



CORNUCOPIA

including the AGFD program and abstracts for the
261st American Chemical Society (Virtual) National Meeting on
April 5 - 16, 2021

YOUNGMOK KIM & LINSHU LIU
Program Chairs

**VIRTUAL PROGRAMMING
HOW DOES IT WORK ?**

See page 10

Mask Up!

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

MESSAGE FROM THE CHAIR

For all humankind in the world, 2020 was a very special year due to the pandemic that we have not been well-prepared to confront. We have lost many people including beloved family members, friends, colleagues, neighbors and many others to the pandemic. We were confused, lost in direction and scared at the beginning since no one has experienced such a huge outbreak that was prevalent over the whole world. Now COVID-19 testing is widely available, the nationwide positivity rates are declining and the promise of vaccinations eradicating this virus is plausible. However, we recognize that we are still a leap away from normalcy. Therefore, after the ACS has unceasingly worked to mitigate or eliminate risks associated with the pandemic, it was decided the 2021 spring meeting will again be all virtual. I hope everyone remains safe and healthy until we see each other in person in upcoming ACS meetings.

First, I would like to give a summary of what this spring meeting looks like and what the division has accomplished over the last six months even though it has been a historically unprecedented time and environment for us all. This spring meeting will be the second virtual meeting after the first 2020 virtual fall meeting, which was programmed with 100% pre-recorded presentations. However, now we are more comfortable with speaking virtually and the technology is seamlessly providing a virtual friendly environment, therefore the speakers will be asked to present in a live format (pre-recorded presentation is also allowed), in which speakers and audiences could interact more easily on a real-time basis. The live portion will take place on April 5-16, followed by 2 weeks of on-demand access. The poster sessions will provide the capability of live interactions and virtual event rooms are available for networking, both in scientific sessions as well as in social networking forums. A total of 290 abstracts were accepted in the AGFD spring program for both oral and poster presentations, and 33 sessions will be held in 8 symposia which covers a broad range of recent food and agricultural topics. I want to thank the co-program chair, Linshu Liu, for his time and dedication to organize this spring meeting along with me and for developing future AGFD programs. I would also like to thank all symposium organizers, presiders, speakers, and the AGFD executive committee members for their participation, contribution and dedication to the AGFD spring program. I feel honored that the AGFD is hosting the presidential symposium which was organized by the ACS president H.N. Cheng, a former AGFD chair Liangli (Lucy) Yu, Mike Appell and Mike Morello, who all put in tremendous efforts to host this honorable symposium within the AGFD program. A total of 66 well-recognized professionals will present their research work in the presidential symposium which will consist of 10 separate sessions. Details including speaker information can be found in the Cornucopia.

I congratulate all the award winners. Rickey Yada at the University of British Columbia won the Advancement of Application and Agricultural and Food Chemistry award which recognizes and encourages outstanding contributions to pure and/or applied agricultural and food chemistry. This honorable award is sponsored by IFF (International Flavors and Fragrances). Xiaonan Lu at McGill University won the Young Scientist Award which recognizes outstanding research in agricultural and food chemistry by a young scientist. The AGFD Roy Teranishi Graduate Fellowship in Food Chemistry, which is awarded to support and encourage graduate students who display outstanding potential early in their program, was given to Holly Childs at the University of Maryland. I appreciate award chair, Mike Morello, for organizing all the awards.

I thank Liangli (Lucy) Yu for her leadership as a program and AGFD chair last year. Although last year was full of uncertainties for the division and all of us, her strong leadership brought us much success. I also thank Brian Guthrie for leading the development of the sustainable and green technology subdivision, and establishing an AGFD division young industrial scientist achievement award. Thanks also go to Alyson Mitchell, Mike Morello, Mike Appell, Brian Guthrie, Xuetong Fan, and Lucy Yu for their support and advice with developing programs, and managing division-wide events. Thank you Stephen Toth for keeping our budget healthy and Carl Frey for publishing Cornucopia. As a 2021 AGFD chair, I appreciate you and your invaluable services to the division. I am honored to have the opportunity to serve you as AGFD 2021 chair. Thank you.

Youngmok Kim AGFD Chair 2021

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General Manager	P. White
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FUTURE PROGRAMS

ATLANTA August, 22-26, 2021

ACS Meeting Theme: Resilience of Chemistry

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

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

Feeding the Gut: What Drives a Healthy Gut Jason Soares Jason.w.soares.civ@mail.mil Guodong Zhang guodongzhang@umass.edu Wei Chen zjuchenwei@zju.edu.cn Karley Mahalak Karley.mahalak@usda.gov

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

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

Japanese Food: Ingredients and Culture Masuko Kobori kobori@affrc.go.jp Wally Yokoyama wally.yokoyama@wrcc.usda Hiroshi Nabetani nabetani-h@tokyo-kasei.ac.jp Linshu Liu linshu.liu@usda.gov

Chemistry, Health Benefits and Future Prospects of Kimchi as a Korean Health-promoting Fermented Vegetable Hak-Jong Choi hjchoi@wikim.re.kr Jungeun Cho jecho@wikim.re.kr Youngmok Kim youngmok.kim@finlays.net

Analytical Methods for Health Beneficial Bioactive Components and Hazards in Ethnic Foods Kwang-Geun Lee kwglee@dongguk.edu Hyang-Sook Chun hschun@cau.ac.kr Youngmok Kim youngmok.kim@finlays.net

Hemp, Medicinal and Aromatic Crops: Production, Phytochemistry, & Utilization Charles Cantrell charles.cantrell@usda.gov Valtcho Jeliaskov valtcho.jeliaskov@oregonstate.edu

JAFC Best Paper Award Presentation Thomas F. Hofmann jafc@jafc.acs.org

History of Carbonated Beverages (title to be determined) Alyson Mitchell aemitchell@ucdavis.edu

General Papers & General Posters Linshu Liu linshu.liu@ars.usda.gov

SAN DIEGO March, 20-24, 2022 and Beyond

ACS Meeting Theme: Evolving Biomolecular Sciences

Advances in the in Development of In-Silico Taste and Extra-Oral Nutrition Receptors Brian Guthrie Brian_Guthrie@cargill.com Antonella Di Pizio a.dipizio.leibniz-lsb@tum.de Soo-Kyung Kim skkim@wag.caltech.edu

Tree Nuts Alyson Mitchell aemitchell@ucdavis.edu

Water Alyson Mitchell, aemitchell@ucdavis.edu Mike Qian Michael.qian@oregonstate.edu

Food Macromolecules: Functionality, Health Benefits, Delivery Systems Wallace Yokoyama wally.yokoyama@ars.usda.gov Fang Zhong fzhong@jiangnan.edu.cn Nitin Nitin nnnitin@ucdavis.edu

Chemistry of Traditional Chinese Medicine Wallace Yokoyama wally.yokoyama@ars.usda.gov Jinlin Guo guo596@163.com Yue Zhang, yue.zhang@unl.edu

Chemistry of Aged Beer Nick Flynn nflynn@wtamu.edu;

Impact of Global Disasters on Food Quality, Safety and Security Alyson Mitchell aemitchell@ucdavis.edu Michael Morello mjmorello226@gmail.com Liangli (Lucy) Yu lyu5@umd.edu

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Carbohydrate-Based Fat Replacers TBD

Advances in Nanomaterials for Food and Agricultural Applications Bosoon Park Bosoon.Park@USDA.gov
Sechin Chang Sechin.Chang@USDA.gov

Green Polymers & Active Polymers LinShu Liu linshu.liu@ars.usda.gov Riasha Gorshkova Jinwen

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

AGFD Award Symposium Honoring Prof. Rickey Y. Yada Youngmok Kim, Xiaonan Lu, Michael Morello



The International Chemical Congress of Pacific Basin Societies 2021 – A Creative Vision for the Future Honolulu Dec 16-21, 2021

<https://pacifichem.org>
Call for submissions (closes April 11, 2021)

Flavor and Bioactive Compounds in Fermented Foods and Beverages (#156)

Symposium co-organizers: Michael C. Qian (michael.qian@oregonstate.edu), Philip Marriott, Zhen-Yu Chen,
Chi-kun Wang, Hirotohi Tamura, Yanping L. Qian, Young-Suk Kim, Mingwei Zhang

- 1) Flavor/off-flavor characterization and identification, flavor generation during fermentation and storage.
- 2) Chemistry/biochemistry of bio-active compounds, including identification of bioactive compounds in fermented foods, metabolism of bioactive compounds, and mechanism of fermented foods in preventing disease and improving human health.
- 3) Analytical methodologies including new developments in sample prep, chromatography, identification, structural elucidation.

also symposia on

New Developments in Food Processing (#118) and Food Bioactives, Inflammation and Gut Health (#176)

Executive Committee Meeting Minutes

Sunday, August 16, 2020 (virtual meeting on Zoom)

Takes place at each ACS National Meeting

Attendees: Terry Acree, Michael Appell, Keith Cadwallader, Juhong Chen, Kathryn Deibler, Laurel Doherty, Xueting Fan, John Finley, Carl Frey, Brian Guthrie, Thomas Hofmann, Lauren Jackson, Tony Jin, Youngmok Kim, LinShu Liu, Kathleen Luo, Hang Ma, Karley Mahalak, Michael Morello, Bhimu Patil, Michael Qian, Fereidoon Shahidi, Tony Shao, Jason Soares, Mathias Sukan, Stephen Toth, Michael Tunick, Lucy Yu, Yuzhu Wang, Guodong Zhang, Zhizhao Zhang

AGFD Chair Lucy Yu called the meeting to order at 3:04 p.m. Eastern time.

Thomas Hofmann gave the **Journal Report** first because of his time constraints. He announced the JAFC Best Paper of the Year Awards. JAFC will probably have 9000-10,000 submissions in 2020, compared with 5500 five years ago. The acceptance rate is holding steady at 20%, with less than 80 days from submission to acceptance. Two new journals have been established: ACS Agricultural Science and Technology, edited by Laura McConnell, and ACS Food Science and Technology, edited by Coralía Osorio Roa. The first issues of both are expected in January.

The **minutes** of the previous meeting were approved with no changes.

Stephen Toth gave the **Treasurer's Report**. The division spent only \$15,338 this year, and received \$10,000 from donations, \$8700 from dues, \$30,000 from the ACS allotment, and about \$4300 from investment income, royalties, etc. The net (revenues minus expenses) for the year so far is \$37,600, giving AGFD \$768,755 in the bank and investments. The division is financially healthy.

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The **Awards Committee** report was given by Mike Morello. The following people are responsible for the awards that AGFD presents: Mike Morello, IFF Award; Fereidoon Shahidi, AGFD Fellows Award; Mike Granvogl, Young Scientist Award; Lucy Yu, Teranishi Award; and Kathryn Deibler, Graduate and Undergraduate Student Symposia. In addition, Mike Appell is our contact for the Hendricks Award, Sarah Leibowitz for the Spencer Award, and Thomas Hofmann for the JAFC Best Paper Awards. Pictures of the awardees with their plaques and the student award posters should be posted on our web site, and descriptions of the reasons the honorees received their awards should be in the Cornucopia. Mike will check to see if recorded versions of the award lectures, or variations of the presentations, could be also be posted to the site. The award application due dates have been consolidated to October 15 and February 1. ACS prefers eight papers per session, so the Graduate Student Symposium, which normally has six presenters, could be combined with another award symposium session. Mike Tunick volunteered to manage the Distinguished Service Award, and Mike Appell will assist Mike Morello in coordinating the nominations for the ACS Fellow Award. The criteria for the AGFD Fellow Award should be modified to give consideration to industrial chemists who cannot present proprietary information. An award for younger industrial chemists, who have the same restriction, may be established. Brian Guthrie, Mike Morello, Mike Qian, Fereidoon Shahidi, and Mathias Sucan will form a working group about this issue. Mike Morello also said that a long-term distinguished service award, for at least 25 years of active service to AGFD, should be established. It turns out that such an award was secretly created by several Executive Committee members over the previous few months and that Mike M. was the first winner, in recognition of his exemplary leadership. Cynthia Mussinan also received an award in recognition of industrial career achievement. The name of the honor will tentatively be the AGFD Exemplary Leadership Award. Several members are celebrating 50 years of AGFD membership, and Mike M. will look into costs of mementos such as baseball caps, pins, ties, and scarves with our logo.

Kathleen Luo reported that the **Student Committee** was mostly on hold since there were no in-person National Meetings this year. Alternatives for student participation will be discussed.

Youngmok Kim gave the **Program Report** for the virtual Fall Meeting and indicated that were 21 symposia and 34 sessions. The Spring Meeting slated for San Antonio has 21 symposia scheduled. If that meeting is also virtual, we can cover the registrations of up to five speakers per session. Youngmok moved that we do that, and the motion passed. Steve Toth suggested a \$35,000 budget for San Antonio if the meeting is held in person, and that motion was also approved. Pacifichem has been postponed a year, until December 2021.

In **Subdivision Reports**, Jason Soares, Laurel Doherty, and Karley Mahalak, officers for the new Diet and Gut Microbiome Subdivision, introduced themselves. Jason reported that they have met to discuss upcoming symposia they are considering. Flavor Subdivision Tony Shao reported that there are 17 on-demand oral technical presentations, including four broadcast presentations, for the flavor symposium at this meeting. Another symposium will be organized for Spring 2020. Hang Ma stated that the Functional Foods & Natural Products Subdivision will have to postpone the 3rd Global Symposium on Chemistry and Biological Effects of Maple Food Products. Youngmok Kim reported that the Nutrition Subdivision will organize symposia in San Antonio and Atlanta. Xiaohua He sent a report saying that the Food Safety Subdivision plans two symposia for San Antonio.

Councilor Reports were given. Mike Tunick reported that there has been a suggestion that ACS hold one virtual meeting and one in-person meeting every year. John Finley reported that diversity on Council is being improved. Mike Appell noted that Council consists of 80% Local Section Councilors and 20% Division Councilors, and that participation in Local Section activities should help. Lauren Jackson said that ACS membership may become more a la carte in the future, with reduced benefits for a reduced membership fee. The Council has concerns about sustainability. AGFD may add a subdivision focusing on that topic. Mike Appell, John Finley, and Brian Guthrie will for a working group on this.

The **Nominations report** was given by Immediate Past Chair Xuotong Fan. The slate of officers will be Youngmok Kim, Chair; LinShu Liu, Chair-Elect; and Mike Granvogl, Vice Chair. Three people, Brian Guthrie, Lauren Jackson, and Alyson Mitchell, are being nominated for two Councilor positions for the 2021-24 term. The Alternate Councilor nominee is Keith Cadwallader.

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Cornucopia editor Carl Frey said that there were no printed copies this year since there were no in-person meetings. He had to edit 500 pages of abstracts supplied by ACS down to 70 pages for the Cornucopia. Youngmok Kim had to assign AGFD abstract numbers to them.

Mike Tunick reported that there was no activity in **Hospitality/Public Relations** since we had no Philadelphia or San Francisco meetings.

Membership Chair Michael Qian said that AGFD has about 3000 members and that the number is holding steady.

In the **Communications report**, Mike Appell said our website, agfoodchem.org, costs less than \$200 a year to operate. It works on all devices and presentations can be linked to it with the DOI number. Its YouTube channel can also be used for adding presentations.

There was no **Old Business**. In **New Business**, Lucy Yu mentioned the possibility of having a virtual Executive Committee meeting in advance of the San Antonio meeting. Keith Cadwallader pointed out that a short meeting can always be scheduled if needed.

The meeting adjourned at 6:08 p.m.

Submitted by Michael Tunick, substituting for AGFD Secretary Alyson Mitchell

In Memorium

G. K Jayaprakasha



Guddadarangavvanahally K. Jayaprakasha (Jay), Ph.D, Research Professor, Vegetable and Fruit Improvement Center (VFIC), Department of Horticultural Sciences at Texas A&M University (TAMU), College Station, died of brain cancer on October 25, 2020.

After earning degrees (B.S. in chemistry, physics, and mathematics and M.S. and Ph.D in chemistry) from the University of Mysore, India he worked in the food industry and at the Central Food Technological Research Institute, Mysore. In 2004, he joined TAMU, eventually becoming a VFIC Research Professor in 2014. As a leading authority in natural products and health Jay developed methods for isolating and characterizing fruit and vegetable bioactive compounds, assessing their role in promoting human health as well as preventing disease. He authored >151 research publications, 31 book chapters and edited five books and 12 proceedings/reviews in organic chemistry, natural products, nutrition, and health. He presented 183 abstracts at national and international conferences and filed 24 patents in the US, Europe, and India.

For his significant work he was awarded Royal Society of Chemistry Fellow, AGFD Fellow, Indian Association of Food Scientists and Technologists Fellow, Indian Chemistry Fellow and the VFIC Director's Award of Excellence 2014. He served as Chair of the AGFD Functional Foods and Natural Products Subdivision and organized and presided over several ACS symposia.

He taught food technology, mentoring >70 undergraduate and graduate students and 10 visiting scientists. His dedication and his exemplary work ethic inspired students and colleagues at the VFIC and beyond.

Jay is survived by his wife Savitha, two children Shreyas and Swathi, father Krishnareddy Kommein, four siblings and in-laws Vasudevareddy and Savitramma. He embodied humility and empathy. Jay is missed by friends and colleagues. His friends at AGFD miss him and extend condolences to his family.

GOLDEN GATE GRID

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66						67			68			
69						70					71	

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

ACROSS

- | | | | |
|---|---|---|---|
| 1 Six-pack muscles | 46 Fa, sol, la, -- | 5 Family Dr. | 36 What 50 Across does |
| 4 -- & Food Division | 47 Jr's dad | 6 Civilian airspace overseer | 37 Hairstyle |
| 6 Newborn horse | 48 ----- <i>Waldo?</i> | 7 Here I come, ready -----! | 39 <i>Goosebumps</i> author Stine |
| 10 Foolish ones | 50 Resident of 40 Across | 8 Displaying a flamboyant air | 41 --, go home! |
| 13 Sass | 51 Mulish remark: --- Haw! | 9 To undergo cell breakdown | 42 Do, --, mi |
| 14 SFPD's <i>Dirty</i> ----- | 52 Cubical Star Trek nemesis | 11 3 component sandwiches | 45 Juan Ponce – Leon |
| 15 SF bell ringing transport | 53 sports drink: Gator --- | 12 Red, White or Black --- | 48 You and me |
| 17 SF's Oracle Park team | 55 H ₂ O purification method | 13 --- Vegas | 49 ----- mud in your eye! |
| 18 Accounts at bars | 57 Refuse to sign into law | 14 Make advances towards | 50 --here or --pay or --habit |
| 19 Hrs. beyond 40/wk. | 60 SF's ----- State Warriors | 16 Trucker radio | 51 Line from <i>Jerry Maguire</i>
You had me at -----. |
| 20 Santana's --- <i>Como Va</i> | 62 California mania of 1849 | 17 Monopoly corner square | 52 Make weary by repetition |
| 21 Sauna locations | 66 Parts in plays & films | 21 Stirrup ear bone | 53 ----culture or ----business |
| 24 Three strikes equivalent | 67 Peppy beverage: Mtn. ---- | 22 Game participant | 54 Entryway |
| 26 Separation on a flat plate | 68 Brown tone of old photos | 23 W/67 Down: an Australian
rock band with a slash | 55 Switch option |
| 27 Synthetic polymers
derived from cellulose | 69 Element at center of heme | 25 You and me | 57 'I do' or 'I solemnly swear' |
| 31 <i>Law & Order</i> role (abbr) | 70 Approximately 0.39 in. | 27 More impolite | 58 Chicago rail transport |
| 33 Abuser recovery org. | 71 Secret agent | 28 Inert gas inside lightbulbs | 59 NFL 6 pointers |
| 34 Ripens or ages | | 29 Abominable snowmen | 61 Home for a bear or wolf |
| 37 Uno y uno | | 30 MSDS prescriber | 62 Ruby, emerald, or diamond |
| 38 SF's Transamerica ----- | | 31 Title of many lab heads | 63 Delivery via a brown truck |
| 40 Alcatraz Island | | 32 Requesting | 64 Tiny taste |
| 43 Slithery sea creature | | 34 A post-BA degree | 65 Make --- while the sun shines |
| 44 Arbitrate | | 35 Before noon | 67 See 23 Down |

DOWN

- 1 As easy as ---
2 It can be a constrictor
3 Weep
4 78% N₂+21% O₂+1% Ar

AGFD DIVISION MEMBERSHIP APPLICATION

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

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

At ACS National Meetings you can discuss division activities at the AGFD information table located near the AGFD technical session rooms. Join >3000 AGFD members via the application form (below) or on-line at www.agfoodchem.org or www.acs.org (click on Communities, Technical Divisions, Technical Division List) or call ACS (800)333-9511 (in US) or 616-447-3776 (outside US). Payment by Visa/Master Card or AmEx.

