared Spectroscopy Stephania Imbachi-Ordonez1,2, simbachiordonez@agcenter.lsu.edu, Kevin McPeak2, Gillian Eggleston1. (1) Audubon Sugar Inst., Louisiana State Univ., St. Gabriel (2) Chemical Engineering, Louisiana State Univ., Baton Rouge Analysis of sugarcane quality is of vital importance for sugarcane factories, as it impacts factory efficiency and is involved in the cane payment system; however, analysis of these quality parameters is time-cost prohibitive. In addition, the quantification of extraneous matter (leaves, tops, and soil), which negatively affects factory efficiency, is not currently measured since there are no practical methodologies available. Near-infrared (NIR) spectroscopy is a rapid, non-destructive analytical technique that could solve these problems. This research was undertaken to evaluate the potential of NIR spectroscopy for the analysis of multiple quality parameters of sugarcane relevant to the payment system. Samples of shredded cane, pressed cane, and pressed juice were collected from a Louisiana sugar factory during the 2020-2022 processing seasons. Mixtures of known concentrations of clean cane, soil, and leaves were also prepared. Partial least squares regression models with k-fold cross-validation were developed relating NIR spectra to reference values. Press juice provided the most accurate predictions of Brix (R2=0.984) and pol (R2=0.977) compared to shredded cane. Soil content based on ash analysis yielded better calibration (R2=0.929) than sediment analysis (R2=0.152). For the first time ever reported, green leaves (R2=0.864), brown leaves (R2=0.950), and total leaves (R2=0.921) could also be predicted. This successfully demonstrates the practical use of NIR spectroscopy for rapid and accurate determination of multiple quality parameters of sugarcane.

Constituents isolated from Brazilian propolis as natural pesticides Victor P. Ribeiro1, vitorpena10@gmail.com, Jairo K. Bastos2, Alden S. Estep3, Kumudini Meepagala1. (1) Npuru, USDA Agricultural Research Service, Oxford, Mississippi(2) Pharmaceutical Sciences, Univ. de Sao Paulo Faculdade de Ciencias Farmaceuticas de Ribeirao Preto, São Paulo, Brazil(3) Mosquito and Fly Research Unit, USDA Agricultural Research Service, Gainesville, Florida Propolis is a resin with a viscous consistency produced by Apis mellifera bees using plant parts, wax, and their own salivary secretions. As a result, it has a rich and complex chemical composition. Brazil, known for its biodiversity, produces different types of propolis, with the main types categorized as green, red, and brown based on the color. Our objective was to isolate the compounds from these three main types of Brazilian propolis and evaluate their pesticidal activities, including antifungal, phytotoxic, and larvicidal properties. To isolate the compounds, each type of propolis was extracted with using hydroalcoholic solution of ethanol and water (7:3). The crude extracts were fractionated using column chromatography, and these fractions were further purified using high-performance liquid chromatography. From green propolis, kaempferol, drupanin, artepellin C, and baccharin were isolated. Red propolis yielded vestitol, isoliquiritigenin, formononetin, neovestitol, methylvestitol, medicarpin, oblongifolin A, and gutiferone E. Brown propolis provided the compounds isopimaric acid, abietic acid, communic acid, and totarol. The compounds derived from green and brown propolis exhibited weak activity against Aedes aegypti larvae, whereas the red propolis compounds demonstrated significantly higher larvicidal activity, with all of them being effective. We also conducted a TLC bioautography assay to evaluate the antifungal activity of these fractions against the fungal plant pathogen Colletotrichum fragariae. Compounds from green propolis, as well as red propolis compounds, exhibited the largest inhibitory zones against C. fragariae. In contrast, the compounds isolated from brown propolis showed no activity against C. fragariae. Furthermore, all the isolated compounds demonstrated phytotoxic activity against Agrostis stolonifera, with medicarpin showing total germination inhibition.

AGFD CORNUCOPIA

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

Sun. March 17	noon-1:00pm	Special Topics Meeting	Hilton - Riverside – Compass rm
Sun. March 17	7:00pm-9:00pm	Poster Session & Reception	Morial Conv. Ctr. Hall C
Mon. March 18	noon-1:00pm	AGFD Leader Luncheon	Morial Conv. Ctr. rm 245
Mon. March 18	1:00-2:00pm	Future Programs	Morial Conv. Ctr. rm 245
Mon. March 18	5:00pm-8:00pm	Executive Committee	Marriott - Warehouse Arts – Cypress rm
Mon. March 18	6:30-8:30pm	Urban South Brewery Tour	registration required (see page 4)
Tues. March 19	6:00-8:00pm	AGFD Chair's reception	Palace Café 605 Canal St.
Tues. March 19	10:30-12:15pm	C4-Communicating Culinary Chemistry Competition	Dickie Brennan's Steakhouse 716 Iberville Street