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

	APPLICATION FOR AGFD DIVISION MEMBERSHIP (7623P)
Title	
Name	
1 st address line	
2 nd address line	
City	
State	
Zip code	
Country	
e-mail address	
Phone	
check one	MEMBERSHIP FEE
<input type="checkbox"/>	I am an ACS member and wish to join AGFD (\$10.00)
<input type="checkbox"/>	I am not an ACS member and wish to join AGFD (\$15.00)
<input type="checkbox"/>	I am a full time student and wish to join AGFD (\$10.00)
Be cool JOIN AGFD	Return application, with payment (payable to American Chemical Society), to AGFD Membership Chair: Michael Qian, Professor Department of Food Science and Technology Oregon State University Corvallis OR 97330

ROSTER OF AGFD OFFICERS & COMMITTEE LEADERSHIP

Chair - Serves 1 year. Preside over Division meetings & appoint committees
Youngmok Kim
Finlays, North Kingstown RI
youngmok.kim@finlays.net

Chair-Elect - Serves 1 year. Substitute for the chair as needed
LinShu Liu USDA-ARS-ERRC
linshu.liu@ars.usda.gov

Vice-Chair - Serves 1 year. Assist Chair-elect. Develop future technical programs.
Michael Granvogl
michael.granvogl@uni-hohenheim.de

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

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

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

Councilors - Represent Division for 3 years on ACS council.
Alyson Mitchell (thru '23)
aemitchell@ucdavis.edu
Lauren Jackson (thru '23)
lauren.jackson@fda.hhs.gov
Michael Tunick (thru '21)
mht39@drexel.edu

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

Student Activities - Attract and retain graduate/undergraduate student members.
Kathleen Luo kkluo@ucdavis.edu
Zhichao Zhang yntzhang@ucdavis.edu

Nominations - Develop officer slate.
Served by Immediate Past Chair.
Liangli (Lucy) Yu lyu5@umd.edu

Public Relations - Publicize Division.
Alyson Mitchell aemitchell@ucdavis.edu

Alternate Councilors - Substitute for Councilors. Serves 3 years.
Keith Cadwallader (thru '23)
cadwlldr@uiuc.edu
Kathryn Deibler (thru '21)
kdd3@cornell.edu
Michael Qian (thru '21)
Michael.qian@oregonstate.edu

At-Large Executive Committee Members - Assist in Div. management Serves 3 years.
Terry Acree (thru '21)
tea2@cornell.edu
Jane Leland (thru '23)
JLelandEnterprises@gmail.com
Robert McGorin (thru '23)
robert.mcgorin@oregonstate.edu
Mathias Sucan (thru '21)
Mathias.sucan@gmail.com

Awards - Solicit nominations, oversee awards process.
Chair Michael Morello
mjmorello226@gmail.com
Fellow Awards Fereidoon Shahidi
fshahidi@mun.ca
Young Scientist Awards
Michael Granvogl
Michael.Granvogl@uni.hohenheim.de
Teranishi Fellowship
Liangli (Lucy) Yu lyu5@umd.edu
Student Awards
Kathryn Deibler kdd3@cornell.edu
Canvassing
Stephen Toth
stephen.toth@iff.com

Finance - Monitor Division's finances for 1 year. Led by Immediate Past Chair
Liangli (Lucy) Yu lyu5@umd.edu

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

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

Multidisciplinary Program Planning - Help coordinate nat'l mtg programming
John Finley jfinle5@lsu.edu

Sub-divisions Develop symposia.

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Chair, Sam Alcaine sda23@cornell.edu
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Vice-Chair, Tianxi Yang
Tianxu.Yang@fda.hhs.gov
Secretary, Majher Sarker
Majher.Sarker@usda.gov

Flavor
Chair, Jonathan Beauchamp
jonathan.beauchamp@ivv.fraunhofer.de
Chair-Elect, Yu Wang yu.wang@ufl.edu
Vice-Chair, Gal Kreitman
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Secretary, Xiaofen Du xdu@twu.edu
Coralia Osorio Roa cosorior@unal.edu.co (22)

Food Safety
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jhchen@vt.edu
Chair-Elect, Tony Jin Tony.Jin@usda.gov
Vice-Chair, Reuven Rasooly
reuven.rasooly@ars.usda.gov
Secretary, Xiaonan Lu
Xiaonan.lu@ubc.ca

Functional Foods & Nat. Products
Chair, Yu Wang yu.wang@ufl.edu
Chair-Elect, Xian Wu
Wux57@miamioh.edu
Vice-Chair, Jianping Wu
Jwu3@ualberta.ca
Secretary, Kenny Xie KYX@usp.org
Yingdong Zhu yzhu1@ncat.edu (22)

Diet & Gut Microbiome
Chair, Jason Soares
jason.w.soares.civ@mail.mil
Chair-elect, Guodong Zhang
guodongzhang@umass.edu
Vice-Chair Karley Mahalak
Karley.mahalak@usda.gov
Secretary Laurel Doherty
Laurel.a.doherty.civ@mail.mil

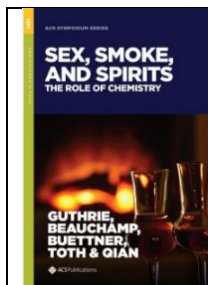
Nutrition
Chair, Mina Kim minakim@jbnu.ac.kr
Chair-Elect, Mathias Sucan
Mathias.sucan@gmail.com
Vice-Chair, Hye-Seon Kim,
hyeseon.kim@usda.gov
Secretary, Hae Won Jang
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AWARDS and other GOOD NEWS



Rickey Y. Yada won the 2021 **Award for the Advancement of Application of Agricultural and Food Chemistry**. This award recognizes outstanding contributions to pure and applied agricultural and food chemistry. The award celebrates Professor Yada's research which has focused on the structure-function relationships of food and non-food related enzymes using molecular biology and various physico-chemical techniques (e.g., circular dichroism spectroscopy, micro-calorimeter, small angle neutron scattering, ultracentrifugation, enzyme kinetics, etc.), carbohydrate metabolism in potatoes as it related to process quality. His research provides insight on the factors that affect enzyme activity, such as the thermodynamics, formation of an enzyme-substrate complex, enzymatic catalysis, enzymatic kinetics, and enzyme inhibition. Highlights of Prof. Yada's research

include improving pulse protein functional properties and digestion through application of enzymatic modifications, providing opportunities to develop palatable plant protein based food products with many health benefits and revealing anaerobic respiratory enzymes contribute to low-temperature sweetening of potato, enabling chip process quality enhancement by guiding postharvest storage. Dr. Yada has authored over 230 peer reviewed journal papers, 10 books and 27 book chapters, including 2 ACS Symposium Series ebooks. Currently Professor Yada is Dean Faculty of Land and Food Systems, University British Columbia. This award is sponsored by International Flavors and Fragrances.



Sex, Smoke and the Spirits by AGFD members Brian Guthrie, Jonathan Beauchamp, Andrea Buettner, Stephen Toth, and Michael Qian was 2020's third most accessed/purchased ACS Symposium book from ACS Publishing.

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

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

AGFD Awards Committee : AAAFC IFF/AGFD Awards (Mike Morello), AGFD Fellow Awards (Fereidoon Shahidi), AGFD Distinguished Service Awards (Mike Morello), Student Awards – Teranishi Fellowships (Liangli [Lucy] Yu), Graduate & Undergraduate Student Symposia (Kathryn Deibler), Young Scientist Awards (Michael Granvogel), Sterling B. Hendricks Memorial Lectureship (Michael Appell), Spencer Awards (Sarah Leibowitz)

VIRTUAL PROGRAMMING – HOW DOES IT WORK ?

See the ACS **Frequently Asked Questions** page on the website (link below) for the upcoming virtual meeting.

<https://www.acs.org/content/acs/en/meetings/acs-meetings/registration/meeting-and-expo-questions-and-answers.html>

Oral technical sessions will have presenters in a Zoom session sharing their desktop. ACS will post the individual presentation recordings of those that opt to make their presentation available on-demand from April 19-30.

Poster presenters upload their poster in PDF or PowerPoint format and may choose to record a brief accompanying video available on demand throughout the meeting.

Organizers of Spring 2021 AGFD Technical Program Symposia

Youngmok Kim = organizer for the symposia:

General Posters

Recent Trends in Food Analysis

Upcoming Topics in Food Analysis

Modern Food Chemistry

Recent Topics in Food Chemistry

Nutritional Science in Food Chemistry

Chemistry of Fruits and Vegetables

Yu Wang & Jonathan Beauchamp = organizers for the symposia:

Food-flavor Dynamics Assessments via Real-time Mass Spectrometry –

-Part I: From Developments to Nosespace

-Part II: Headspace and Beyond

Michael Morello, Tony Jin, Xuotong Fan, Timothy Duncan, John Finley, John, Koontz = organizers for the symposia:

Food Packaging Materials: Safety, Active Packaging & Sustainability -

-Safety of Food Contact Materials

-Active Packaging (Nanotech and Antimicrobial Polymer Systems

-Sustainability to Reduce Food Waste (Active Packaging)

Jashbir Singh, Bhimu Patil, Nitin Dhowlaghar = organizers for the symposia:

Beyond Chemistry: Consumer Acceptance of Flavor, Food Safety and Health Benefits of Fruits and Vegetables –

Genomics Assisted Breeding/Region and Cultivar Specific Melons

Sensorial Qualities and Microbial Decontamination of Melons

Effects of Natural Compounds for Food Safety Interventions

Crop Improvement/Bioactive Compounds and Health Benefits of Fruits and Vegetables

Food Processing-impacts on Quality Sensory

Innovative Approaches in Horticulture Technology

Youngmok Kim & Linshu Liu = organizers for the symposium:

Sci-Mix

Liangli (Lucy) Yu, Michael Morello, Michael Appell, H.N. Cheng = organizers for the symposia:

Presidential Symposium Sustainability: Advances and Applications -

-Overviews

-Biobased Polymers

-Biobased Molecules

-Biprduct Utilization

-Waste Product Utilization

-Food-Energy-Water Nexus 1

-Food-Energy-Water Nexus 2

-Nanotech that Drives Sustainability

-Food Safety and Security

-Sustainable Food Systems for Health

Youngmok Kim; Hyang-Sook Chun; Kwang-Geun Lee; Mina Kim = organizers for the symposium:

Chemistry and Health Benefits of Fermented Foods

Zhuohong Xie & James Harnly = organizers for the symposium:

Food Authentication and Adulteration Detection

Michael Tunick & Elvira de Mejía = organizers for the symposia:

Chemistry of Fermented Hispanic Foods -

-Beverages

-Other Foods

AGFD TECHNICAL SESSION ABSTRACTS

MONDAY MORNING 4/5/21 start 6:00 AM end 8:00 AM

General Posters

AGFD001A 3558823 poster 1 **Taste-modulating pyroglutamyl dipeptides from mushrooms** Andrew Moore amoor140@vols.utk.edu An activity-guided fractionation approach was applied to enzymatically hydrolyzed mushroom protein with the goal of identifying saltiness enhancing and taste-modulating substances. This approach led to the identification of several pyroglutamyl dipeptides that exhibited saltiness and kokumi enhancing effects in a low sodium chicken broth. The dipeptides were identified in the mushroom hydrolysates through pairing sensory analysis with mushroom hydrolysate fractions obtained through solid-phase extraction (SPE), gel permeation chromatography (GPC), and semi-preparative reverse-phase high-performance liquid chromatography (RP-HPLC). The taste modulating thresholds of the pyroglutamyl dipeptides were determined in a NaCl (0.2%) aqueous broth containing a mixture of 5'-nucleotides and amino acids at the concentrations measured in the hydrolyzed mushroom samples. A liquid chromatography-tandem mass spectrometry (LC-MS/MS) method was then employed to quantitate the pyroglutamyl dipeptides in the samples. The levels of the dipeptides in the hydrolysate were determined to be below their taste modulating thresholds. Interestingly, each pyroglutamyl dipeptide (alone) showed no taste modulation activity in the model broth when prepared at the concentrations determined in the hydrolysate. However, when all the dipeptides were added together, there was a significant enhancement of both the salty and the kokumi taste qualities, suggesting a sub-threshold synergistic taste modulating effect. The results of this work lay the groundwork for future studies aimed at the application of pyroglutamyl dipeptides derived from mushrooms for flavor enhancement in reduced-sodium foods.

AGFD001A 3552156 poster 2 **Detection of krill, a crustacean shellfish allergen, using real-time PCR** Anne Eischeid Anne.Eischeid@fda.hhs.gov FDA has received consumer complaints about food products, most notably sardines, containing krill as an undeclared crustacean shellfish allergen. The Food Allergen Labeling and Consumer Protection Act (FALCPA) requires that food products containing crustacean shellfish be labeled with the type of crustacean. Antibody based assays such as ELISA, which are most often used for allergen detection, cannot distinguish type of crustacean, so there is a need for additional methods. Previous work at FDA-CFSAN has resulted in the successful development of real-time PCR based assays for differentiation of crustaceans through detection of their DNA. Purpose: The purpose of this work was to develop and evaluate a real-time PCR based method for specific detection of krill contamination in foods, with a focus on detection in sardines. Methodology: While krill is morphologically similar to shrimp, it is not a close relative taxonomically and therefore cannot be expected to give a similar response in DNA assays. Methodology included first examining the response of the current crustacean real-time PCR assays to krill, and then adapting a previously developed shrimp assay to specifically detect krill through modification of primer and probe sequences. Results: Two different sets of modified primer and probe sequences were found to work equally well. Both yielded specific detection of krill in sardines with lower limits of detection at 0.1-1 mg/kg and linearity over 7-8 orders of magnitude. The krill assay does not cross-react with shrimp. Conclusion: FDA consumer complaints about undeclared krill have highlighted the

need for a detection assay specific for this crustacean. While krill is not a close taxonomic relative of shrimp, this work has shown that minor changes in shrimp primers and probe were nonetheless able to yield an effective and specific krill assay.

AGFD001A 3558285 poster 3 **Arsenic (III and V) metal contamination of romaine lettuce (*Lactuca sativa*) through hydroponic means** Beatriz Lopez beatriz.lopez01@utrgv.edu One of agriculture's major problem is the large of accumulation of arsenic (As) found in the groundwater used for irrigation. Arsenic pollution originates from the natural occurring high concentrations of arsenic in the deeper levels of groundwater. The accumulation of arsenic contamination in food plants is of major concern since Arsenic has the potential to be extremely toxic even at low concentration. In our research, we have measured the absorption of As by germinating lettuce seeds, through hydroponic means, with arsenic (III) and arsenic (V) contamination over a two-week growth period, and then determined the level absorption of the heavy metal in the leaves, roots and stems of the plant. The experimental design involved the following steps: Once the seedlings had been germinated, the sprouts were then placed into a Hoagland solution, a nutrient solution highly capable of providing every necessary nutrient for promoting plant growth. Along with the Hoagland solution, the plants were contaminated with 1, 2, 5 ppm of As (III) and As (V) each. Samples of the leaves, roots, and stems were freeze-dried, followed by acid and peroxide digestion for As analysis by Inductively Coupled Plasma-Optical Emission Spectrometry (ICP-OES). Our data indicates that the higher concentrations of As were detected in both the roots and leaves of the plant and the growth of the plants was stunted when the medium contain high concentrations of As.

AGFD001A 3554033 poster 4 **Lifetime and fate of hop (*Humulus lupulus*) acids in craft brewing cultivars by HPLC analysis** Celina Paoletta celina.paoletta.18@cnu.edu There are many chemical changes that take place during wort boiling, to include the oxidation of polyphenols, production of melanoidins via Maillard reactions, protein precipitation, enzyme inactivation, and isomerization of hop acids. Hops are one of the most important raw materials used in the production of beer as it is responsible for the bitter flavor and aroma of beer. The metabolites in hops also provide beer with other qualities like flavor stability, foam stability, microbial stability, color, and mouthfeel. During the wort boiling, the α -acids are isomerized to iso- α -acids. These products can lead to various ratios of the cis/trans-iso- α -acids, which can affect the kinetics of oxidative degradation as well as the bitter taste development in the final product. Environmental changes to the terroir can lead to alterations in the acid profiles of individual hop cultivars. Therefore an accurate assessment of initial α -acid components is clearly important for brewers in determining a consistent product. Additionally, determination of the fate of these compounds throughout the brewing process is of interest for studies focused on the stability and shelf life of the product. Here we present our initial findings of acid profiles from hop pellets and the corresponding isomerization and degradation products as a function of wort boiling at a local craft brewery.

AGFD001A 3548658 poster 5 **Influence of bovine blood with methylation and polymerization on flocculation of kaolin and hematite suspensions** Changhoon Lee changhoon.lee@usda.gov Flocculants are used in the primary step of industrial wastewater

purification to precipitate solids. Bovine blood is a waste product from slaughterhouses, and there is limited evidence in the literature demonstrating that it can be used as a flocculant. The purpose of this study is to more rigorously evaluate bovine blood as a flocculant and to investigate possible modifications to improve its flocculation efficacy. Native bovine blood (NBB) and two types of chemically modified blood (methylated bovine blood (MeBB) and polymerized bovine blood (PolyBB)) were tested against kaolin and hematite suspensions. Flocculation tests and zeta potential measurements were used to study how performance varied with suspension pH and flocculant dosage. NBB and PolyBB performed well with kaolin suspensions only at pH ≤ 5.5 , while MeBB showed high and consistent performance, indicating pH insensitivity in the range from 4.5 to 8.5. pH was set at 5.5 for flocculant dosage tests. A 20 mg/g kaolin dose of MeBB resulted in 98% precipitation in an hour but performance decreased when more than 30 mg/g was added. Since the isoelectric point of MeBB was much higher than pH 5.5, more positive charges of MeBB could attach to the kaolin particles to decrease electrostatic repulsion compared to the NBB. The performance of MeBB with hematite suspensions was poor at all tested doses (2-100 mg/g hematite), whereas a 30 mg/g dose of PolyBB showed 81% precipitation in an hour due to its negative charge and larger molecular size. Based on those results, MeBB was more pH independent and dose effective compared to NBB in the kaolin suspension, and PolyBB was effective in the hematite suspension. Therefore, bovine blood has potential as a high performance, bio-based flocculant for wastewater treatment.

AGFD001A 3549441 poster 6 **Physical and chemical properties of edamame over bean development and application of spectroscopy-based machine learning methods to predict optimal harvest time** Dajun Yu dajunyu@vt.edu Edamame has been widely consumed in China and Japan for centuries as a snack or side dish. In the US, the consumption of edamame has been increasing, and edamame has become the second most highly consumed soy-food after soymilk because it is nutritious and has potential health benefits. The edamame harvest window is narrow but critical for producing high-quality beans. Current methods for determining the optimal harvest time of edamame rely on the ability of experienced edamame growers to detect these changes visually, by touch or taste. These determination methods can be quite subjective and pose a major obstacle for inexperienced growers in the US. Therefore, to foster growth of the domestic edamame industry, a rapid, consistent, and standardized method for determining optimal harvest time is desired. This study aims to understand the physical and chemical property changes of edamame over bean development (R5 to R7 stages) and develop a spectroscopy-based machine learning technique to rapidly predict optimal harvest time. The results showed that pod weight, bean weight, and pod thickness peaked at R6 and remained stable for the remainder of bean development. Sugar, starch, alanine, and glycine contents also peaked at R6 but proceeded to decline thereafter. Meanwhile, fat, fiber and ash contents remained low at the R6 stage. Based on the physical and chemical properties, the harvested edamame samples was labeled as 'early', 'ready' or 'late' to indicate early, ready or late to harvest. The machine learning method based on the spectral reflectance of pods had a high accuracy of 0.95 for classifying "early" and "late" harvested edamame and 0.87 for classifying "early" and "ready" harvested edamame. This work would provide a platform technology for developing rapid and accurate prediction of optimum harvest time of edamame, which is essential to ensure to produce consistent and high-quality edamame for the market.

AGFD001A 3554938 poster 7 **Pinot noir grape polysaccharide analysis by GC-MS after methanolysis and silylation** Danye Zhu zhudany@oregonstate.edu Wine polysaccharides play an important

role in wine aroma and flavor perception. The interaction of polysaccharides with wine aroma may depend on the physical and chemical properties of aroma, structure, and composition of polysaccharides. In addition, wine polysaccharides are closely related to the mouthfeel perceptions due to their interactions with excess tannins and pigments, which further affects the sensation of astringency, sweetness, and body of the wine. However, the actual cause and mechanisms are not well studied. Hence, it is essential to research wine polysaccharide composition. GC or GC-MS can analyze polysaccharide composition after methanolysis and silylation. Methanolysis conditions were investigated using lactose under acidic conditions (0.5 M HCl) in methanol at 75, 80, and 85 $^{\circ}\text{C}$ for 16, 18, and 20 hrs. After the methanolysis, an aliquot of 0.2 mL internal standard myo-inositol in pyridine (0.1 mg/mL) was added, and the mixture was dried under a flow of nitrogen gas. For silylation, 0.1 mL 1-(trimethylsilyl)imidazole (TMSI) was added and incubated at 80 $^{\circ}\text{C}$ for 30 min. The characteristic peaks of sugars were identified by GC-MS with an HP-5MS column. It was found that methanolysis was temperature and time-dependent, lactose was methanolized completely at 85 $^{\circ}\text{C}$, higher than reported in the literature. Sugar standards (glucose, xylose, mannose, arabinose, galactose, rhamnose, fucose, glucuronic acid and galacturonic acid) and Pinot noir grape polysaccharides were methanolized by 0.5 M HCl/MeOH at 85 $^{\circ}\text{C}$ for 18 h and derivatized by TMSI. Under these conditions, glucose mainly gave α - and β -methyl-tetrakis-O-(trimethylsilyl) glucopyranoside. In contrast, galactose gave both furanosides and pyranosides. Similarly, arabinose gave mixtures of α -/ β -1-methyl-O-tris-(3-methylsilyl)-arabinofuranosides and α -/ β -1-methyl-O-tris-(3-methylsilyl) arabinopyranosides. GC-MS analysis showed that Pinot noir grape polysaccharides were composed mainly of glucose, arabinose, rhamnose, galactose, mannose, galacturonic acid and xylose

AGFD001A 3552479 poster 8 **Biological application of capsanthin in the medicine as novel anticancer agents: Importance of scientific data analysis in the medicine** Dinesh Patel dkp.itbhu@gmail.com Herbal medicine has been used in the traditional system of medicine since very ancient time on believe that these products are not toxic to human being and easily available throughout the world. Capsanthin is an important class of phytochemical found to be present in the *Capsicum annum*. In the present investigation, numerous scientific data have been collected from various literature sources to explore the biological importance and therapeutic benefit of Capsanthin in the medicine. Methods: Biological importance and therapeutic application of capsanthin in the medicine have been investigated through scientific data analysis of various research works of the scientific fields. Numerous scientific data have been collected and analyzed in the present research work in order to know the health beneficial aspects of capsanthin in the medicine. Molecular study data have been collected and analyzed in the medicine from various literature sources to know their effectiveness against various form of cancerous disorders. Results: Literature data analysis signified the biological importance of capsanthin in the medicine as it has been used in the medicine for the treatment of various health complications. Literature data analysis signified the biological importance of capsanthin in the medicine for the treatment of various form of cancerous disorders. Molecular study data signified the biological importance of capsanthin in the medicine for their anticancer potential. Conclusions: Literature data analysis of various scientific research works signified the biological potential and therapeutic importance of capsanthin for the treatment of various form of cancerous disorders

AGFD001A 3552485 poster 9 **Therapeutic potential of Irisfloreantin as an anti-parkinsonian drug candidate: Biological**

importance of flavonoidal compounds in the brain disorders Dinesh Patel dkp.itbhu@gmail.com Flavonoids are plant secondary metabolite found to be present in the various medicinal plants and well known for their therapeutic benefit in both the plants body and human being. Flavonoidal compounds have been present in our daily diet due to their presence in the fruit and vegetable. Some scientific study revealed the biological potential and therapeutic benefit of flavonoidal compounds in the brain functions and related disorders such as Parkinson's disease which is disorder of the central nervous system. Irisfloreantin is a flavonoidal compound found to be present in the roots of *Belamcanda chinensis* well known medicinal plant in the traditional Chinese medicine. Methods: in order to know the biological potential of irisfloreantin in the medicine and other allied sectors, effectiveness of irisfloreantin for the treatment of Parkinson's disorder has been studied in the present investigation through scientific data analysis of different research work of scientific fields. Effectiveness of irisfloreantin on acetylcholinesterase (AChE) activity has been also investigated in the present investigation through scientific data analysis of current scientific research works. Molecular mechanisms have been also investigated through scientific data analysis of current scientific research works to know the biological importance of acetylcholinesterase in the brain complication. Results: Scientific data analysis of different research work revealed the biological importance of irisfloreantin in the treatment of Parkinson's disorder as it improves dopaminergic neuron degeneration and signifying their potential to treat Parkinson's disease. Scientific study revealed the biological importance of irisfloreantin on acetylcholinesterase enzymes as it showed significant effect on acetylcholinesterase enzyme. Molecular study signified the biological importance of acetylcholinesterase enzyme in the Parkinson's disease. Conclusions : Scientific data analysis of current research work revealed the biological potential of flavonoidal compounds in the medicine including irisfloreantin for the treatment and development of better medicine against Parkinson's disorders.

AGFD001A 3557046 poster 10 **Combining GC with MS and** olfactory detection for a variety of food, flavor, and fragrance analyses Elizabeth Humston-Fulmer liz_humston-fulmer@leco.com Gas chromatography (GC) coupled with mass spectrometry (MS) is an important tool for the characterization of a wide range of food, flavor, and fragrance samples. The components most likely to contribute to the aroma of a sample tend to be volatile and semi-volatile analytes and GC-MS is well-suited for this type of analysis. Complex samples are effectively separated into the individual analyte components with GC. Time-of-Flight (TOF) MS detection provides important information towards the identification of these potentially important components of the sample with full m/z range data that can be library searched and that is also suitable for deconvolution algorithms. The incorporation of olfactory detection with this data is particularly helpful for connecting the identified features with their contributions to the overall aroma or flavor. This type of sensory directed analysis highlights regions of interest and leads to specific analytes of interest for a focused review of the data. This combination of tools can separate and identify analytes and then determine those that are most important for contributing to the characteristics of the sample. A variety of samples were analyzed with this combination of tools, and the benefits of using the information together are highlighted

AGFD001A 3533934 poster 11 **Synergistic effect of oil type & self-assembled structures on the shape stability of 3D-printed cookies** Ezgi Pulatsu etm4g@umsystem.edu Organogelators are structuring molecules forming a three-dimensional (3D) network within the body of oils to improve the functionality of liquid oils in foods. The use of the organogelation concept in 3D food printing studies is underexplored, especially in investigating the post-processing

capacity of 3D-printed food structures. Moreover, the use of edible liquid oils in cookies is problematic, and liquid oils may interfere with the stability of food inks. Therefore, structuring liquid oils can be an alternative route to obtain printable and structurally stable cookies. This study explores the use of oil structuring agents in 3D-printed cookie formulas and their contribution to structural stability. In this context, carnauba wax in various concentrations (0, 2, and 4 % (w/w)) in either sunflower oil or corn oil were prepared. The polymorphism, crystallinity, and microstructure were evaluated using polarized light microscopy, while rheological studies disclosed the viscoelastic and thixotropic nature of the organogel-based cookies. The printability and shape stability were examined based on dimensional properties of printed and baked structures, respectively. All samples exhibited gel-like behavior with the varying modulus values where the differences of up to three-fold were noted depending on the formulation. The viscosity and the stability of the cookies increased significantly when the wax concentration was increased. Oil type had proven to exert a significant effect on the mechanical properties and microstructural properties of cookies. Oils without organogelator failed to create self-sustained 3D-printed structures, whereas oils reinforced with organogelator (2 and 4 % w/w) produced self-supporting structures stable over baking. Increased storage, loss, and complex modulus that led to reinforced structures can be associated with the strong network formed between the crystalline gelator structure and the oil phase. Considering the outcomes, organogelation is a promising approach to overcome the printability and post-processing related issues in 3D food printing studies

AGFD001A 3551826 poster 12 **Phytonutrient composition in** purslane, spinach and kale: Comparative study Fadwa Al-Taher faltaher1@yahoo.com Leafy greens contain essential nutrients and are important for a healthy diet. The objective of this study was to compare the nutritional and phytochemical components of the two most prevalent leafy greens in the world, spinach and kale, with purslane. Compared to spinach and kale, this investigation shows that purslane is an excellent source of omega-3 fatty acids, minerals, ascorbic acid, and various phytochemicals with antioxidant properties. While the omega-3 fatty acid content in spinach and kale leaves was 10.84 ± 0.86 mg/100 g and 16.69 ± 2.44 mg/100 g, dry weight, respectively, the omega-3 content in purslane was 98.35 ± 6.78 mg/100 g, dry weight. This study also unraveled a higher number of phytochemicals in purslane with over 100 identified, which were not present in either spinach or kale. Two hundred and twenty-eight health-promoting bioactive compounds were identified in the leafy greens (spinach, 71; kale, 105; purslane, 190), including flavonoids, alkaloids, glucosinolates, and phenolic, chlorogenic, and organic acids. These findings prove purslane to be a nutritionally unique and potentially functional ingredient. Furthermore, it is strongly advised that balancing the nutritional benefits of spinach, kale and purslane could be achieved through selective formulation of these freeze-dried powders

AGFD001A 3557395 poster 13 **Antioxidant activity of EGCG** (epigallocatechin gallate) ester derivatives as affected by the acyl chain length in food and biological model systems Han Peng hanp@mun.ca The addition of antioxidants is one of the most critical measures to retard oxidative processes in food and pharmaceutical products in order to extend their shelf-life. To address safety concerns about synthetic antioxidants, various novel alternates have been developed. EGCG, one of the most widely distributed dietary phenolics, serves as an efficient natural antioxidant with numerous health effects but it is relatively poorly-soluble. In this study, the bioactive properties of lipophilic EGCG derivatives prepared enzymatically were evaluated in food and biological model systems. Methods: The acylated EGCG samples were prepared using

a simple and easily controllable enzymatic method. Various saturated fatty acids with 2 to 18 carbon atoms were used as acyl donors to increase the hydrophobicity of EGCG (products obtained included, mono-, di- and even tri-esters in some cases). The purified products were then tested for their antioxidant activity using β -carotene bleaching, LDL (low-density lipoprotein) oxidation, and DNA scission assays. Results: In β -carotene bleaching assay, the bleaching rate of β -carotene was inhibited by both EGCG and its esters. The maximum inhibition was at around 20-35 min under accelerated oxidation condition (50 centigrade), but then decreased gradually during 6-hours of measurement duration. Meanwhile, EGCG monoesters showed a similar inhibition rate to EGCG. In the LDL oxidation assay, a downtrend of antioxidant ability was also observed after the point of maximum antioxidant efficiency. However, compared to EGCG monoesters, EGCG exhibited a lower ability in inhibiting LDL oxidation. In the DNA scission test, the EGCG esters, especially the monoesters acylated with short-chain fatty acids (C2 and C4), showed a similar DNA-anti-scission rate with EGCG, which were higher than other EGCG esters. Conclusion: Overall, EGCG monoesters displayed significant antioxidant activity in all assays employed. In addition, the comparison of antioxidant activities of different EGCG esters in biological/food model systems did not show complete compliance with those from chemical antioxidant tests. The main reasons for the observed differences are the matrix and potency of oxidizing agents in these three model systems. However, the original biological effects of EGCG as an antioxidant were well retained after modification. Thus, acylated EGCG derivatives could serve as viable alternatives to traditional synthetic antioxidants

AGFD001A 3550243 poster 14 **Metabolite profile differences between cow and goat milk yogurt** Heena Sharma s.heenavet@gmail.com Ranjith Ramanathan ranjith.ramanathan@okstate.edu Metabolomics is a systematic analysis of small molecules such as amino acids, tricarboxylic intermediates, and fatty acids in a biological system. Quantification of metabolites provides a real-time snapshot of reactions in a biological system. Yogurt is a fermented dairy product and possesses many health benefits. Characterizing metabolites and changes in their concentration during the storage of yogurt would provide a comprehensive understanding of the technological process used for its manufacturing. The objective was to determine overall changes in the metabolite profiles of cow milk yogurt (CY) and goat milk yogurt (GY) during storage. Yogurt culture (*Lactobacillus delbrueckii* subsp. *bulgaricus* and *Streptococcus thermophilus*) was inoculated at 20 DCU/100 liters of milk. Yogurt samples were stored in polystyrene cups for at refrigeration temperature. The samples were analyzed using a GC-MS based untargeted metabolomics at different storage intervals (day 0, 14, and 28). The metabolites were identified using NIST 17 library, and the mass spectral data were analyzed using R-programming and MetaboAnalyst. Metabolomics analysis indicated 187 compounds in CY and GY. The principal component analysis noted different clusters of metabolites present in between CY and GY on day 14. Upregulation ($p < 0.05$) of free amino acids and dipeptides in GY indicated a stronger proteolytic action of bacteria on goat milk proteins, while tri-peptides were upregulated ($p < 0.01$) in CY, revealing its better texture. The predominance of medium-chain fatty acids in GY resulted in the upregulation ($p < 0.05$) of carboxylic acids and fatty acid derivatives on day 14. Impact pathway analysis showed the association of differentially abundant metabolites of GY with metabolic pathways of amino acids. This work will provide novel insights into the metabolite differences between yogurt prepared from large (cow) and small ruminant (goat) milk and help researchers comprehend key factors in improving yogurt composition and nutrition

AGFD001A 3550618 poster 15 **Development of simultaneous analytical method for imidazolinone herbicides from livestock using LC-MSMS** Hyeong Wook Jo hyeongwook.jo@gmail.com Simultaneous analytical method using LC/MSMS for imidazolinone herbicides from livestock (egg, milk, beef, pork and chicken) for monitoring was developed with QuEChERS preparation. Sample weighing (5 g) in a 50 mL conical tube, added 0.1 M potassium phosphate dibasic solution (5 mL) was shaken for 10 min. After 0.5 mL 6 N HCl, 10 mL acetonitrile were added, it was shaken for 10 min. And QuEChERS extraction salt (Original method, 4 g MgSO_4 , 1 g NaCl) were added to the sample in the 50 mL conical tube. The mixture was strongly shaken for 1 min and was centrifuged at 3,000 g for 10 min. The acetonitrile layer was purification with dSPE (150 mg MgSO_4 , 25 mg C18) and was centrifuged at 13,000 g for 5 min. The supernatant was filtered with a membrane filters (pore size: 0.2 μm) before analysis. ME (% Matrix effect) for almost analytes range were -6.56 to 7.11%. MLOD (Method LOD) and MLOQ (Method LOQ) was calculated by S/N ratio. MLOQs were 0.01 mg/kg. The linear correlation coefficients (r^2) were > 0.99 within the range of 2 ~ 100 $\mu\text{g/kg}$ for all of the 7 imidazolinone herbicides. The percentages (of imidazolinone herbicides) recoveries were in the range of 76.1 ~ 110.6% (0.01 mg/kg level), 89.2 ~ 100.7% (0.1 mg/kg level) and 94.4 ~ 104.4% (0.5 mg/kg level) within the validation criteria (recover; 70-120% with RSD $\leq 20\%$)

AGFD001A 3531651 poster 16 **Double-edged sword of surfactant effect on hydrophobic surface broccoli leaf as a model plant: Promotion to pathogenic microbial contamination and improvement to disinfection efficiency of ozonated water** Hyunjong Song cc9848@naver.com *Salmonella*, which causes salmonellosis, is a major pathogen in food-borne disease related to fresh produce and its contamination rate is significantly influenced by the surface properties of fresh produce. Epicuticular waxes present on the outer layer of the leaf surface provide water repellency to the leaves thereby they reduce the rate of *Salmonella* attachment. Damage or deformation of epicuticular wax crystals by external action, such as pesticide spraying, may increase the rate of *Salmonella* attachment. Meanwhile, the hydrophobic nature of epicuticular wax crystals may possibly reduce the effectiveness of *Salmonella* inactivation in fresh produce. The main purpose of this study is to investigate whether the rate of *Salmonella* attachment increases as pesticides denature epicuticular wax crystals and to test that antibacterial effect of ozonated water can be improved on waxy produce surface by adding surfactant to ozonated water. Leaf disks of three different surface conditions (waxy; with the epicuticular wax crystals, glossy; without epicuticular wax crystals, pesticide-treated waxy) were inoculated with a *S. Typhimurium* inoculum. As a result, significantly lower ($P < 0.05$) *S. Typhimurium* attached to waxy leaf surface than glossy and pesticide-treated waxy leaf surface (3.28 as opposed to 4.10 and 4.32 Log CFU/cm²), suggesting that the pesticide (surfactant) application increased the rate of *S. Typhimurium* attachment on waxy leaf surface. This was confirmed to be the influence of the surfactant per se which deformed the structure of epicuticular wax crystals. The surviving population of *S. Typhimurium* on waxy leaf surface washed with ozonated water was no significant difference when compared with unwashed waxy leaf surface (2.91 as opposed to 2.82 Log CFU/cm²). On the other hand, *S. Typhimurium* were not detected in surfactant-added ozonated water washed waxy leaf surface. These results imply that the surfactant can effectively improve the efficiency of ozonated water on plants with epicuticular wax crystals. Furthermore, disinfection strategy proved in this study will reduce the risk of cross-contamination by maintaining the quality of the washing solution safe and will become an environmentally friendly alternative for washing fresh produce in the food industry.

AGFD001A 3538187 poster 17 **High doses of allyl isothiocyanate** degrade the appearance and postharvest quality of lettuce Hyunjong Song cc9848@naver.com Allyl isothiocyanate (AITC) is a natural compound present in plants belonging to the Brassicaceae family, including cauliflower, cabbage, kale and broccoli. AITC has antimicrobial activity, has been considered as a "generally recognized as safe" (GRAS) compound, thus and has been used as a promising food additive and preservative. However, AITC could often reduce food quality, such as antioxidant activity. Therefore, the objective of this study is to investigate the physiological disorder of lettuce treated with high doses of AITC and to determine the optimal concentration of AITC for inactivation of *Salmonella Typhimurium*. From the lettuce treated with various concentrations of AITC (0, 1, 2.5, 5 and 7.5 $\mu\text{L L}^{-1}$) for 3 days, chlorophyll degradation, cell membrane damage and significantly reduced antioxidant activity were observed with increasing AITC concentration. Moreover, metabolome analysis showed pattern of increased respiratory and cell damage, such as lipid peroxidation. Based on physiological changes, 1 $\mu\text{L L}^{-1}$ was determined as the optimal AITC concentration that significantly reduced *S. Typhimurium* population (4.01 log CFU g^{-1}) on lettuce.

AGFD001A 3541228 poster 18 **Comprehensive SPE** fractionation coupled with GC \times GC-ToF-MS analysis of volatile compounds in Wuliangye baijiu Jia Zheng zhengwanqi86@163.com Wuliangye baijiu is famous Chinese liquor with a protected geographical indication in the bilateral agreement between China and the EU. Due to its volatile composition complexity, fractionation into the simpler composition is often needed for reliable aroma identification and analysis. In this study, solid-phase extraction (SPE) and liquid-liquid extraction (LLE) were used to extract aroma compounds in Wuliangye baijiu. Both extracts were fractionated into ten groups on LiChrolut[®] EN SPE column with different pentane and dichloromethane ratios. All the fractions were subjected to comprehensive GC \times GC-ToF-MS. The work resulted in the identification of a total of 668 volatile compounds in the Wuliangye baijiu. Compared with LLE, more alcohols, aldehydes, aromatics, furans, and ketones were detected in the SPE-based extraction. The fractionation on the LiChrolut[®] EN SPE column was successful, and the elution orders were esters = acetals \leq β -damascenone < alcohols = pyrazine = furans \leq aromatics < fatty acids with increased solvent polarity from 100% of pentane to 100% of dichloromethane. Most esters were eluted in fraction 1 (100% pentane) and fraction 2 (98% pentane in dichloromethane), alcohols were main eluted in fraction 4 (90% pentane in dichloromethane), and acids were main in fraction 10 (100% dichloromethane). The comprehensive fractionation and two-dimensional GC \times GC-ToF-MS analysis revealed the complex volatile composition of Wuliangye baijiu. This is the first report based on the SPE fractionation-GC \times GC-ToF-MS for the study of volatile compounds in baijiu

AGFD001A 3542545 poster 19 **Angiotensin-converting enzyme** (ACE)-inhibitory activity of peanut protein hydrolysate with reduced in vitro allergenicity Jianmei Yu jyu@ncat.edu Hypertension is a controllable risk factor Yu of cardiovascular diseases and angiotensin-converting enzyme (ACE) is a central component of the renin-angiotensin system (RAS) which controls blood pressure. Most of the antihypertensive drugs are ACE-inhibitors which are effective but often cause many side effects. Some food protein-derived hydrolysates/peptides showed significant antihypertensive activity without side effects. Limited studies show that regular consumption of peanuts reduces blood pressure and total/cause-specific mortality. This study evaluated the in vitro allergenicity and ACE-inhibitory activity of peanut protein hydrolysates (PPH) produced by proteolytic

hydrolysis of partially defatted peanut flours. Partially defatted light- and dark-roasted peanut flours with about 50% protein were hydrolyzed with Alcalase for different time. The peanut flour suspensions incubated without Alcalase were used as controls. Samples were taken every 2 hours to inactivate the enzyme. After centrifugation, the supernatants (PPH) were collected and total protein concentrations were determined. The PPH was then tested for IgE-binding, a key indicator of allergenicity, by Western Blot using pooled plasma from 6 peanut allergic patients. The ACE-inhibitory activity of PPH was determined using ACE from rabbit lung. Western blot shows that Alcalase hydrolysis significantly reduced IgE-binding of peanut flour, although the residual of Ara h 6 and proteins/peptides 5-15 kDa remained IgE-binding. The fractions of PPH smaller than 5kDa did not bind to the IgE antibody from peanut allergic patients. Alcalase hydrolysis resulted in PPH with significant ACE-inhibitory activity depending on hydrolysis time and protein concentration. The fraction smaller than 5 kDa exhibited higher ACE-inhibitory activity than crude PPH. The ACE-inhibitory activity of dark-roasted PPH was slightly higher than that of light-roasted PPH at same concentration. Higher ACE-inhibitory activity indicates greater antihypertensive potential. Thus, peanut flour could be an inexpensive and available protein source for producing anti-hypertensive ingredient

AGFD001A 3542590 poster 20 **Quantification of aflatoxins in** organic corn grains by a pre-column derivatization HPLC-FLD method Jianmei Yu jyu@ncat.edu Aflatoxins (B1, B2, G1 and G2) are the secondary metabolites of pathogenic molds, *Apergillus flavus* and *Apergillus parasiticus* and they are classified as a Group 1 human carcinogen by the International Agency for Research on Cancer (IARC). Among these toxins, Aflatoxin B1 (AFB1) is the most toxic and widely present in cereal grains, peanuts, tree nuts and other oil seeds. Accurate determination of aflatoxin content is extremely important to the trade of cereals and safety of human food and animal feed. Due to the ban of most fungicide in organic farming, organic cereal grains may contain higher aflatoxins than conventional cereal grains. The objective of this study was to optimize the extraction and purification procedures for the HPLC quantification of aflatoxins in organic corn grains. The ground corn grains (25g each) was extracted with 100 ml of 80% methanol, 70% methanol with and without 4% NaCl, separately. The extracts were purified with Florosil SPE column conditioned with methanol, acetonitrile and the mixture of methanol and hexane (1:1), separately followed by elution with the mixture of acetone/DI water/formic acid (96:3.7:0.3) at different solvent to sample ratios. After purification, the elutes were dried under nitrogen flush, reconstituted in 40% acetonitrile, and then derivatized with trifluoroacetic acid for HPLC analysis. The results indicate that 80% methanol was the best for extraction solvents which resulted in clean peaks of all aflatoxins; 100% methanol was the best conditioning solution for SPE column, and the elution solvent to sample ratio of 6:5 (v/v) gave highest recovery. Under the optimized the extraction and purification condition, the recoveries of aflatoxin B1, B2, G1 and G2 from ground organic corn grains were 96.01%, 89.04%, 85.09% and 85.01%, respectively

AGFD001A 3550882 poster 21 **Fish glue from fish skin and the** paint art application for children poster watercolor Kangsadan Boonprab ffisksb@ku.ac.th Fish glue (adhesive agent) was the collagen extracted from skin and bone which obtained from the fish processing waste. This report was aimed to develop fish glue from Thai fish skin (1) and its application for poster watercolor for children by using fish glue as adhesive for painting material instead of chemical agent (2). The results showed that (1) Milkfish (*Chanos chanos*) was an appropriate species for glue production from twenty species. Hydroxyproline content was a factor affected on adhesion of glue and suggested that characteristic of glue required hydroxyproline

content at least 213.7 mg/g of glue. The chemical properties of glue including moisture, ash, fat, protein and carbohydrate were 97.26%, 0.061%, 0.342%, 1.214% and 1.127% respectively and the physical properties of glue including pH and viscosity were 3.35 and 18,330 cP respectively. SDS PAGE pattern showed that the glue was collagen type I which was composed of $\alpha 1$ (144 KDa) and $\alpha 2$ (129 KDa) chain. This character corresponded to the FTIR spectrum profile and amino acid composition according to previous report. Yield of glue from milk fish skin was 68.82%. (2) The optimal formula for poster watercolor from fish skin glue (FSG) was the proportion of corn starch: baking soda: acetic acid: FSG (by weight) as 10: 5: 5.5: 5. The product showed fast drying, coagulation (smoothness) and adherence with cracks-free paper painting (at least 30 days) and high viscosity; The proper natural color sources, mixing into adhesive formulation were Butterfly Pea and Beetroot. This product obtained stable color value (L^* , a^* and b^*) for at least 30 days storage. Different containers (clear plastic bottle, opaque plastic bottle, amber glass bottle and clear glass bottle) do not affect the color stability. Organic ingredients represented compostable product and highly safe for specific users. It was equivalent to a commercial product.

AGFD001A 3558551 poster 22 **Near-atomic size novel nanotechnology-based NoPest-Ag5** that effectively kills mosquitos is safer to honey bees, *Apis mellifer L.* Lok Pokhrel lokraj123@gmail.com Pollinators, especially honey bees, are susceptible to certain insecticides. Understanding honey bee susceptibility to pesticide will determine its safe use in the environment as well as when the pesticide should be used in relation to honey bee activity. Acute oral and contact (dermal) toxicity bioassays were conducted with inhouse synthesized novel nanotechnology-based pesticide, NoPest-Ag5, using the honey bee, *Apis mellifera L.*, to determine if field application of NoPest-Ag5 for mosquito control has any effect on the pollinators such as honey bees. Oral exposure followed OECD Test 213 method and contact exposure followed OECD Test 214 method. Young adult worker honey bees were exposed to six doses (0.05-20 mg a.i./L) of NoPest-Ag5 administered orally or dermally, and compared with the negative control (sucrose solution) and Imidacloprid (positive control). Observations of mortality and other signs of toxicity were made for approximately 48 hours after dosing. Cumulative mortality observed in the test groups was used to determine the LD_{50} . Our results showed that NoPest-Ag5 was nontoxic (97%-100% survival) to the honey bees at all doses tested in a 48-hr oral exposure test and all surviving bees appeared normal at test termination. Treatment-related reduction in diet consumption was observed among the Imidacloprid group, where mean consumption ranged from 88 to 198 μ L per replicate. Imidacloprid was deemed to be nontoxic to bees with average survival ranging from 93%-97%, and all surviving bees appeared normal at test termination. The lack of mortality in the Imidacloprid group was attributed to dose avoidance and not tolerance of the honey bees used in the test. NoPest-Ag5 was nontoxic (100% survival) to honey bees at all doses tested in a 48-hr contact exposure test and all surviving bees appeared normal at test termination. However, Imidacloprid was found to be significantly toxic to honey bees with average survival ranging from 10%-77%, and an LD_{50} of 0.11 μ g a.i./bee. Moreover, 46.3% of the surviving bees appeared lethargic in the Imidacloprid group. These results highlight that nanotechnology-based novel pesticide, NoPest-Ag5, designed to control mosquito vectors is safer to the sensitive pollinators such as honey bees.

AGFD001A 3558055 poster 23 **The role of magnesium in the conversion of humulone to isohumulone** Michael Mosher michael.mosher@unco.edu The acyloin rearrangement of humulone during the boiling process during beer brewing results in the

formation of cis- and trans-isohumulone. These compounds contribute the primary bitterness found in beer. The rate of rearrangement appears to be mediated by magnesium ions to the largest extent. We have evaluated the binding of magnesium to humulone by polarimetry, UV-vis titration, and other methods. Although the binding constant is relatively small, the effect on the structure, as determined by computational analysis, results in a tremendous rate enhancement of the rearrangement. The results of the analyses and the implications to the process of beer brewing will be discussed

AGFD001A 3557044 poster 24 **Determining the kinetic order of the degradation of L-ascorbic acid through spectroscopic analysis** Nisa Syed nisa.syed@pop.belmont.edu L-ascorbic acid, commonly known as vitamin C, is an antioxidant that the human body needs to protect itself from illnesses and diseases. It can be found in many different fruits and in a variety of vegetables. For convenient consumer consumption, many fruits and vegetables are processed into juices. Research has shown that the juice processing techniques these fruits and vegetables go through affect the degradation of L-ascorbic acid, decreasing the concentration of vitamin C present. However, many studies do not agree on the kinetic order of this degradation process. In this study, L-ascorbic acid solutions were prepared using two different solvents: deionized (DI) water and 9.78×10^{-5} M acetic acid. Six L-ascorbic acid standard solutions (ranging from roughly 4.0×10^{-4} M – 4.0×10^{-6} M) were prepared using each of these solvents. UV-Vis spectroscopy was used to measure the absorbance values ($\lambda = 255$ nm) for each standard solution. This data was used to generate two calibration curves. 3.80×10^{-4} M and 4.13×10^{-4} M L-ascorbic acid testing solutions were prepared in DI water and 9.78×10^{-5} M acetic acid, respectively. Samples of both solutions were stored at 25.1°C (benchtop) and 3.8°C (refrigerator). Absorbance data was collected over a three-day period. Based on the four testing solutions, initial results indicate that L-ascorbic acid degradation likely follows either first-order or second-order kinetics. In order to explore these conflicting results, additional trials will be run, analyzing the degradation of each testing solution over a longer period of time

AGFD001A 3558577 poster 25 **Study of wheat kernel characteristics and their correlation with Peleg parameters** Reihaneh Abdi rabdi@uoguelph.ca Knowledge on the relation between kernel characteristics and the water absorption behavior of wheat is crucial to optimize soaking parameters for specific wheat samples. From a processing and engineering point of view, it is important to know how fast the penetration of water through the grain could be achieved; but also, the effect of other variables on the water absorption behavior needs to be simultaneously evaluated. In this project, 30 wheat varieties, varying in hardness from super soft to hard, were immersed in water for 8 h. The increase in sample mass in function of soaking time was considered as the increase of moisture in the kernel. Mathematica 12.0.0 was used in order to run a non-linear regression analysis routine and obtain the Peleg constants. The Peleg equation resulted in R^2 higher than 0.99 for all the varieties, indicating a proper fit of the Peleg equation to the experimental data. Two different phases in the water absorption curves were distinguished (0-2 h of soaking and 2-8 h of soaking). The correlation among the characteristics of wheat kernels including hardness, diameter, weight, protein content, ash content, initial moisture content, and Peleg parameters was also studied. Peleg rate in the first phase of soaking was negatively related to the protein content and kernel hardness. The ash content was negatively correlated with the second phase Peleg rate. There was no other significant correlation among Peleg parameters and kernel

characteristics. Kernel hardness had a significant positive correlation with protein content (as expected) and diameter. The weight was also found to be significantly positively related to diameter (as foreseen), and negatively to protein content. A significant negative correlation was shown between ash content and first phase initial moisture content. Additional data analysis is currently done to look for non-linear relations and combined effects.

AGFD001A 3550930 poster 26 **Pyrethrins elicit olfactory response and spatial repellency in *Aedes albopictus*** Ru Yan 11916109@zju.edu.cn Pyrethrum from dry flowers of *Chrysanthemum* is a well-known botanical insecticide and repellent. Its insecticidal activity attributes to its six insecticidal esters, collectively known as pyrethrins. Pyrethrins and its synthetic analogs pyrethroids exert their toxic action by modifying the function of voltage-gated sodium channels. Aside from insecticidal activity, pyrethrum has also been used to repel mosquitoes for centuries. Today, pyrethrum continues to be used as an active ingredient in mosquito coils and other mosquito-repellent devices globally. However, the mechanism of pyrethrum repellency remains largely unknown. Here we report that pyrethrum vapor induced spatial (non-contact) repellency in *Aedes albopictus*, a major vector of dengue and West Nile viruses. Using electroantennogram (EAG) recordings from adult antennae, we found that pyrethrum elicited EAG response in a dose-dependent manner. We then isolated the six insecticidal esters, pyrethrins I and II, cinerins I and II, jasmolins I and II from pyrethrum extract and discovered that five of the six esters, except jasmolin I, all elicited EAG responses. Furthermore, pyrethrins I and II, cinerin II and jasmolin II induced repellency, whereas cinerin I and jasmolin I did not. Of the six pyrethrins, four of them, pyrethrins I and II, cinerin II and jasmolin II, activate ORNs (olfactory-receptor neurons) and elicit spatial repellency in *Ae. albopictus*. Our study provided a foundation for future structure-function studies of pyrethrins, their cognate olfactory receptors and efficacies of repellency and for the development of new and more effective mosquito repellents for controlling vector-borne human diseases.

AGFD001A 3555088 poster 27 **Comparison of stir-bar sorptive extraction-GC-MS and solid-phase micro-extraction -GC-MS for volatile phenol analysis in wine to assess the smoke impact** Ruiwen Yang yangru@oregonstate.edu Smoke taint has become a significant concern for the wine industry, partly due to climate change. Smoke taint is an off-aroma describing the wine with smoky, medicinal, and ashy characters. This unpleasant taint is caused by grapes or grapevine exposed to bushfire smoke before grape harvest. Guaiacol, 4-methylguaiacol, o-, m-, p-cresols, and other volatile phenols have been found to be related to smoke taints. When the grapes and the grapevines were exposed to wildfire smoke, they will absorb these volatile phenols and convert them to the corresponding glycosides or other bound forms. These glycosides and the bound form precursors do not exhibit aroma themselves, but can be converted back to the odorants during the winemaking and wine aging process. Grape maturity, grape varieties, and bottle aging can all influence smoke taint intensity in wines. Thus, it is crucial to analyze these volatile phenols in grapes and wine reliably. In this study, solid-phase microextraction-GC-MS (SPME-GC-MS) and stir bar sorptive extraction-GC-MS (SBSE-GC-MS) methods were compared and verified for volatile phenol analysis. For SPME-GC-MS analysis, stable isotope standards need to be employed, guaiacol, 4-methylguaiacol, 4-ethylguaiacol, and o-cresol m-cresol, p-cresol, 4-ethylphenol can be analyzed in 30 min in wine. For SBSE-GC-MS analysis, an ethylene glycol-polydimethylsiloxane (EG-PDMS) copolymer was used for volatile phenol extraction. The wine pH was adjusted to 7 to minimize the extraction of fermentation fatty acids from the wine. Both methods can quantitate volatile phenols down to 0.1 ug/L in wine, with good repeatability and linear response. The

methods can also be used to analyze total volatile phenols after acid hydrolysis.

AGFD001A 3554996 poster 28 **Comparison of aflatoxin and ochratoxin A levels in home-style and commercial Doenjangs (soybean paste) prepared with traditional and modified methods** Seung Yoon Kang tmddbs1457@naver.com Doenjang is known as a traditional fermented soybean-based food in Korea, but safety concerns have been raised as it can be contaminated with fungi that produce aflatoxin (AF) and/or ochratoxin A (OTA) during the fermentation process. To address this, the modified method of adding selected microorganisms to starter (meju) or soybean, is sometimes used in homes and factories. The purpose of this study is to optimize and validate the method of analyzing AF and OTA in doenjang matrix, and to compare the levels of AF and OTA in home-style and commercial doenjangs prepared with traditional and modified methods. The optimized method was validated in terms of linearity ($R^2 \geq 0.9999$), limit of detection (0.015-0.173 µg/kg), limit of quantification (0.047-0.526 µg/kg), recovery (intra-day: 84.5-98.3%, inter-day: 84.0-100.0%), and precision (intra-day: 2.72-6.25%, inter-day: 2.93-7.44%). Using the method, we analyzed AF and OTA levels of a total of 60 (15 each) home-style and commercial doenjang samples prepared with traditional and modified methods. AF and OTA were detected in 11 out of 30 home-style doenjangs and in 7 out of 30 commercial doenjangs. All mycotoxins (AFB1, AFB2, AFG1 and OTA) except AFG2 were detected in doenjang prepared with traditional method, but only trace amounts of AFB1 were detected in doenjang prepared with modified method. In the commercially available traditional and modified doenjangs, total AF (sum of AFB1, AFB2, AFG1 and AFG2) was in the range of 0.54-37.89 µg/kg and 0.18-0.39 µg/kg, respectively. On the other hand, in homemade traditional and modified doenjangs, total AF was 1.72-281.92 µg/kg and 0.23 µg/kg, respectively. OTA was in the range of 1.25-32.64 µg/kg in traditional doenjang, but was not detected in modified doenjang. These findings suggest that the AF and OTA levels of modified doenjang are lower than those of traditionally prepared doenjang

AGFD001A 3552374 poster 29 **Synthesis and biological activity evaluation of 5-demethylnobiletin prodrugs** Shiming Li shiming3702@yahoo.com Polymethoxyflavones (PMFs) from citrus peels possess multiple biological activities such as antioxidant, inhibitory effects against chronic inflammation and chemoprevention. However, both aqueous and lipid solubility of PMFs is poor, which hinders the evaluation of the biological activity of PMFs. In this study, a version of lipophilic prodrugs of 5-demethylnobiletin was synthesized for the bioactivity testing. Nobiletin was first demethylated in aqueous ethanol with the catalysis of hydrochloric acid. The resulted 5-demethylnobiletin was esterified with lauric acid under a coupling reagent or lauroyl chloride in the presence of an amine base such as triethylamine. Detailed reaction conditions will be reported

AGFD001A 3545434 poster 30 **Fabrication and characterization of dextran/zein hybrid nanofibers with tailored properties for controlled release of curcumin** Shiyuan Luo lsytsn@163.com Electrospinning has emerged as a promising technique to create and fabricate micro to nano-sized fibers with desired functional, physicochemical, and mechanical properties. In recent years, the interest in the use of electrospun nanofibers for various food application has been increased due to the biocompatibility, biodegradability, high loading capacity and sustained release, and safety aspects because the electrospun nanofibers are usually made from natural polymers. In this study, novel hybrid nanofibers comprising various concentrations of zein with dextran were successfully fabricated and characterized for food applications. The

zein addition modified the fiber-beads morphology of pure dextran nanofibers and the diameter showed an increasing trend with an increase in the zein contents. When zein was added at low concentrations (5% and 10%), the dextran and zein showed poor miscibility, reflected by the significantly decreased viscosity of the solutions and poor mechanical properties of the derived nanofibrous films. The hydrophobicity of the nanofibrous films was increased due to the surface dispersion of hydrophobic zein molecules. When zein was added at medium concentration (15 - 25%), hydrogen bonds were formed between dextran and zein molecules, indicated by the red shift of FTIR peaks and the β -sheet to α -helix structural transformation. The intense interactions between dextran and zein molecules resulted in significantly decreased water contact angle for D50Z15, and the hydrophobicity increased gradually by increasing zein content into the D50Z25, which showed a most hydrophobic surface with a contact angle of 116.9° . The homogenous dispersion of dextran and zein resulted in the improved mechanical properties in terms of elastic modulus and elongation at break. When zein was added at a rate of 30%, caused a significant decrease in the hydrophobicity, and also endowed the desired mechanical properties. The curcumin encapsulated dextran/zein nanofibers exhibited strong radical scavenging activities along with the desired functional properties of controlled release behavior for curcumin delivery by maintaining its inherent antioxidant potential.

AGFD001A 3552337 poster 31 **Simple chromatographic determination of aflatoxins in Korean fermented soybean products Doenjang, Ganjang, and Gochujang with comparison of derivatization methods** So Young Woo mochalatte9@naver.com Some fungal contamination in the production of the common Korean fermented soybean products Doenjang, Ganjang, and Gochujang sauces can produce harmful aflatoxins (AFs); therefore, there is a need for simple and effective methods for AF determination in these complex food matrices. AFs in three commercially available Korean fermented soybean sauces were analyzed by HPLC with fluorescence detection. The best AF extraction efficiency from Doenjang, Ganjang, and Gochujang sauces was achieved using methanol:water (70:30, v/v) as the solvent, and polyethylene glycol as the extraction additive. Pre-column derivatization of the AF extracts was performed using trifluoroacetic acid (TFA), and post-column derivatization was performed in a photochemical reactor for enhanced detection (PHRED). Both derivatization methods resulted in acceptable performances with suitable linearity ($R^2 \geq 0.999$), recovery (71–118%), and precision ($\leq 10.6\%$) values. The mean recovery and precision obtained with pre- and post-column derivatization were similar, but the limit of detection and limit of quantification were superior with post-column derivatization. The procedures based on TFA or PHRED described herein can therefore be implemented for the routine AF analysis of Korean Jang products and but also various types of fermented soybean products, such as Japanese Miso and Shoyu, Chinese Dajiang, Doubanjiang and Chiangyu, and Nepal Kinema. The validated method was applied in the analysis of commercial Doenjang, Ganjang and Gochujang, which showed that their contamination levels were extremely low. Among the 42 tested samples, 26% were contaminated with at least one AF in the concentration range of 0.08–0.41 $\mu\text{g/kg}$, which are significantly lower values than those of current regulatory limits

AGFD001A 3557147 poster 32 **Metal-organic frameworks (MOFs): Advanced technology of architectural instabilité against moisture** Souad Djaoui s.djaoui@univ-boumerdes.dz Les cadres métalliques et organiques de contrôle de stabilité chimique et structurale sont bien liés à l'étape de synthèse ainsi qu'à l'étape de modification post-synthétique, qui permet au MOF d'être orienté vers une application spécifique. L'instabilité à l'humidité provoque un

effondrement structurel et une forte baisse de surface d'environ 80% pour le MOF-5 après une semaine d'exposition à l'humidité, ce qui reflète une réduction significative de la capacité de sorption. Pour ce qui suit, un travail comparatif est effectué avec la modification d'approche post-synthétique du ligand par des groupes hydrophobes également par stabilisation de la barrière énergétique de l'activation structurale contre l'eau afin de stabiliser les interactions métal-ligand

AGFD001A 3557377 poster 33 **ANOVA for unbalanced data with missing cells: Using spreadsheets to evaluate SAS Type IV sums of squares** Thomas Klasson thomas.klasson@usda.gov Student and researchers are often introduced to Analysis of Variance (ANOVA) Statistics by first studying one-way ANOVA examples. They then move on to factorial ANOVA statistics, for example two-way ANOVA, but often this is limited to balanced data. Balanced data are when the number of data values for each of the category (or group) is the same. When this is the case, the calculations are simple to do and the equations can easily be written to allow for each of the values needed to construct an ANOVA table. When unbalanced data are encountered, which is often the case in agricultural field studies, the data are often entered into a statistical program such as SAS to construct the ANOVA table. The most complicated situation is when data are completely missing in a two-way ANOVA design for some treatment combination(s). This can be handled by a SAS Type IV evaluation in the SAS GLM Procedure. In this presentation we will show how dynamic spreadsheets can be constructed to produce SAS Type IV sums of squares for two-way ANOVA tables using hypotheses testing. Different hypotheses can be constructed by the user

AGFD001A 3554185 poster 34 **Accelerated stability study of phytochemical active compounds and antioxidant activity in whole coffee cherry extract powder** Tiffany Gallegos-Peretz Tiffany.GallegosPeretz@futureceuticals.com An accelerated stability study was conducted on FutureCeuticals' coffeeberry extract product, NeuroFactor[®] (CoffeeBerry 40% Chlorogenic Acids (CGA)), in powder form at two different storage temperatures/relative humidity (RH) (25°C/ 60% RH and 40°C/ 75% RH) for up to six months. The objective of this study was to determine if any functional changes in the product's chemical properties existed during storage that might influence quality. Chemical analyses were performed to determine the stability of whole coffee cherry extract. Results showed that the active chemical components of the NeuroFactor[®] powder that were evaluated were stable during storage. The antioxidant capacity, the total chlorogenic acid (CGA) content and the individual chlorogenic acid components, 5-CQA, 4-CQA or 3-CQA, the trigonelline content and the caffeine content for this product were determined to be stable for up to six months. The stability of NeuroFactor[®] powder suggests that it can be stored at room temperature (25°C) for 2 years without any effects on its active chemical components

AGFD001A 3551996 poster 35 **Estimation of the contribution of SPLET and HAT reaction mechanisms to the overall radical scavenging activity of catechol-flavones** William Whaley whaley@tarleton.edu The flavonoids are phenolic compounds present in fruits and vegetables. Due to their activity as scavengers of reactive oxygen species (ROS), there is interest in using flavonoids as nutritional supplements and as lead structures for drug development. The stable free radical 2,2-diphenyl-1-picrylhydrazyl (DPPH) is often used to determine IC_{50} , which is the concentration of antioxidant needed to diminish the absorbance of DPPH ($\lambda=515\text{ nm}$) by one-half in 30 minutes. This parameter discriminates flavonoids based on differences in total radical scavenging activity (RSA). It does not reflect differences in the rates at which flavonoids scavenge DPPH in the early part of the assay. ROS are aggressive and

mechanisms for their fast reduction are relevant for protection of living cells. DPPH reacts with catechol flavones in methanol solvent by several mechanisms with overlapping time domains. A rapid single proton loss electron transfer (SPLET) reaction is over within milliseconds after reagent mixing. Fast to moderate hydrogen atom transfer (HAT) reactions continue about 300 seconds while slow HAT reactions may last 30 minutes after mixing. The five catechol flavones, α -tocopherol (Vitamin E), quercetin, rutin and pomiferin were assayed with DPPH using continuous recording of absorbance for 30 minutes. The absorbance values at 12, 300 and 1800 seconds were compared to estimate the proportion of the RSA due to each mechanism. The compound 7,8-dihydroxyflavone exhibited SPLET almost exclusively. Vitamin E and the other catechol flavones exhibited different degrees of SPLET, fast HAT and slow HAT. This modified DPPH assay can identify flavonoids that react by the SPLET and/or fast HAT mechanisms and may compete with Vitamin E for scavenging ROS.

AGFD001A 3552717 poster 36 **Determination of the location & orientation of catechol-flavones and catechol-isoflavones in aqueous SDS micelles by ^1H -NMR spectroscopy** William Whaley whaley@tarleton.edu Vitamin E (α -tocopherol) is a vital antioxidant that protects lipid structures in living cells from being damaged by reactive oxygen species (ROS). Dietary flavones and isoflavones that bear catechol (ortho-dihydroxy) groups also scavenge ROS at a significant rate and may prevent Vitamin E depletion. There is evidence that catechol-flavonoids may have a protective role in cellular models of Alzheimer's disease (AD), Parkinson's disease (PD) and Huntington's disease (HD). Using a Mn²⁺ titration assay, based on ^1H -NMR spectroscopy, it was previously demonstrated that daidzein (7,4'-dihydroxy-isoflavone) incorporated into aqueous sodium dodecyl sulfate (SDS) micelles and occupied a time-average location near the sulfate "head" groups. In contrast genistein (5,7,4'-trihydroxy-isoflavone) incorporated into SDS micelles but was located within the hydrophobic micelle core. The results from the assay of quercetin, rutin, 7,3',4'-trihydroxy-isoflavone (7,3',4'-THIF) and pomiferin are now reported. Quercetin and pomiferin both were located within the hydrophobic micelle core. In contrast, 7,3',4'-THIF (3'-hydroxy-daidzein) was located near the aqueous interface, much like daidzein. Rutin was located at the aqueous interface with the rutinose portion exposed to the aqueous phase and the aromatic flavone portion buried within the hydrophobic micelle core. Each catechol-flavone or catechol-isoflavone reacted with 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical in methanol solution and exhibited an IC_{50} value in the range of 5 μM to 20 μM . The aqueous SDS micelle system could be used as a model to investigate how the position and orientation of flavonoids in lipid structures may affect scavenging of ROS.

AGFD001A 3545450 poster 37 **Fabrication & characterization of fast dissolving glycerol monolaurate microemulsion encapsulated gelatin nanofibers with antimicrobial activity** Xinyan Zhang shelden2403@163.com Due to the advantages of low cost, easy operation, and large surface area to volume, electrospun nanofibers has long been researched as a proper delivery system in the food industry. Gelatin has been researched as an ideal candidate for fast dissolving nanofibrous film fabrication. Glycerol monolaurate (GML) is approved as a generally recognized as safe food additive by the US Food and Drug Administration. However, the physical properties of GML such high melting point and poor solubility in water lead to difficulties in its use as an antimicrobial. Emulsion electrospinning has been rapidly developing for its effectiveness of encapsulating both hydrophobic and hydrophilic bioactive for controlled release and bioactivity. The gelatin/GML microemulsion nanofibers were fabricated by solubilizing GML in Tween 80 and

then mixed with gelatin for electrospinning. The addition of GML microemulsions did not affect the electrospinnability and uniform morphology was observed. The solutions with GML microemulsions showed more pronounced shear-shinning effects and the intermolecular interactions between gelatin and GML microemulsion resulted in a higher average diameter of the D64 nanofibers (1147 nm) compared to the gelatin nanofibers (560 nm). FTIR analysis suggested the hydrogen bonding between gelatin and GML microemulsions. The thermal analysis and XRD results indicated the amorphous structure of gelatin/GML microemulsion nanofibers, even though a small amount of GML crystalline exists. The nanofibers with GML microemulsions showed higher thermal stability and facilitated the gelatin degradation upon heating. The gelatin/GML microemulsion nanofibrous films showed super-hydrophilicity and fast dissolution properties, which was due to the high surface to volume ratio property, the amorphous structure, and the improved surface hydrophilicity of nanofiber surface. The nanofiber with 5% (weight ratio respect to nanofiber) GML (D64) showed effective antimicrobial activity against *E. coli* and *S. aureus*, which has potential application as edible antimicrobial food package.

AGFD001A 3552431 poster 38 **Cloning & expression of a novel thermal-activated β -galactosidase from *Bacillus aryabhattai* Gel-09** Xuguo Duan xgduan@njfu.edu.cn β -galactosidase (EC 3.2.1.23), catalyzing the hydrolysis of β -1,4 or β -1,6 galactosyl bonds in disaccharides as well as transglycosylation, is a kind of glycoside hydrolase that plays a important role in dairy industry. In this study, a novel thermal stable β -galactosidase (lacZBa) was characterized from *Bacillus aryabhattai* GEL-09. It showed that the lacZBa encoding gene was composed of 1950 bp open reading frame (ORF), which encodes a protein containing 649 amino acid residues. Phylogeny and amino acid sequence analysis indicated that this enzyme belonged to family 42 of glycoside hydrolases. The lacZBa encoding gene was over-expressed in *E. coli* BL21(DE3) and the recombinant enzyme was purified to homogeneity. The molecular weight of the recombinant β -galactosidase was estimated to be about 75.4 kDa by SDS-PAGE. The recombinant β -galactosidase exhibited maximum activity at 45°C, and pH 6.0, and it maintained 92%, 96% and 47% relative activity at 40°C, 50°C and 55°C, respectively. The activity of enzyme can be activated when it was incubated at 45°C for several minutes. Moreover, the residue activity of the purified enzyme remained about 150% after being stored at 45°C for more than 100 h, and its half-life was 36 h at 50°C. In the presence of Co^{2+} , Mn^{2+} , Zn^{2+} , Fe^{3+} , Mg^{2+} , Ca^{2+} , the activity of the recombinant enzyme was enhanced, however, copper ion and EDTA had a significant inhibitory effect on enzyme activity. In addition, the kinetic analysis showed that the michaelis constant (K_m) value was 14.38 mM and the maximum rate of enzymatic reaction (V_m) value was 11.66 U/mg when oNPG was used as the substrate. In this study, a solution with a concentration of 5 g/L lactose was used to simulate the commercial milk, and the lactose substrate was completely hydrolyzed within 2 h with addition of 7 U/mL of pure enzyme at 45°C. These results suggested that the β -galactosidase identified in this study has potential applications in the dairy industry.

AGFD001A 3554096 poster 39 **Natural flagella-templated Au nanowires as a novel adjuvant against *Listeria monocytogenes*** Yanhong Liu yanhong.liu@ars.usda.gov A simple method was developed for the extraction and purification of bacterial flagella with a yield of a concentration of 113.22 ± 5.64 mg/mL. Gold (Au) nanowires were synthesized using the bacterial flagella as the template. Transmission Electron Microscopy (TEM) analysis showed that the nanowires were scarcely clustered as stiff (no tendency to bend or fold) and straight nanorods with homogeneous surface and a

uniform aspect ratio over 60. Fourier Transform Infrared (FT-IR) spectroscopic studies revealed the deep involvement of the functional groups located within and on the surface of flagellin, including C-N, N-H, O-H, and C=O. The profound transformation observed in the absorption profiles of these groups supported the notion that both chemical (reduction) reaction and physical (electrostatic) binding of Au occurred during the formation of Au nanowires. Verbascoside, oleuropein, and olive leaf extract (OLE) have been shown to inhibit the growth of *Listeria monocytogenes* completely at their respective Minimal Inhibitory Concentrations (MICs) of 20, 64, and 64 mg/mL. In contrast, the synthesized Au nanowires demonstrated high electrocatalytic activity and reduced the MICs of the three antibacterial compounds by half. Moreover, results from the AMES assays indicated that the synthesized Au nanowires had no mutagenic activities at the catalytic concentration used, 128 mg/mL. Therefore, the Au nanowires fabricated in this work have the potential to be used as new antimicrobial food packaging materials to enhance food safety.

AGFD001A 3556886 poster 40 **Encapsulation of garlic oil and diallyl disulfide with β -cyclodextrin for garlic white rot control**
YanPing Qian yan.ping.qian@oregonstate.edu White rot, a disease caused by the soil-borne fungus *Sclerotia cepivorum*, is a severe enemy of garlic and onion production in California, Oregon, and Washington. It is desirable to use sulfur-containing organic compounds to trigger sclerotia germination in the absence of a host to control the sclerotia. Previous research has shown that diallyl disulfide (DADS) can reduce fungus soil levels by 90 to 98 % in field trials. However, soil incubation studies found that volatile organic sulfur compounds have strong interaction with the soil. Depending on the types of soils, organic matter, and soil microorganisms, the sulfur compounds can bind to soil particles or be metabolized by microorganisms. In either case, it reduces the efficiency of volatile sulfur compounds. This study was conducted to encapsulate commercial DADS and garlic oil with β -cyclodextrin (β -CD) to protect sulfur volatiles from reacting with soil and against oxidation, heat, light-induced degradation, and evaporation. Also, volatile sulfur compounds' encapsulation may allow for slower release and increase their efficacy for sclerotia germination. Inclusion complexes of DADS and garlic oil with β -cyclodextrin were prepared by the coprecipitation method with the DADA/garlic oil ratio β -cyclodextrin of 15:85 (w/w), which achieved the maximum inclusion efficiency of β -cyclodextrin. Oil analysis showed that the garlic oil was successfully encapsulated with greater than 90% powder recovery. Encapsulated oil analysis also showed that the micro-encapsulation process did not change the chemical compounds, but their proportions were altered. Microencapsulated commercial DADS oil contained 63% diallyl disulfide, whereas the encapsulated garlic oil had 75% diallyl disulfide. Further research will study the release of volatile sulfur compounds from the encapsulation complex in different soils and its effects on sclerotia germination.

AGFD001A 3556316 poster 41 **Aging of titanium dioxide nanoparticles relieved the original phytotoxicity and enhance the nutrient quality of soil grown carrots**
Yi Wang ywang10@miners.utep.edu The effect of surface-functionalized nanomaterials (NMs) on the development of agricultural plants, especially the belowground root crops, has attracted increased interest. After release, NMs may remain in the soil for an extended period and undergo significant transformation reactions. In this study, carrots (*Daucus carota* L.) were grown in soils amended with titanium dioxide nanoparticles (nTiO_2), pristine, hydrophilic- or hydrophobic-surface coated) at 100, 200, and 400 mg/kg until full-plant maturity. To investigate the aging effect, nanoparticles were weathered in native soil for four months before the cultivation of plants. In carrots treated by the freshly exposed

nTiO_2 , the taproot fresh biomass was significantly decreased by all nTiO_2 forms at 400 mg/kg compared with control. An abnormal increase of taproot splitting was found. The accumulation of Mg, Mn, and Zn in the taproot was decreased. However, after the aging process, all the negative impacts listed above were alleviated, both in a surface coating and concentration dependent-manner. The aged surface-coated nTiO_2 improved taproot and leaf fresh biomass and plant height compared to control. The Fe in leaves, Mg in taproots, and Ca, Zn, and K in roots were enhanced by exposure to the aged nTiO_2 . These results may contribute to the development of safe and sustainable applications of nTiO_2 in nano-enabled agriculture.

AGFD001A 3558217 poster 42 **Development of DNA computing and self-generating system**
Yu-Chen Lo bennylo@stanford.edu
Gu Ren rengui@shu.edu.cn Hiroshi Honda chrishonda@yahoo.com This paper presents a facile development of a self-generating system automated similarly to the DNA-protein system of the living organism.

AGFD001A 3552432 poster 43 **Development of chemical synthesis of azamacrocyclic systems related to polypyrrolic macrocycles**
Yu-Chen Lo bennylo@stanford.edu Hiroshi Honda chrishonda@yahoo.com This paper presents the development of the chemical synthesis of azamacrocyclic compounds and derivatives.

AGFD001A 3557484 poster 44 **Synthesis & characterization of hydrophobic deep eutectic solvents based on lignin derivatives**
Yuxuan Zhang yx.zhang@uky.edu Hydrophobic deep eutectic solvents (DESSs) have gained increasing attention as sustainable and environmentally friendly alternatives to the conventional organic solvents. In this work, we prepared several new hydrophobic DESSs based on lignin derivatives and characterized their physicochemical properties using experiments and molecular simulations. We investigated the melting point and thermal decomposition temperature of the new DESSs using thermogravimetric analysis and the level of their hydrophobicity based on their static contact angle on a glass or plastics surface. Molecular simulations were conducted to investigate the structural and dynamic properties of molecular association, especially hydrogen bonds in these DESSs. This work provides the promising role of lignin derivatives in developing hydrophobic DESSs with features suitable for applications as solvent and extraction medium.

AGFD001A 3548703 poster 45 **Tandem solid-phase extraction columns for simultaneous aroma extraction and fractionation of Wuliangye and other baijiu**
Zhanglan He hezhanglan@wuliangye.com.cn Wuliangye is one of the most famous baijiu in China. Several hundreds of esters have been identified in Wuliangye baijiu, and these esters are abundant. Their aromas are similar, which makes it challenging to analyze other compounds with unique aroma quality. Thus, it is desirable to fractionate the aroma extract into subgroups based on functional group or polarity to simplify the analysis. However, the high alcohol content in aroma extract often deteriorates fractionation efficiency on normal phase chromatography. In this study, a new approach was attempted to achieve simultaneous aroma extraction and fractionation using tandem LiChrolut EN and silica gel solid-phase extraction (SPE) columns. The baijiu sample (10 ml, diluted in 40 ml of water) was first pass through the LiChrolut EN (1.0g) column. After dried with air, the LiChrolut EN (1.0g) column was connected with a silica gel (5.0g) SPE column with anhydrous Na_2SO_4 (10.0g) in between. The aroma compounds were eluted from the LiChrolut EN column and simultaneously fractionated on the silica gel column with increased solvent polarity (40ml of each fraction). The simultaneous extraction and fractionation enabled the

collections of all esters in less polar fractions, and the acids, alcohols, pyrazines, furans, phenols, hydroxy esters, and other compounds in the more polar fractions. This method successfully solved esters' interference with other aroma analysis in baijiu. It has the advantages of integrating adsorption and fractionation, fast and straightforward operation, low solvent consumption, and minimum selective extraction and adsorption for aroma compounds. This technique was used to study the polar aroma compounds in Wuliangye, Moutai, and Fenjiu baijiu.

MONDAY MORNING 4/05/21 start 9:00 AM end noon

Food-flavor Dynamics Assessments via Real-time Mass Spectrometry - Part I: From Developments to Nosespace

AGFD009A 3547964 9:05 AM **Atmospheric pressure chemical ionization (APCI) for real-time odor analysis** Andrew Taylor flavometrix@btconnect.com The 1990s saw a move to complement the analysis of food flavor composition (using techniques like Solvent Assisted Flavor Evaporation followed by GC-MS), with methods to measure the odor profile released from foods before and during eating. The rationale was that the odor profiles in the headspace and "nosespace" were very different from the compositional profile, due to factors like odor partition and volatility but these were the profiles that actually activated the odor receptors and might help researchers better understand the link between the perceived flavor of a food and its flavor composition. Direct mass spectrometry was an obvious analytical option but presented challenges such as obtaining sufficient sensitivity (odor concentrations in the gas phase are several orders of magnitude lower than in foods), dealing with the high humidity in human breath and collecting data fast enough to accurately map odor release on a breath-by-breath basis. APCI-MS offered many advantages for this analytical task, for example, the ease of interfacing human breath with the hi-vacuum MS using venturi, the fact that water can be used as the charge transfer reagent in APCI (thus humidity of breath samples is not an issue) and the ready availability and simplicity of the APCI interfaces fitted to mass spectrometers. Like all techniques, there were also limitations, some of which could be overcome by "work arounds", others which are inherent to the technique. A description of the APCI ionization process and the design of the interface will be given along with the pros and cons of this technique for monitoring the real-time release of odors from foods. This presentation is dedicated to my long-term collaborator in the development of APCI-MS, Jun Hatakeyama from Nichirei Foods, Japan, who tragically died in 2020.

3567957 9:00 AM **PTR-MS: Sampling matter(s) - from the importance of sample introduction to the diversity of innovative solutions** Christian Lindinger The majority of complex scientific data generated in the food, flavor and fragrance research sectors relies on modern mass spectrometric methods. This is due to obvious advantages in terms of objectiveness, reliability, comprehensiveness and accessibility. In the early days only experts were skilled enough to use this technology. But from the first day on, when such complex instruments started to be well manageable in standard laboratory environments, the success of their applications never declined. One of the common persistent challenges relates to the introduction of the sample into the analyzer. Because of its importance, diversity and accumulated knowledge for PTR-MS in this field, this presentation will provide a short overview about past hurdles, achieved solutions and an outlook on new developments for flavor-research applications and beyond.

AGFD009A 3553114 9:00 AM **Comprehensive aroma analysis with selected ion flow tube mass spectrometry (SIFT-MS)** Diandree Padayachee diandree.padayachee@syft.com Selected ion flow tube mass spectrometry (SIFT-MS) is a direct mass spectrometric

technique that has contributed significantly to better understanding of food-flavor dynamics in food processing and in vivo studies. In SIFT-MS, rapid switching of multiple reagent ions and cooling of reagent ions to consistent energies before sample introduction, provides speed, selectivity and enables an in-built compound library. This simplifies method development, quantitation and compound identification, making for a more user-friendly experience. This talk reviews some recent applications of SIFT-MS in food aroma analysis. A few highlights of flavor analysis applications, such as flavor release, sensory, food origins, quality testing and food processing, are discussed. The power of SIFT-MS combined with chemometrics for both targeted and untargeted analysis is also demonstrated. Packaging can also impact food quality and flavor. While packaging can play a significant role in maintaining food freshness, inferior grade packaging could lead to food taint. SIFT-MS investigations into packaging are discussed, along with the benefits of using automated SIFT-MS to improve both speed and precision of headspace measurements. A recent development – thermal desorption (TD)-SIFT-MS – is also introduced, which adds extra functionality to analysis of packaging materials, by utilizing thermal extraction analysis. Finally, the potential and future direction of SIFT-MS in food-flavor analysis is presented.

AGFD009A 3555828 9:00 AM **Molecular mechanisms behind the phenomenon of food aroma persistence** Carolina Munoz Aroma persistence plays a major role in food choices and liking, and thus, its understanding might be important to formulate food products sensorially appreciated by consumers. The aim of this work was to unravel the molecular mechanisms behind the phenomenon of aroma persistence by using a global approach. The release and metabolization of 5 food aroma compounds (linalool, pentan-2-one, nonan-2-one, hexan-2,3-dione and octanal) from different chemical classes was studied after their exposure to ex vivo models of oral mucosa (oral cells+saliva) by Gas-Chromatography Mass Spectrometry (GC-MS). Then, in vivo dynamic instrumental and sensory experiments were carried out to validate the ex vivo findings in a more realistic context. To do that, in vivo aroma release was monitored by Proton Transfer Reaction-Mass Spectrometry (PTR-MS) (n=54). Moreover, the intensity of two aroma descriptors was evaluated using a dynamic time-intensity sensory evaluation (n=26). Ex vivo experiments showed that oral mucosa reduced the release of all aroma compounds assayed and that cells and saliva metabolized aroma compounds in a compound-dependent manner ($p < 0.05$). Interestingly, in vivo experiments confirmed that the compounds metabolized ex vivo disappeared quicker in the breath than the compounds not metabolized by cells and saliva ($p < 0.05$). The same trend was observed in the sensory experiments, which confirmed the sensory meaning of these findings. Overall, results from this work suggest that aroma persistence is driven by both, biological and physicochemical mechanisms.

AGFD009A 3553772 10:00 AM **Nosespace PTR-MS analysis with simultaneous TDS or TCATA sensory evaluation: Release and perception of the aroma of dark chocolates differing in sensory properties** Jean-Luc Le Quere jean-luc.le-quere@inrae.fr Perception of flavor is a dynamic process during which the concentration of aroma molecules at the olfactory epithelium varies with time as they are released progressively from the food in the mouth during consumption. However, how the various components combine to produce a sensory impression is still not completely understood. Real-time mass spectrometry (MS) techniques that measure aroma compounds directly in the nose (nosespace) aim at obtaining data patterns that are supposed to reflect the way aromas are released in real time during food consumption. These patterns are supposed to be representative of the retronasal stimuli perception. Real-time sensory methods, such as time-intensity, or the more recent

Temporal Dominance of Sensations (TDS) and Temporal Check All That Apply (TCATA) procedures, are used to account for the dynamic and time-related aspects of flavor perception. Combined together, preferably simultaneously in a fully real-time in vivo approach, both chemical and sensory methods should provide fundamental results to understand the link between aroma release and aroma perception better. The present lecture will present an overview of the advances made for combining real-time nosespace analysis with simultaneous temporal sensory evaluation. In order to analyse conjointly the two sets of data, a statistical procedure will be presented and discussed. These advancements will be illustrated and discussed through the study of the flavor of three dark chocolates differing in sensory properties, analyzed by a panel of 16 assessors in nosespace with a PTR-ToF-MS instrument and simultaneous TDS or TCATA sensory evaluation. Results obtained with TDS and TCATA will be compared.

AGFD009A 3555761 10:00 AM **Combination of in-vivo** nosespace analysis and dynamic sensory methods for better understanding of flavour release and sensory perception of composite foods Iuliia Khomenko iuliia.khomenko@fmach.it Many of the regularly consumed foods are composite foods, which consist of multiple components differing in composition and properties, i.e. toppings and condiments combined with vegetables or potatoes, sauces and spreads combined with bread or crackers. The characteristics of each component can differ considerably and may influence physically and chemically flavour release and sensory perceptions of the other components. Characterizing composite foods has recently gained interest not only due to their increased sensory complexity, but also because composite foods are more representative of the natural consumption context and may be a way to address eating behaviours issues. An optimal experimental approach for the investigation of the flavour evolution of composite food during oral processing is the combining of dynamic sensory methods with simultaneous nose-space analysis by high sensitivity direct injection mass spectrometry. In this work we discuss two case studies related to important food combinations: i) the influence of different carriers on the flavour release and perception of extra virgin olive oil (EVO); ii) investigation of the effect of food structure and composition on aroma release and sensory perception of chocolate-hazelnut spreads. In both cases Temporal-Check-All-That-Apply (TCATA) was coupled with in vivo nose space analysis using a commercial PTR-ToF-MS (Proton Transfer Reaction Time-of-Flight Mass Spectrometer, Ionicon Analytik, Innsbruck, Austria). In the first case study 2 different EVO oils were tested alone and with 2 carriers (bread and chickpea) by 10 panellists wearing a glass nosepiece connected to the PTR-ToF-MS with a (PEEK tube (50 cm at room temperature and then heated at 110°C). In the second case study three different formulation of chocolate-hazelnut spread varying in fat and sugar content (high fat/high sugar; high fat/low sugar; low fat/high sugar) together with 2 carriers (bread and wafer) were evaluated by 8 subjects. The spreads were spiked with 5 aroma compounds (Benzaldehyde, Filbertone, δ -decalactone, Isovaleraldehyde, 2-methylpyrazine). For this study a heatable nosepiece system (Ionicon Analytik, Innsbruck, Austria) was used for nosespace analysis. In both case studies the effects of different products, addition of carriers and interindividual differences were observed. We are currently working on the investigation of the relationship between volatile release during nosespace analysis and sensory response.

AGFD009A 3553641 11:10 AM **Real time nose space** monitoring by SIFT-MS allows to get insights on biological and behavioral factors affecting the inter-individual variability on flavor release Leonardo Menghi leonardo.menghi@unitn.it It is known that factors affecting flavor release during food consumption comprise a complex interplay between biology and eating behaviors.

However, evidence supporting the effect of both components on representative sample sizes using an ecologically valid method are still lacking. Mounting evidence suggests that real time MS in-vivo monitoring the volatile organic compounds exhaled from the nose during food consumption, also called nose-space analysis, still remains the most direct way to non-invasively investigate the dynamics of flavor release and, therefore, it ought to be considered as the gold standard method when such studies are thought to be performed. Hence, this contribution aims to get insights on the inter-individual variability on flavor release of a representative healthy population, monitored in real time, by taking into account both some biological (i.e. gender, age, BMI) and behavioral variables. To address this later issue, Food Neophobia, a widely studied eating behaviour trait that measures the reluctance to eat what is unfamiliar, and trait anxiety were chosen. Eighty-three subjects (57.8 % female; aged 22 to 68 yo) consumed, according to a fixed chewing procedure supported by a video tool, a strawberry jelly candy chosen as reference food to study aroma release. Simultaneously, nose-space analysis with Selected-Ion Flow-Tube Mass Spectrometry (SIFT-MS) was carried out by monitoring in real time the release of 7 key aroma compounds (5 esters, 2 alcohols). Flavour profiles information based on parameters commonly used to analyze time-intensity (T-I) curves (i.e. AUC, I_{max} , I_{mean} , T_{max} , T_{end} , Slope) revealed a slightly negative effect of age and BMI on flavor release. No gender effect was observed. Moreover, individuals with lower Food Neophobia and trait anxiety tendencies showed a higher extent of flavor release, probably due to a longer oral processing and lower anxiety-related physiological responses (such as breathing rate). These results confirm that real time MS nose space monitoring is an efficient tool to unravel the dynamics of flavor release. As a final remark, we advocate the usage of both representative sample sizes and to consider its multidimensional nature once mechanisms underlying flavor release are under investigation.

AGFD009A 3555610 11:00 AM **Characterization of product & panel effect on in vivo aroma release and sensory perception** Michele Pedrotti michele.pedrotti@wur.nl Proton Transfer Reaction Mass Spectrometry has been described has particularly suited to provide “in vivo” on-line flavor monitoring during food consumption. In the last years, the technique has been applied to different food matrixes. Due to analysis rapidity and high sensitivity, the technique has become a reference tool for the investigation of the complex phenomena related to flavor perception. In this work we describe a PTR-MS nose-space approach coupled to different dynamic sensory methods to investigate the influence of product properties and participants characteristics on in-vivo aroma release and perception. In the first part, the influence of food properties on in-vivo aroma release and perception will be explored. Case studies on chewing gum formulation, composite foods and on raw and cooked cabbage will be presented. For the chewing gum the effect of gum base and aroma concentration on aroma and sweeteners release and flavor perception was tested. The approach was also tested on commercial samples to evaluate samples differences. In the composite food study mayonnaises varying in fat content (high/low) and viscosity (high/low) were consumed alone and in combination with carriers differing in moisture absorption capacity (bread, potato) and hardness (hard/soft). The same approach was applied to evaluate the effect of both condiment and carrier properties on in vivo aroma release and lemon perception through time intensity sensory test. In the last study another kind of sensory test, Temporal Dominance of Sensation was applied to characterize flavor differences of raw and cooked cabbage samples. In the second set of studies, the effect of physiological parameters (oral cavity volume, salivary flow and papillary count), gender and ethnicity in flavor perception and aroma release was investigated by using chewing gum and cabbage as food

product. Overall, the results of the studies suggest a multimodal effect of aroma release on both flavor and sweetness intensity. Individual differences due to physiological, biochemical and physicochemical phenomena may have a relevant effect in aroma perception and thus in sensory flavor perception. Real time direct injection mass spectrometric analysis coupled with dynamic sensory methods, is confirmed as a powerful tool to investigate flavor perception mechanisms and highlight physiological and cultural biases.

MONDAY AFTERNOON 4/05/21 start 1:00 PM end 4:00 PM
Food-flavor Dynamics Assessments via Real-time Mass Spectrometry - Part II: Headspace and Beyond

AGFD009B 3549302 1:05 PM **Applications of on-line mass spectrometry (MS) in flavor research** Andrew Taylor flavometrix@btconnect.com Commercial on-line MS systems have been available for over 20 years, and their application to flavor research has been reviewed for SIFT-MS¹ and PTR-MS² but not for APCI-MS. Here, we present some of the pioneering applications developed at the University of Nottingham, UK. These include the initial studies on the patterns of aroma release from foods during eating, which led to the conclusion that the retronasal aroma profile varied over the time of eating and was very different from the flavor composition of the food and the headspace measured above the food³. Efforts to reduce sugar, and fat in foods, while maintaining the original flavor, initiated studies on the connection between the physicochemical factors of the food matrix and aroma release⁴. In response to an enquiry about the flavor-fade in chewing gum, significant taste-aroma interactions between sweetness and minty odours were discovered⁵. To measure the aroma profile in fresh tomatoes when eaten, a rapid technique was developed to mimic the disruption of the tomato tissue, while simultaneously measuring the pre-formed aroma compounds as well as the formation of the enzymically-generated aroma compounds⁶. Combining APCI-MS with physiological methods showed the relationship between chewing, breathing and swallowing during the eating of foods⁷. The effect of sugar crystallisation on the rate of the Maillard reaction was monitored using FT-IR and APCI-MS⁸, while the effect of water content on the first few steps in the Maillard reaction showed the reaction flux was highly dependent on water levels⁹. Lastly, the dynamic binding of aromas to Odour Binding Protein (OBP) in the nasal passages was used in an *in vitro* system to study competitive binding of aromas to OBP¹⁰.

AGFD009B 3551018 1:00 PM **Swiss cheese flavor: Volatile organic compounds and descriptive sensory attributes indicate mechanisms** Sheryl Barringer barringer.11@osu.edu Minimizing flavor variation in cheeses in order to produce a consistent product is a challenge in the Swiss cheese industry. This study evaluated the flavor variability of cheeses without defects, based on correlations of volatile flavor compounds and sensory attributes. The headspace concentrations of volatile compounds were analyzed using selected ion flow tube-mass spectrometry (SIFT-MS), while the sensory attributes were evaluated using descriptive sensory analysis and consumer testing. The important discriminating volatile compounds were classified into five functional groups: sulfur-containing compounds (methyl mercaptan, hydrogen sulfide, dimethyl disulfide, dimethyl trisulfide, and methional), organic acids (propanoic acid, acetic acid, 3-methylbutanoic acid), aldehydes (3-methylbutanal, butanal, and 2-methylpropanal), a ketone (2,3-butanedione), and an ester (ethyl hexanoate). The interactions between discriminating volatile compounds indicating interactions in the underlying mechanisms of volatile formation. Correlations were identified among volatile compounds and between volatile compounds and

sensory attributes. Only a small number of volatile compounds strongly correlated positively or negatively to a specific sensory attribute. Nutty malty, milkfat lactone, salty, umami, and sweet positively correlated to overall liking and nutty flavor liking of Swiss cheese. Evaluation of cheese flavor using correlations between volatile compounds and sensory attributes provided further understanding of the complexity of flavor and flavor variability among Swiss cheeses manufactured from different factories, and the underlying mechanism of flavor formation in Swiss cheese.

AGFD009B 3550836 1:00 PM **Application of proton transfer reaction mass spectrometry (PTR-MS) for wine taste & quality analysis** Joseph Timkovsky j.timkovsky@gmail.com Wine perception is very subjective and leads to many discussions, having multiple scales to assess wine, etc. It would be very beneficial to be able to objectively characterize wine taste. This is what we have performed by using proton transfer reaction mass spectrometry (PTR-MS) for monitoring on a commercial basis large amounts of wine samples in terms of quality and taste. We considered a few elements of the standard form for wine assessment and made it objective based on PTR-MS and some basic chemical parameters (pH, total reducing sugars, ethanol, total acidity, etc.) measurements. In particular, we objectified the following parameters using PTR-MS measurements: flavour intensity, aroma&flavour characteristics, development, etc. Also, we considered off-notes presence in wines by setting up threshold values for a number of the off-note compounds (hexanal, 4-ethylphenol, ethyl acetate, etc.). In the presentation, we will discuss in more detail how these parameters have been quantified and also provide a few examples where differences were observed between the professional tasting panel observations and the measurements. All in all, using PTR-MS measurements has been successfully applied to automatically process thousands of wine samples on a yearly basis and assess their quality and taste in an objective way.

AGFD009B 3557325 1:00 PM **Influence of fat replacer use on volatile organic compound release in muffins** Patrick Silcock pat.silcock@otago.ac.nz Solid fat plays an important role in food, in particular baked goods where it improves texture and modifies flavor. However, pressure exists on the food industry to eliminate trans-fatty acids and decrease of amount of saturated fat. Organic gelators or oleogels have been identified as suitable for solid fat reduction. Oleogels are 3-dimensional gel networks containing an entrapped organic liquid, which in this instance was a liquid vegetable oil entrapped in a crystalline monoglyceride network. Using a plain muffin as a model baked system the substitution of hydrogenated coconut oil (HCO) for canola oil/monoglyceride oleogels or canola oil on the volatile organic compounds (VOCs) generated by baking was investigated. Muffins were prepared from oleogels containing 6, 8, 14 and 25% monoglycerides in canola oil. Muffins were also prepared containing HCO at two levels or canola oil. VOC release was measured using proton transfer reaction time of flight mass spectrometry (PTR-ToF-MS) during baking and upon cooling on the baked muffins (crust and crumb measured separately). Differences were observed in the VOCs released during baking of the muffins depending upon the fat source used in the muffins. VOCs released into the headspace above the cooled muffins varied systematically depending upon the fat source. Generally higher levels of VOCs were observed released from the crust of the muffins compared to the crumb

AGFD009B 3555843 2:00 PM **Analyses of volatile compounds released by fresh Atlantic salmon stored at 4°C for upto 16 days** Patrik Spanel spanel@jh-inst.cas.cz Fish are highly perishable and it is important to have reliable spoilage assessment methods. Most effort has been devoted to chemical methods of characterizing freshness: assays of TVBN (total volatile basic nitrogen), TMA

(trimethylamine), nucleotide derivatives using the H, K and K⁺ ratios and assay of fatty acids. Other methods include spectroscopic, microbiological, texture assessment, study of electrical properties and determination of biogenic amine composition. Atlantic salmon is rich in bioactive proteins, antioxidants, vitamins and omega-3 fatty acids, making it rich source of essential nutrients. However, it is highly susceptible to biochemical, physicochemical and microbial spoilage. The aim of the study was to use natural antioxidants in oregano and dill extracts in combination with modified atmosphere packaging MAP (CO₂:N₂:O₂:60:40) to retain the quality and delay lipid oxidation in Atlantic salmon (*Salmo salar*) during storage. Extract treated samples and controls (both vacuum packed and in MAP) were stored under chilled conditions (4±1°C) for 0-16 days. Quality changes during storage were assessed in terms of drip loss, microbial growth, colour, pH, protein solubility and lipid oxidation. Primary and secondary lipid oxidation products were determined by means of peroxide value, conjugated dienes and TBARS. In parallel, volatile compounds were analysed using GC-MS, SIFT-MS and SESI-MS. GC-MS indicated 29 recognizable VOCs present in the headspace of the salmon samples. SIFT-MS quantification was carried out for ammonia and the following VOCs: Ethanol, acetaldehyde, butyric acid, acetic acid, pentanal, hydrogen sulphide, trimethylamine and pentane. Changes of the measured concentration with storage time can be used to monitor freshness and spoilage and the effect of natural antioxidants in oregano and dill extracts can be observed.

AGFD009B 3551692 2:00 PM **Characterizing the volatolome of live-packed blue mussels (*Mytilus edulis*) stored under high-O₂ modified atmospheres** Susana Endah Ratnawati SusanaEndah.Ratnawati@UGent.be Modified atmosphere packaging (MAP) is frequently applied for living mussels in order to preserve their quality under refrigerated storage conditions. However, the shelf-life of these products is still very limited because of inevitable microbiological and (bio)chemical degradation processes. Combining optimized MAP conditions with efficient quality monitoring is thus of primary importance for their quality control. In the past, selected-ion flow-tube mass spectrometry has been successfully used for monitoring the real-time accumulation of spoilage-related volatile organic compounds (VOCs) in different seafood products; however, information about the volatolome of bivalves and its evolution under commercially realistic storage conditions is still limited in the scientific literature. The aim of this study was thus to characterize the VOC production in blue mussels (*Mytilus edulis*) as a function of storage time under different high-oxygen atmospheres (%v/v CO₂:O₂:N₂: 30/40/30, 40/60/0 and 0/60/40). SIFT-MS was used for quantifying 23 VOCs directly from the package headspace during up to 16 days at 4 °C. The results of the study showed that VOC production could be linked with the loss of viability and increase in microbial growth. Ethanol and sulfuric compounds became eventually dominating over storage time, greatly exceeding their human olfactory thresholds as well as the concentration ranges of the other quantified VOCs. These compounds are not only associated with offensive off-odors, but also widely recognized as seafood spoilage indicators. Real-time quantification of these compounds could thus be considered a promising way to monitor mussel quality under the tested conditions.

AGFD009B 3561490 3:10 PM **The emission of volatile thermal degradation products during the early stage of deep-frying: emission profile determination using PTR-TOFMS** Tomasz Majchrzak tomasz.majchrzak@pg.edu.pl Deep-frying improves digestibility and palatability of food. The aroma volatile compounds produced during frying include secondary oxidation products (SOPs) of fatty acids, such as saturated and unsaturated aldehydes. Release of these

compounds may pose health hazards due to their toxic nature and be indicative of thermal degradation of oils. The emission profile of SOPs can depend on many parameters, including the type of oil, frying time and temperature, and the type of fried food. Precise determination of the emission pattern, however, requires adequate measurement tools that enable true real-time analysis. This can be achieved using direct infusion mass spectrometry, e.g. proton transfer reaction time-of-flight mass spectrometry (PTR-TOFMS). The described study involved immersion of food in hot oil and measuring the changes of the amount of released thermal degradation products. It was possible to capture the sudden burst of SOPs at the time of food immersion, which is explained by the immediate emission of water vapour, which, as it is released from the oil surface, facilitates rapid release of volatile organic compounds. The role of crust formation on the emission of SOPs was also observed. The study also revealed a link between the emission of volatile compounds and the deterioration of oil quality, making it possible to estimate the degree of oil degradation with progression of frying, and the measurement itself is done without stopping the process and collecting an oil sample. Hence, using PTR-TOFMS, it is possible both to monitor the formation of SOPs and to identify the link between the degree of oil degradation and the emission of volatile compounds.

AGFD009B 3555988 3:00 PM **Shaken, not stirred – analysis of aroma compounds in alcoholic spirits through direct injection mass spectrometry** Jonathan Beauchamp jonathan.beauchamp@ivv.fraunhofer.de Conventional aroma compound analysis of alcoholic spirits by gas chromatography with mass spectrometric and/or olfactometric detection (GC-MS/O) requires a certain degree of prior sample workup, typically involving sample distillation and pre-concentration. Although this approach provides a comprehensive characterisation of aroma constituents in a sample, it is not suitable for screening a large number of samples within a easily manageable timeframe. Direct injection mass spectrometry (DIMS) techniques, such as proton transfer reaction time-of-flight mass spectrometry (PTR-TOFMS), offer a complementary approach to analysing constituent aroma compounds, with reduced sample preconditioning and rapid and immediate compound detection. In the case of spirits, however, the presence of ethanol in high abundance poses an analytical challenge due to reagent ion sequestration and a concomitant saturation of ethanol-related product ions in the reaction chamber. The use of a fastGC in combination with PTR-TOFMS, which exhibits rapid runs of ca. 1 min that do not compromise analysis time, overcomes this issue by achieving an early elution of ethanol and thereafter an ethanol-free matrix for subsequently eluting compounds. This analytical configuration can be enhanced by the use of a peripheral liquid calibration unit (LCU), which vaporises volatile constituents from aqueous solutions by use of a heated chamber and a nebuliser under a high-pressure gas flow. While the intended use of the LCU is to establish stable gas concentrations for calibration of PTR-TOFMS, it can be repurposed to vaporise volatile constituents in liquid samples, such as alcoholic spirits. The present work demonstrates the combined use of an LCU with fastGC-PTR-TOFMS to directly analyse and quantify predominant aroma compounds in different alcoholic spirits; shaken, not stirred.

TUESDAY MORNING 4/06/21 start 9:00 AM end 11:55 AM
Food Packaging Materials: Safety, Active Packaging, & Sustainability - Safety of Food Contact Materials
 AGFD007A 3536700 9:05 AM **Safety evaluation of food packaging materials: A regulatory overview of FDA's food contact substance notification (FCN) program** Raymond Brinas raymondpeter.brinas@fda.hhs.gov One of the public health responsibilities of the U.S. Food and Drug Administration (FDA) is to ensure the safety of the U.S. food supply. Within that scope, FDA

evaluates the safety of substances added to food (i.e., direct food additives) and food contact materials (i.e., food contact substances, FCSs). This presentation will focus on the premarket safety evaluation of FCSs through the food contact substance notification (FCN) process, a premarket approval process by which FDA regulates FCSs. The regulatory framework for the safety evaluation of an FCS, including considerations in the determination of the level of migration of an FCS to food, calculating consumer exposure, and safety assessment, will be discussed.

AGFD007A 3548797 9:00 AM **Screening and identification of chemicals migrating from paper and plastic food contact materials** Yelena Sapozhnikova yelena.sapozhnikova@usda.gov Over 10,000 chemicals are intentionally used in the manufacturing of food contact materials (FCMs). For many of these chemicals, information on their identity, potential migration into foods, and effects on human health is lacking. Identification of chemicals migrating from FCMs is a complex analytical challenge because of lack of public information on the substances used in manufacturing of FCMs, limited spectral databases for their identification, and unavailability of authentic analytical standards for their unambiguous identification. Non-targeted analysis with high-resolution accurate mass is advantageous to meet this challenge. The goal of this study was to investigate migration of chemicals from paper and plastic FCMs. Identification of migrated chemicals was performed with gas chromatography (GC) and liquid chromatography (LC) with Orbitrap mass spectrometry (MS) to identify a wide range of migrated chemicals with high confidence based on high resolution accurate mass measurement. Samples of paper-based FCMs (pizza boxes, butcher paper, liquid egg containers) and plastic FCMs (stretch film, storage bags, oven bags, meat trays and microwavable meals trays) of different brands were collected around the Philadelphia, PA area. Migration experiments were performed following the US FDA migration protocols regulating the length of migration, temperature, volume-to-specimen ratios and food simulants based on food packaging type and use. Migrated chemicals were identified with mass error <5 ppm using existing mass spectral libraries and databases (NIST MS library, ChemSpider, Extractable and Leachable high-resolution accurate mass database). Most of the identified migrants were associated with substances used in production of FCMs, i.e. common plastic additives, siloxanes, hydrocarbons, etc. However, other migrated chemicals were products and derivatives of commonly used food contact substances, and some were reported for the first time. Examples of identification and identified migrants will be presented. These findings are important to inform decision-makers of migrating chemicals to improve the safety of packaged food.

AGFD007A 3530508 9:00 AM **DART-MS methods development and validation for WEEE signatures in food contact polymers** Luke Ackerman Luke.Ackerman@fda.hhs.gov Recycling of polymers can reduce resource use and contamination. However, municipal waste streams struggle to maintain recycled polymer purity due to comingling & multi-polymer articles. Retail and or captive venues can supply higher purity recycled polymer. However, these niche streams will never close the post-consumer loop. Contract manufacture and spot purchases of recycled polymers risk unknown contaminants being incorporated into the final products. One example is brominated flame retardants (BFR) and waste electronic and electrical equipment (WEEE) in food contact articles (FCA). BFRs and WEEE components are not approved for food contact materials and need to be screened out. Methods to detect WEEE contaminants have used X-ray Florescence (XRF) of bromine, extraction GC-MS of BFRs, ICP-MS of rare-earth elements, and pyrolysis GC-MS for polymer degradants. If a rapid screening could be more specific for BFRs, inorganics or polymer mixes, then WEEE contaminated polymers could be identified and re-purposed sooner, recycled

polymer more easily and routinely tested, and contaminated food contact materials (FCM) could be identified. Direct Analysis in Real Time, a thermal desorption and chemical ionization source for mass spectrometry, (DART-MS) was used to evaluate over a dozen polymer samples (including FCAs) with known concentrations of various BFRs, polymers, and WEEE components. Similarly, pure resins, BFR-free formulations, pure WEEE standards, and new reference materials were analyzed. The DART-MS spectra of BFR and WEEE compounds, their transformations in samples and polymer reference materials, and their ion reactions were evaluated to develop the sensitive/selective ions for their detection, identification, and screening in FCAs. WEEE components, such as Antimony, were identified in WEEE contaminated polymers by DART-MS, and all BFRs in the samples were independently identified in the same samples by DART-MS.

AGFD007A 3530030 10:05 AM **Managing the safety of food contact materials through preventive engineering approaches and innovation** Olivier Vitrac olivier.vitrac@agroparistech.fr A new consensus is emerging between experts. Food contact materials are the primary sources of chemical contaminants in foods. The substances originate from materials in contact with food, but also from cross-mass transfer between all materials used during food production, handling, and distribution [1]. Generalized recycling and repeated use complexify the management of finished materials' safety exponentially. One decade ago, the broad adoption of conservative migration modeling contributed to reducing compliance testing costs in the EU, the US, and China. The presentation will offer an overview of preventive and safe-by-design approaches, supported by new generations of models from the molecular to the supply chain scale. Atomistic calculations alone or combined with proper molecular theories (Flory, hole free-volume) enable to predict the thermodynamic and transport properties of almost any substance [3-6]. Tested substances can only be hypothetical or suspected [7]. Bottom-up methods (FMECA: Failure Mode Effects and Criticality Analysis) adapted from the aerospace industry to mass transfer problems provide quantitative and comprehensive scores (severity) for systems as large as supply chains and recycling loops [8]. 3D evolutive design and multicriteria optimization are promising techniques to prototype safer, greener, and more efficient packaging [9]. Global problems will not be solved without strong interdisciplinary training and education programs. Seven European institutions are cooperating to create the first open-source and open-access platform covering all aspects of food packaging design [10].

AGFD007A 3551875 10:00 AM **Safety and regulatory compliance of plastic resins in the food packaging supply chain, a polymer manufacturer's perspective** James Graham james.e.graham@exxonmobil.com Presentation will highlight a polymer manufacturer's role on the safety and regulatory compliance of plastic resins in the food packaging supply chain. Topics to be discussed will include the qualification of incoming raw materials, good manufacturing practices, product certification, and the safety and regulatory compliance of plastic resins marketed for intended uses in food contact applications.

AGFD007A 3552498 11:05 AM **Sustainable packaging adhesives prepared with polysaccharide polyelectrolyte complexes** Wei-Shu Lin wzl5281@psu.edu While adhesives play an indispensable role in packaging, limited research has focused on the development of high-performance alternatives that are sustainable and compostable. In this research, polysaccharide polyelectrolytes were employed to form complexes (PPCs) to investigate the feasibility of PPCs as adhesives. Synthesizing parameters including pH, concentration and plasticizer content have been investigated and found to impact adhesive performance. Testing performed on paperboard suggests

optimized PPC based adhesives may be useful for a wide variety of packaging applications.

AGFD007A 3545802 11:00 AM **Film packaging or direct coating: Which is the better antimicrobial packaging method?** Tony Jin tony.jin@ars.usda.gov An antimicrobial packaging system encompasses any packaging technique used to control microbial growth in food products. Application of antimicrobial packaging can be in the form of film packaging or direct surface coating. The purposes for using antimicrobial film or coating are to inactivate foodborne pathogens and spoilage microorganisms present in food products, thus enhancing their safety and extending their shelf life. Either method has advantages and disadvantages. Antimicrobial film packaging must come into direct contact with the surface of food to exert an antimicrobial effect. The direct coating method may be more suitable for foods with irregular shapes or rough surfaces, where films cannot directly contact food surfaces without vacuum-packaging. However, preparation of coating solutions and coating/drying procedures might slow down production speed. In contrast, antimicrobial films can be customized within current film manufacturing lines, pre-made by a packaging company, and used as regular packaging materials. In this presentation, side-to-side comparisons will be used to evaluate the difference in antimicrobial effectiveness between antimicrobial films and coatings. For example, when 150 micro liter mustard oil with 1-gram chitosan was used to directly coating on grape tomatoes, 3.5 log reduction of Salmonella populations were obtained while similar reduction was achieved when 150 micro liter mustard oil released from a composite chitosan package film. However, 150 micro liter mustard oil encapsulated in 1-gram polylactic acid only reduced 0.5 log of Salmonella. These case studies discussed in the presentation will provide valuable information for researchers and food processors to make a choice for a suitable method based on their preference, convenience, availability, and cost effectiveness

TUESDAY AFTERNOON 4/06/21 start 1:00 PM end 3:55 PM
Food Packaging Materials: Safety, Active Packaging, & Sustainability - Active Packaging (Nanotechnology and Antimicrobial Polymer Systems)

AGFD007B 3552331 1:05 PM **Development of novel food coating materials based on chitosan, gelatin and jabuticaba (Myrciaria cauliflora) peel extract: rheological and morphological characterization** Mirella Bertolo mirella.bertolo@usp.br Chitosan is a natural and biodegradable biopolymer that can be associated with gelatin, a protein derived from collagen, in materials with potential application as food coatings. The aim of this association is to extend the shelf-life of foods, contribute to a smaller waste generation and minimize the worldwide use of plastic packaging. To improve the antioxidant and antimicrobial properties of these materials, the addition of plant extracts has been explored. The aim of this study was to evaluate the effects of jabuticaba peel extract (J) incorporation on the rheological and morphological properties of chitosan and gelatin-based materials. J was isolated by immersing jabuticaba peels in an acidified ethanolic (85 %, v/v) solution for 12 h. Chitosan (7.4 % acetylated) was obtained from squid pens (Doryteuthis spp.) and a 1 % (w/w) chitosan solution (C) was prepared by dissolution in 1 % (w/w) lactic acid. A 1 % (w/w) gelatin solution was prepared by solubilization in water at 60 °C (G). The polymers were mixed (1:1) and J ethanolic solutions (50%, v/v) were added at 0, 2.5 and 5 mg extract g⁻¹ of the mixture (CG, CG2J and CG5J samples). Furthermore, the component addition order was evaluated, since it can affect the materials final properties: J was first added to C, followed by combination with G (C2JG and C5JG samples). Rheological properties were investigated using a stress-controlled rheometer (AR – 1000N – TA Instruments). All materials exhibited pseudoplastic behavior and their initial viscosity decreased as J

concentration enhanced. An increase in viscosity values was observed when J was initially added to C. Materials were freeze-dried and their porosity was evaluated, ranging from 85 to 92 %. In conclusion, both rheological and morphological properties of chitosan/gelatin materials were affected by changes in concentration and order of addition of J, whereas concentration had stronger influence.

AGFD007B 3547849 1:00 PM **Visible-light-responsive graphitic carbon nitride/chitosan composite films for antimicrobial packaging** Hongchen Shen hongchenshen@gwmail.gwu.edu Food borne microorganisms, especially foodborne pathogens, result in significant illness and deaths. However, conventional food contact materials, such as plastic, paper, wood, stainless steel, etc., for food packaging are vulnerable to initial pathogen attachment and subsequent biofilm development. And numerous efforts for antimicrobial and anti-fouling food packaging suffer from low stability, high cost, loss of food taste, and leakage of bactericidal reagents. Herein, we propose to develop an antimicrobial food packaging material based on the visible-light-responsive graphitic carbon nitride (g-C₃N₄) and one earth-abundant biopolymer, chitosan. The antimicrobial potential of g-C₃N₄ against biofilms and planktonic bacteria under visible light irradiation has been well demonstrated in previous studies. After being incorporated into chitosan, a flexible polymeric composite film with promising antimicrobial effectiveness and robustness was achieved. Our study aims to understand the bactericidal mechanism of the composite under visible light irradiation and to seek opportunities to utilize the material for food packaging. g-C₃N₄ powder was first prepared via thermal polycondensation of melamine, cyanuric acid, and barbituric acid with an optimized ratio to achieve desired photocatalytic performance, and the powder was added to the chitosan matrix to fabricate the g-C₃N₄/chitosan composite. The properties of the composite were characterized by Brunauer-Emmett-Teller (BET) analysis, scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR). The results of confocal laser scanning microscopy (CLSM), SEM, and optical coherence topography (OCT) demonstrated that the composite material inhibited Staphylococcus epidermidis and Pseudomonas aeruginosa biofilms formation under the irradiation of visible white light emitting diodes (LEDs). Moreover, mature biofilms were removed from the surface of composite films after exposure to white LED light. The reactive oxygen species (ROS), i.e. singlet oxygen and superoxide anion radicals, identified during the photocatalytic process are believed to play an important role in biofilm inhibition and removal. In addition, the effectiveness of the composite material against the notorious foodborne pathogen, Escherichia coli O157:H7, is also very promising. Our study will have great impacts in food industry, by developing a new generation of antimicrobial food packages to protect public health.

AGFD007B 3554276 1:00 PM **Neem oil encapsulated electrospun polyurethane nanofibrous bags for seed storage application** Mrunalini Gaydhane ch15resch11008@iith.ac.in An ex-situ conservation of seeds is necessary to preserve the active germplasm of crops for longer period to protect their viability and longevity. The Indigenous seed storage systems causes considerable seed-grain losses which accounts nearly 1.3 billion tons worldwide. The primordial factors contributing in storage losses are nature of seeds, temperature and moisture which also promotes fungal or insect growth. Present research attempts to overcome the qualitative and quantitative seed storage losses by designing the polyurethane based nanofibrous bags containing uniformly distributed neem oil. The neem oil is a bio-pesticide effective over 600 species of pests

including insects, nematodes, fungi and viruses. While polyurethane has been chosen for its excellent mechanical and thermal properties along with water resistivity. The bags are fabricated by an easy and effortless technique called electrospinning. The material characterizations performed were, SEM, FTIR, TGA, contact angle, mechanical testing, water vapor transmission rate, and microbial assay. The as fabricated bags are hydrophobic, have high load carrying capacity and lower water vapor permeability due to their nano topography and the values are comparable to the commercially available bags. The real time application of as fabricated seed storage bags has been tested by storing seeds at normal room temperature and moisture conditions for 75 days and compared with commercial storage bags in terms of inhibition of seed borne fungi. The antifungal testing performed by incubating the stored seeds on Sabouraud Dextrose Agar infers that, less than 10% seeds from nanofibrous bags were infected with storage borne fungi, *Aspergillus niger*, whereas nearly 70% seeds were infected from commercial polypropylene bags.

AGFD007B 3555115 2:05 PM **Incorporating curcumin grafted cellulose nanofiber into chitosan films with strong and high UV barrier properties** Mingming Guo mingguo@zju.edu.cn Chitosan has attracted much attention for antimicrobial food packaging because of its unique antibacterial property and excellent film forming ability, however their poor barrier and mechanical properties limit the application. Thus, in this study, curcumin grafted cellulose nanofiber was applied to improve the mechanical and UV shielding properties. Modified cellulose nanofiber was obtained via grafting curcumin to TEMPO-oxidation cellulose, then bio-nanocomposite films composed of chitosan (100-67 wt%) and modified cellulose (0-33 wt%) were prepared by casting method. Infrared spectroscopy and X-ray photoelectron spectroscopy results indicated that cellulose was successfully modified. Scanning electron microscopy images and X-ray diffraction analysis showed that the addition of modified cellulose noticeably affected the morphology and crystal structure of the composite films. Moreover, the appropriate proportion of modified cellulose improved the oxidation resistance, tensile strength and UV barrier properties compared to pure chitosan films. It is also worth mentioning that the composite films maintained equivalent antibacterial activities incorporating with modified nanocellulose, although the ratio of chitosan was decreased. Furthermore, the water solubility of films decreased with the addition of modified cellulose nanofiber. It is concluded that curcumin grafted cellulose nanofiber significantly improved the mechanical and UV barrier properties of chitosan films. The findings in this work would provide useful information for application of chitosan in food packaging

AGFD007B 3530746 2:00 PM **Use of lipid nanoemulsion-doped anti-fungal packaging films to control postharvest disease in small fruits** Valentina Trinetta valentina.trinetta@gmail.com Postharvest losses can occur anywhere from harvesting to handling and shipping. In 2014, approximately \$30 billion of fresh produce were lost in the United States food supply chain. In particular, small fruits shelf-life can be reduced by weight loss, stem scar injury, gray mold and ripe rot. It is important therefore find sustainable packing alternative to protect produce, increase shelf-life, minimize waste and preserve resources. Purpose: The objective of this study was to evaluate the mechanical, physical and anti-fungal properties of packaging films loaded with essential oil (EO) nanoemulsions. Methods: Food-grade emulsions with sub-micron droplets were used to encapsulate cinnamaldehyde (CY), eugenol (E) and thymol (T) within a refined coconut oil (carrier) in pullulan packaging systems (formulated in a previous work). Different film combinations (5 - 10% Pullulan, 1 - 2 % EO, 0 - 50 % water, 0.5 - 1 % gum concentrations) loaded with EO nanoemulsions were investigated. Tensile strength, moisture content and antifungal activity against

Rhizopus stolonifer, *Alternaria* spp. and *Aspergillus niger* were measured and compared to control pullulan systems. Results: A lower tensile strength ($P > 0.05$) was measured for combinations loaded with EO nanoemulsions as compared to films without active lipid solutions: 5.7, 7.9, 6.8 and 17.1 MPa for CY, E, T and control system, respectively. Nevertheless, the active combinations presented good elasticity and ductility. Active films moisture contents were lower as compared to film without EO ($P < 0.05$). The control formulations showed no antifungal activity. Conversely, active combinations exhibited significant inhibition zones ($P < 0.05$). Film containing CY had the biggest inhibition halos: 13.7, 15.7 and 14.5 mm were measured against *R. stolonifer*, *Alternaria* and *A. niger*, respectively. Significance: This study demonstrates the potential application of pullulan packaging films loaded with EO nanoemulsions as a mean of controlling and reducing postharvest disease in small fruits during shipping and storage.

AGFD007B 3557428 3:05 PM **Antiviral and bacteriostatic evaluation of chitosan-based films embedded with grape seed extract against murine norovirus, *Escherichia coli* and *Listeria innocua*** Melvin Pascall pascall.1@osu.edu This study developed and evaluated edible chitosan films impregnated with grape seed extract (GSE) and tested their antimicrobial activities against murine norovirus (MNV-1), *Listeria innocua* and *Escherichia coli* K12. During the study, GSE at 1, 1.5, 2.5 and 5%, and at 5, 10 and 15% concentrations were tested in the film forming solution and then in the films, respectively. Results showed that the 1, 1.5 and 2.5% GSE solutions caused MNV-1 plaque reductions ($p < 0.05$) of 1.75, 2.60 and 3.58 log PFU/ml, respectively after 3 h. For the 2% (w/w) chitosan solutions with 2.5 and 5% GSE, the MNV-1 titers had reductions ($p < 0.05$) of 2.68 and 4.00 log PFU/ml, respectively, after 3 h. When the GSE was incorporated into the chitosan films the results showed significant reductions against MNV-1, *L. innocua* and *E. coli* K12. For the 5, 10, and 15% GSE in the chitosan films, MNV-1 reductions of 0.92, 1.89 and 2.27 log PFU/ml, respectively were obtained after 4 h incubation. After 24 h incubation, the 5 and 10% GSE films produced 1.90 and 3.26 log PFU/ml, respectively, while the 15% GSE film reduced MNV-1 to undetectable levels. When *E. coli* K12 was tested, the results showed reductions of 2.28, 5.18 and 7.14 log CFU/ml after 24 h exposure to the 5, 10, and 15% GSE films, respectively. For *L. innocua*, bacterial reductions of 3.06, 6.15 and 6.91 log CFU/ml were obtained by the 5, 10 and 15% GSE films, respectively. This study illustrated that GSE has potential for use as an antiviral and a bacteriostatic ingredient in edible films and coatings that could be used in various food packaging applications. Since the GSE showed significant effectiveness against these organisms in the film forming solutions, it may have antiviral and bacteriostatic potential as a food additive.

AGFD007B 3529901 3:00 PM **Antimicrobial active packaging synthesized by reactive extrusion of polypropylene and polylysine, a natural antimicrobial** Noah Doshna nad66@cornell.edu Active packaging technologies have shown significant progress in recent years in improving food quality and safety. Yet, a lack of commercial success highlights the need for new and translatable active packaging technologies. This study employed reactive extrusion, a process that alters common polymers through compounding or cross-linking functional compounds to provide desired characteristics. A novel antimicrobial packaging was synthesized through reactive extrusion of polypropylene and ϵ -pol-L-lysine, a natural antimicrobial. ϵ -pol-L-lysine was grafted onto the polypropylene base polymer using a dicumyl peroxide catalyst in a twin-screw extruder. Fourier transform infrared spectroscopy, x-ray photoelectron spectroscopy, scanning electron microscopy, and contact angle measurements were used to characterize film surface chemistry. No changes in hydrophobicity of the polymer surface were observed in contact angle measurements,

suggesting the polymer still allows for the free flow of liquid or semi-liquid foods. The presence of hydrophilic amine groups, indicated by increased absorbance at 1650-1580 cm, was confirmed via Fourier transform infrared spectroscopy. A high degree of correlation ($R^2 > 0.999$) was found between amine density (39.7 nmol/cm^2), determined through an acid-orange 7 assay, and total protein ($12.67 \text{ } \mu\text{g/cm}^2$), determined through a bicinchoninic acid assay, when converting amine density to protein density. This correlation shows that the antimicrobial is evenly distributed by the extrusion process, and amine groups emerge largely unaltered by the process, a key factor in retaining antimicrobial character. Antimicrobial activity towards spoilage microbes was characterized by the effect of films on the density of *Lactobacillus plantarum*, a common food spoilage organism. The polymer achieved a 2-log reduction against *Lactobacillus plantarum* compared to untreated polypropylene. This novel polymer, produced through scalable technology, shows promise as a new form of active packaging, to improve food safety & reduce food waste while meeting consumer demands for cleaner labels.

TUESDAY AFTERNOON & EVENING 4/06/21

start 5:00 PM end 7:55 PM

Food Packaging Materials: Safety, Active Packaging, & Sustainability - Sustainability to Reduce Food Waste (Active Packaging)

AGFD007C 3538940 5:05 PM **Overcoming technical hurdles to translation of active packaging technologies** Julie Goddard goddard@cornell.edu The increasing volume of food wasted due to spoilage represents an emerging threat to the environmental and economic sustainability of our food system. Approved food additives can be added to products to help retain quality and safety, yet there is a widespread effort to remove such additives to address Clean Label demands, which is likely to result in an unintended increase in food wasted due to spoilage. Much proof-of-concept research has demonstrated that active packaging technologies may enable removal of additives without the typical corresponding loss in product quality. While promising, there remain translational hurdles in technology development and stakeholder acceptance that have prevented successful commercialization of most proposed active packaging concepts. Herein we describe research designed to overcome technical hurdles to scalable production of active packaging materials. Techniques such as laminated photografting, emulsion polymerization, and reactive extrusion have been developed with the end goal of producing a thermoplastic active packaging material capable of converting to standard packaging formats on existing equipment. The resulting active packaging materials can support addressing converging consumer demands of additive removal and reduction of food wasted due to spoilage

AGFD007C 3553146 5:00 PM **Natural polymer based electrospay for active food packaging: A study of water soluble yellow mustard mucilage** Ying Wu ywu@tnstate.edu Electrospay is an emerging technology with a low cost, non-thermal and simple process. It can produce functional nano- and microparticles embedded with bioactive components for antimicrobial or/and antioxidant purposes to extend product shelf life. Natural polymers are attracting increasing attention for fabrication of packaging materials due to their biodegradability, biocompatibility, and sustainability. Innovative approaches have recently been introduced for electrospay and electrospinning of natural polymers, including coaxial electrospay and emulsion electrospay assisted with a commercially available microfluidizer. Emulsification approach can encapsulate immiscible compounds with better efficiency, stability, and with a controlled release profile. Material properties such as molecular weight, morphology, viscosity, surface tension and tendency to form a gel have been reported to be of key

importance in electrospay. In the current study, a novel ingredient, water soluble yellow mustard mucilage from yellow mustard bran, were isolated and used together with starch for electrospay. A type of essential oil, carvacrol, was used as a model core component. Two objectives have been achieved: 1. Fabricate micro and nano-particles using electrospay of WSM and starch; 2. Evaluate physicochemical and functional properties of the fabricated materials. Emulsions were prepared using microfluidizer at a pressure of 10,000 psi with the droplet size ranged from 100-500 nm with various concentrations of starch WSM and carvacrol. Scanning electron microscopy was utilized to evaluate the particle properties. Antimicrobial properties of the fabricated particles were evaluated using *E. coli* and *S. aureus* assays. The results indicated that all the carvacrol embed particles exhibited antimicrobial and controlled releasing properties. Further studies will be carried out to optimize the formula of the nano/micro- emulsion, and the effect of antimicrobial and shelf-life prolonging properties after addition of multiple bioactive components in the materials.

AGFD007C 3530102 5:00 PM Modified atmosphere packaging

for small fruit with or without slow-release disinfectants to enhance postharvest quality and safety Jinhe Bai jinhe.bai@usda.gov Commercial (COM) packaging used for small fruits, such as sweet cherries and grape tomatoes, have been designed with wide openings, and therefore cannot benefit from modified atmosphere packaging (MAP) and humidity control. This research was aimed to replace the COM clamshells by a modified humidity (MH) clamshell which has fewer and smaller openings and that can reduce water loss and maintain small fruit quality without excessive change of oxygen and carbon dioxide levels, which can be harmful to fruit quality. The in-package water condensation may be an undesirable factor in marketing even without decay. Controlled-release chlorine dioxide, carvacrol and thymol were developed, and showed substantial capacity to control pathogenic and spoilage microorganisms when MH clamshells were used. In COM clamshells, the redundant venting leads to insufficient accumulation of the active gas in the headspace

AGFD007C 3553745 6:05 PM Antioxidant, free radical scavenging activities and efficacy as bio-control agent of Calotropis procera in food safety Devendra Kumar

devendranagar14@gmail.com In general organophosphates and carbamates pesticides are used at very high doses for pest management as an effective strategy to protect food and other agricultural crops. Synthetic pesticides also pose serious threats to the environment and non-target organism. As an alternative safe strategy natural bio-pesticide based on phytochemicals as active ingredients obtained from plants hold a viable option and being popular due to their eco-friendly and non-toxic properties. *Calotropis procera* is a weed known for its high medicinal properties in Indian system of medicine for the treatment of various ailments. Its antioxidant and free radical scavenging activities followed by bio-efficacy of methanol, hexane and chloroform soluble extracts were studied to explore their potential for pest control in food crops and assure food safety. Total phenolic contents were ranging from 25.6 to 39.4 mg/g gallic acid equivalent (GAE), antioxidant 45.6 to 67.4% and free radical scavenging activity by using DPPH (1,1-diphenyl-2-picrylhydrazyl) varied from 35.8 to 39.6 %. The extract showed potential insecticidal efficacy against experimental pest at 16.7% at 0.007 % lowest dose and 63.3% at 0.5% highest dose. Further, hexane highest (66.7%) at 0.5% and chloroform fraction showed highest (66.7%) mortality at 0.5% dose. The LD_{50} and LD_{90} data obtained for crude extract 0.080 and 9.411 % at fiducial limits of 0.026 to 0.485 and 1.027 to 18.147 respectively. The methanol extracts of aerial parts and their fractions were also screened alone and in combination to assess their insecticidal properties. The combination (1:1) of *Calotropis procera* and

Lantana camara extracts showed synergistically enhanced (2.5 fold) activity. Application of plants in particular weeds as free radical scavenger and bio-control agent in the management of pest in food safety will be presented.

AGFD007C 3554098 6:00 PM **An ent-abietane diterpenoid from the North American plant Stenotus armerioides inhibits the growth of the foodborne pathogen listeria monocytogenes** Yanhong Liu yanhong.liu@ars.usda.gov Antimicrobial compounds isolated from plant extracts showed promise for food safety since they are generally regarded as safe (GRAS). Listeria monocytogenes is a foodborne pathogen of public concern due to the high mortality rate associated with listeriosis. In this study, over 1000 plant extracts were screened for the inhibition of the growth of L. monocytogenes. A plant extract from Stenotus armerioides (Thrift mock golden weed) was identified with significant antimicrobial activity. The plant extract was further fractionated and a compound (abieta-7,13-dien-18-yl succinate) from the extract was purified, identified, and characterized. The Minimal Inhibitory Concentration (MIC) of this compound was 32.5 µg/ml, which is comparable to the known antibiotics used in clinical studies. To further confirm this result, the compound was synthesized and tested. The synthetic compound showed the same antimicrobial activity as the compound purified from plant extract. Results from Ames tests showed that this compound has no mutagenic activity. This compound did not show antimicrobial activity against other pathogens that were tested. Taken together, our results showed that thrift mock golden weed extract has the potential to be used as a sanitizer or in packaging material in the food industry to control L. monocytogenes

AGFD007C 3556096 7:05 PM **Formulations of anti-browning and anti-Listeria coating to maintain freshness and microbial safety of fresh-cut apples** Xuotong Fan xuotong.fan@usda.gov Fresh-cut apples have become popular in recent years, being carried in major chain restaurants and supermarkets. To control browning and maintain freshness of fresh-cut apples, the fresh produce industry employs dipping solutions, mainly an ascorbic acid-based formulation applied by either submerging or spraying. However, the anti-browning solutions do not have any antimicrobial property, and can be contaminated with Listeria monocytogenes, a human pathogen causing miscarriage and other serious diseases. As a result, there have been a number of fresh-cut apple recalls due to contamination with the pathogen. Therefore, formulations that have both anti-browning and anti-Listeria activities are needed to address both freshness and microbial safety of cut apples. Over the last few years, several formulations that are capable to inactivate Listeria in anti-browning solutions and on cut apples while inhibiting surface browning of the fruit have been developed. Those formulations involve combinations of natural antimicrobials and antioxidants such as organic acids, amino acids, alcohols, and ascorbate. For example, a formulation comprised of citric acid, ascorbic acid and L-acetylcysteine in the ratio of 2/2/1 was able to reduce L. monocytogenes populations by 5 logs, and maintained the shelf life of fresh-cut apples by 21 days at 4°C. Future research direction will be discussed to further improve the safety and quality of cut fruits.

AGFD007C 3556328 7:00 PM **Antimicrobial packaging to control postharvest decay and retain fruit quality of fresh fruits** Chang-Lin Xiao Chang-Lin.Xiao@ars.usda.gov Postharvest decay caused primarily by fungal pathogens results in significant losses of fresh fruits during storage and transit and in the market. Controlling postharvest decay and maintaining fruit quality is important to consumers' acceptance and the profitability of the fresh fruit industry. In this presentation, the use of antimicrobial packaging with or without modified atmosphere (MA) to control postharvest fruit decay and maintain fruit quality of fresh fruits is presented. In our research

on blueberries, sulfur dioxide-emitting packaging pads, liners, sheets, or bags with MA capability were evaluated for the effectiveness in controlling decay, reducing water loss, and maintaining fruit quality. In one study, Dual SO₂-emitting pad (SO₂ was initially released up to 10 ppm and then declined and stabilized at a low concentration), Slow SO₂-emitting pad (SO₂ was released at a low and constant concentration), or MA bag alone significantly reduced fruit rots during cold storage compared to nontreated control. Dual SO₂ pad in combination with MA bag or Slow SO₂ pad in combination with MA bag provided even better control, but Dual SO₂ pad can cause bleaching on blueberry fruit due to SO₂ injuries. In another study, SO₂-emitting liners with modified atmosphere capability was effective in reducing fruit rots, reducing water loss and maintaining fruit quality. Our results showed that the combination of Slow SO₂-emitting pad and MAP bag is a promising method for control of postharvest fruit rots while maintaining blueberry fruit quality and that SO₂-emitting liners are also an effective means of preserving blueberry quality during extended storage, particularly when combined with MA. The simplicity of assembling a package with a single liner versus using a conventional liner followed by a SO₂-emitting sheet or pad could be of benefit to blueberry packers. Challenges and prospects of antimicrobial packaging for fresh fruits will also be discussed.

WEDNESDAY MORNING 4/07/21 start 9:00 AM end 11:40 AM
Beyond Chemistry: Consumer Acceptance of Flavor, Food Safety & Health Benefits of Fruits and Vegetables - Genomics Assisted Breeding/Region & Cultivar Specific Melons

AGFD011A 3557221 9:05 AM **Fruit quality of new melon hybrids from the Texas A&M breeding program** Kevin Crosby k-crosby@tamu.edu In order to assess the contribution of 12 elite muskmelon inbred lines to fruit quality attributes, 34 F1 hybrids and the parents were planted at Uvalde, Texas while a subset was planted at College Station, Texas in 2019. All plants were grown with commercial practices, drip irrigation, black plastic mulch, at 12 inch spacing in the rows. All plots were established by transplanting 5-week old seedlings. Fruit were harvested from 3 replicated plots at full maturity. Fruit size, firmness, abscission zone size, flesh thickness and total soluble solids were recorded. Data was subjected to analysis of variance to determine any significant differences among the hybrids and to high parent heterosis values were calculated for the Uvalde data. At Uvalde, hybrids 19x65, 26x96, 52x96 and 26x65 all had high brix of 11-12 and medium orange flesh color. Hybrids 19x65 and 26x96 also had very firm flesh with 77 N and 91 N, respectively. Hybrids 19x65 and 52x96 had thick flesh, and almost no air space in the seed cavity. Hybrids 19x65 and 26x65 both evinced high parent heterosis for brix, while hybrids 26x96 and 52x136 expressed heterosis for flesh firmness. At College Station, hybrids 19x65, 40x65, 52x70, and 52x136 all had fruits with average brix of 12, while 52x96 fruit averaged 14 brix. Average flesh firmness was greatest in 52x96 (105 N) while 26x96 (95 N) fruit were also very firm. Both of these hybrids also had very good flavor compared to the firm-fleshed commercial check, Infinite Gold. The hybrids 19x65 and 52x70 were early to mature fruit, 7 days before the other entries. All of these hybrids will undergo further trials in multiple regions of the U.S. to determine the top 3 for release as new muskmelon cultivars.

AGFD011A 3556105 9:00 AM **Variety evaluation of yield and quality for two types of melons** Joara Candian candian@uga.edu In Spring 2018 and 2019, eight varieties of cantaloupe (Cucumis melo var. cantalupensis) and honeydew (Cucumis melo (Indorus Group)) were evaluated for yield and quality characteristics in Tifton, Georgia. This variety trial was part of a larger nationwide trial that

evaluated the impact of the environment on the variation of quality traits in melons as well as the ability of human pathogens to adhere to the surface of melon fruit. Melons were planted on March 27, 2018 and April 3, 2019, and grown using plastic mulch and drip irrigation following standard practices for the region. The trial was a randomized complete block design with four replicates. Fruit was harvested 66 days after transplanting (DAT) in 2018 and 78 DAT in 2019 and individually weighed to get size classifications. Fruit from a representative harvest was analyzed for rind thickness, firmness (8 mm probe), total soluble solids, seed cavity area, and netting pattern. In 2018, 'Athena' which is an industry-standard was the highest yielding cantaloupe (37,818 kg/ha⁻¹), though it was not significantly different from 'Aphrodite' (36,741 kg/ha⁻¹), 'Infinite Gold' (35,945 kg/ha⁻¹), and 'DaVinci' (27034 kg/ha⁻¹). 'Athena' had the highest yield of 9-count fruit and average fruit weight of 1.9 kg. 'Infinite Gold' and 'DaVinci' were had the highest flesh firmness ratings, while F-39 had the lowest firmness of all fruit. 'HD252' was the highest yielding honeydew, with a yield of 38,433 kg/ha⁻¹. In 2019, despite 'Athena' had the highest yield, there was no difference from the other cantaloupe varieties for total yield (average of 47,026 kg/ha⁻¹). 'Athena' was the highest average fruit weight of 2 kg, though it was not significantly different from 'Samoa' (1.7 kg) and 'Infinite Gold' (1.7 kg). 'Samoa' (12.5 °Brix) and 'DaVinci' (12.4 °Brix) were had the highest soluble solids, while 'Infinite Gold' (3.4 kgf) and 'DaVinci' (3.9 kgf) had the highest flesh firmness ratings. 'HD252' was the highest yielding and flesh firmness ratings honeydew variety, with a yield of 77,639 kg/ha⁻¹ and 3 kgf. Overall, our data suggest that current industry standards are performing adequately in terms of yield and quality; however, new varieties may offer improved characteristics for food safety purposes.

AGFD011A 3557488 9:00 AM **Melon cultigens and their adaptation** in the southeastern United States when grown in North Carolina Jonathan Schultheis jonathan_schultheis@ncsu.edu Melon cultigens (cultivars and advanced lines) were evaluated in 2018 and 2019. In 2018, 24 entries were evaluated, 8 from seed companies and 6 from Texas A&M Univ. Entries were mainly orange flesh types (22). In 2019, 18 entries were evaluated, 7 from seed companies, and 11 from Texas A&M Univ. As in 2018, most entries were orange flesh, the exceptions being HD150, HD252 and USAM16203 (green flesh) and SFR3079 and SFR3083 (white flesh). In both studies, the Athena cultivar was used as the standard since it is the most grown and marketed cultivar in the region. Transplants were set in the field 21 and 2 May in 2018 and 2019, respectively. Each plot consisted of 10 plants and cultigen treatments were replicated four times and arranged and analyzed as a randomized complete block design. Harvests began 9 July and ended 3 August totaling 12 harvests in 2018. Harvest started 24 June and ended 26 July totaling 14 harvests in 2019. Each fruit was harvested and weighed when ripe, and soluble solids and flesh firmness were obtained from 5 fruit per replication for each entry. In 2018, highest total fruit yields over 12 harvests (>23,465 fruit/ha) were obtained with SVM 2690, Master's Choice, Oui, DaVinci, Electra, and USAM14836 cultigens. Average cumulative yield across all 24 cultigens was 19,970 fruit/ha. Athena, the standard cultigen yielded 16,947 fruit/ha. Average fruit size across cultigen entries was 2.4 kg. All of the highest yielding cultigens had average fruit weights less than 2.0 kg. Soluble solid values were high for most cultigens and averaged 11.8. Highest values were obtained with SVML2690 (13.6), Katza (13.2) and DaVinci (13.1), while the lowest cultigen values were Master's Choice (9.3) and USAM16155 (9.7). In 2019, the highest cumulative yields (>30,875 fruit/ha) over 14 harvests were obtained with SFR3079, TH6, SFR3083, TH3, F39 and DaVinci. At least 30% of the cultigens that yielded the highest fruit number per

acre were in the less than 1.4 kg category, with SFR 3079 and TH6 producing at least 60% of their fruit in that size category. Fruits less than 1.4 kg is considered too small for orange flesh melons sold in the eastern U.S. markets. Melons which are specialty white flesh types potentially could be sold as a smaller sized melon. Athena cultivar averaged 2.2 kg per fruit. Most Texas A&M cultigens had relatively small sized fruit compared with Athena. TH3 fruit (1.8 kg) had the most comparable size to Athena with high soluble solids (13.0).

AGFD011A 3551263 10:00 AM **Environmental and genotypic variation of fruit yield and quality traits in melon in south Texas** John Jifon jljifon@ag.tamu.edu This study characterized the contributions of genotype, environment, and their interactions on variations in the fruit yields and quality traits for six cultivars of melon (Cucumis melo L.; cv 'HoneyDew 252', 'HD150', 'OC164' 'DaVinci', 'Infinite Gold', and 'Chujuc') and evaluated the stability of these traits across environments. Field experiments were conducted during the 2018 and 2019 spring growing seasons at two locations in Texas (Uvalde and Weslaco) using a randomized complete block design with four replications in each location. Main and interactive effects of treatments on total and marketable yields, average fruit weight, soluble solids content (SSC), and fruit firmness were measured. The genotype × environment effect was significant for total and marketable yields, and SSC, but not for average fruit weight or fruit firmness which varied by the main effect of genotypes. Marketable fruit yield ranged from 25.7 to 56.2 t/ha and was largely influenced by genotype (63.2% of the total sum of squares variation) versus 4.8% by environment, and 11.2% by the genotype × environment interaction. SSC varied from 9.0 to 13.6% and was explained by 15.4, 21.1, and 31.7% of the environment, genotype, and their interactions, respectively. The Mean vs. Stability view for genotype plus genotype-by-environment (GGE) biplot analysis indicated that 'Honeydew 252' (50.9 t/ha) and 'HD150' (46.9 t/ha) had higher mean marketable fruit yield but appeared less stable than 'DaVinci' (31.6 t/ha) or 'Chujuc' (30.0 t/ha). 'Infinite Gold' was the most stable with yield (41.8 t/ha) just slightly higher than the grand mean (40.6 t/ha). The GGE biplot analysis also indicated that both 'DaVinci' and 'HoneyDew 252' had higher SSC values (average 12.2 %), however, 'DaVinci' showed the highest stability across environments. These results indicate that 'Honeydew 252' was the most resilient cultivar in terms of productivity and quality across the two environments.

AGFD011A 3548441 10:00 AM **Wild relatives of melon** (Cucumis melo L.) as potential source of bioactive principles. Chidambara Murthy kncmurthy@gmail.com Cultivating crops from more natural habitats, such as wild types, can help maintaining biodiversity and sustainable agriculture. Identifying and characterizing wild relatives of melons, and providing genetic materials for crop breeding, play a vital role in agriculture. The current study was focused on characterization of a diverse set of wild relatives of melon (Cucumis melo L.) to understand the possible nutrition and explore the health benefits. Four wild types namely Putti kaayi (acidulous), Budamekaayi (kachri), Small melon (callosus), and an unknown botanical type collected from different parts Karnataka state of Southern India. All the four types were used in the study to identify major human health properties. The total sugar content in these ranged from 25-54 mg/ 100 g fresh weight and the range of reducing sugar was 0.67-1.47 mg/ 100 g fresh weight indicating these are non-sweet. The Total soluble solid content was 4.02-3.29 °B and titrable acidity was 0.22- 0.24 %. All four samples showed ascorbic content of 34.5 ± 2.0 mg/ 100 g fresh weight and total polyphenols content was 18 mg/ 100 g fresh weight in case of kachri and callosus. The average total carotenoid content among four group of samples was 5.0 ± 1.2 µg/ g fresh weight. Both kachri

and callosus exhibited 80 ± 2 % radical scavenging activity at 100 ppm concentration as measured by DPPH assay. The nitric oxide (NO) scavenging activity was 63.59 (acidulous), 87.16 (unknown botanical type), 71.69 (kachri) and 82.34% (callosus), respectively at 200 ppm concentration. Additionally, all the four samples exhibited more than 50% ACE inhibition activity at 100 ppm indicating they can serve as potential source of bioactive principles and can be a part of healthy diet. Details of these results will be discussed in comparison with some of the reference bioactive molecules in the presentation.

AGFD011A 3554821 10:00 AM **Assessment of carotenoids and sugars contents in melon cultivars harvested from five different locations in the United States** Jashbir Singh jashbirsingh@gmail.com Melons (*Cucumis melo* L.) are an important commercial fruit crop with global popularity due to their numerous retail and consumer preference attributes such as sweetness, flavor, flesh color, nutrition and health benefits. Melon quality traits such as appearance (color) and health attributes are related to their carotenoid contents. Most melon cultivars contain a wide array of carotenoids which are responsible for the distinctive flesh (mesocarp) colors. Besides genetic makeup, carotenoid and sugar accumulation are strongly influenced by management and environmental factors such as production location, soil characteristics, etc. A better understanding of the role of these factors on carotenoid content and composition is important for fruit quality improvement through genetics. In the current study, we characterized carotenoid and sugar contents in different melon cultivars grown in five different locations in California, Texas, Georgia, Arizona, and North Carolina (U.S.A). Mesocarp sugar (sucrose, glucose and fructose) and β -carotene concentrations varied significantly as a function of production location and variety. Among the cantaloupe (western shipper) varieties grown in North Carolina had higher total sugar contents compared to the other cultivars. A significantly higher concentration of β -carotene was observed in Tuscan type (Da Vinci) grown in Texas and Georgia than in fruits grown elsewhere. The Casaba type (TAM Orange Pacal) grown in Texas had significantly higher β -carotene levels compared to other locations and cultivars. While some of the location effects may be due to crop husbandry, they also highlight the impacts of weather conditions and edaphic factors. The data also highlight the stability of key quality attributes such as sweetness and appearance across various environmental conditions. This study demonstrated that growing location had a significant influence on the phytonutrient contents, which should be considered for the selection and improvement of melon varieties rich in sugars and carotenoids.

AGFD011A 3531102 11:00 AM **RNA-sequencing analysis to study transcriptomic profile changes during melon fruit development** Xiaoning Qian xqian@ece.tamu.edu In order to understand the dynamic molecular changes during fruit development for different melon varieties, the research team has harvested melons at different maturing stages and different locations. RNA-sequencing (RNA-seq) data has been collected from both leaf and fruit samples. In this presentation, we review the challenges of analyzing such a complex RNA-seq dataset for extracting meaningful knowledge about melon fruit development. We have developed a bioinformatics analysis pipeline for analyzing RNA-seq data with complex temporal and spatial confounding factors, which can help detect dynamic changes in transcript profiles with the integrative analysis of metabolites to characterize melon fruit development.

WEDNESDAY AFTERNOON 4/07/21 start 1:00 PM end 4:00 PM
Beyond Chemistry: Consumer Acceptance of Flavor, Food Safety and Health Benefits of Fruits and Vegetables - Sensorial Qualities and Microbial Decontamination of Melons

AGFD011B 3557635 1:05 PM **Relationships between descriptive and consumer sensory attributes of melons** Rhonda Miller rmiller@tamu.edu Production characteristics have been used to develop melon varieties and have not incorporated flavor and texture attributes and consumer liking as components of selection. Our objective was to develop descriptive melon flavor and texture attributes and understand their relationship to consumer melon liking. Melons and 2 honeydew varieties were planted in 7 US locations (Arizona, California, North Carolina, Georgia, Indiana, Uvadle TX and Weslaco, TX) over 3 years. Whole and cut melon appearance, aroma, flavor, and texture were evaluated using an expert trained descriptive sensory panel. Additionally, consumers evaluated liking for appearance, aroma, flavor, texture and overall liking using 9-point hedonic scales. Whole melon appearance and aroma liking were not closely associated with cut melon consumer liking. However, cut melon consumer liking attributes were very closely related. Melon identity, overall sweet, sweet and honey descriptive attributes were closely associated with cut consumer liking attributes. Hard melons with musty/earthy, green, bitter, and sour descriptive attributes were negatively related to consumer liking. Juicy melons with more surface moisture and higher levels of overripe and fermented flavors were preferred by consumers to a greater extent than melons that were hard and had with sour, musty/earthy, green, and bitter descriptive attributes. In conclusion, melon descriptive flavor and texture attributes can be used to assess attributes to improve melon consumer liking and selection of melons with positive flavor and texture attributes are a tool for use in development of advanced melon varieties.

AGFD011B 3549538 1:00 PM **Consumer willingness to pay for melon cultivars** Ruixin Jia rjia@tamu.edu Melon cultivars may develop different characteristics under different regional environmental conditions. Consumer purchase satisfaction revealed by willingness-to-pay (WTP) may also differ from consumption satisfaction in sensory scale measures. We investigate consumer's WTP of different melon varieties using a two-stage non-hypothetical Vickrey second-price auction on appearance of the whole melons and taste. Meanwhile, we measure consumer sensory satisfaction using a 9-point scale evaluation and a 15-point expert flavor and texture descriptive sensory evaluation. We recruited around 580 subjects from the general population and conducted economic auction experiments and sensory surveys for over 10 melon cultivars from 7 regions (6 states, two regions located in Texas). We find that the consumers' WTP elicited from auction experiments is consistent with the sensory panel analysis. No one variety obtained the highest WTP across all the study regions. Instead some varieties seem to perform better agronomically and also have higher acceptance by the tasting panel and consumers. In particular, commercial Tuscan type (Davinci, TT-DV) produced the highest WTP across several U.S. States. Sensory attribute evaluation scores show that TT-DV is one of the cultivars liked by a large proportion of consumers with sensory descriptive attributes, such as overall liking, cut appearance, and sweetness.

AGFD011B 3554762 1:00 PM **Aroma volatile profiles of cantaloupe (*Cucumis melo* var. *cantalupensis*) from different cultivars grown in five locations in the United States** Rita Metrani ritametrani@tamu.edu Cantaloupe fruit (*Cucumis melo* L. var. *cantalupensis*) is highly valued for its sweet and refreshing flesh; however, the flavor is highly influenced by aroma, which is dictated by volatile organic compounds. Gas chromatography-mass spectrometry (GC-MS) is widely used to identify and quantify volatile compounds at the picogram levels. Using our optimized GC-MS-solid phase microextraction (SPME) method, we performed a multi-location trial for cantaloupes planted in 2019 and grown using uniform management practices in California, Arizona, Texas,

Georgia, and North Carolina. The study included two varieties Western Shipper (F-39) and Tuscan type-Da Vinci (TT-DV) and six hybrids (TH1, TH2, TH3, TH4, TH5 and TH6). Our GC-MS-SPME identified and quantified 167 volatile compounds including esters, alcohols, aldehydes, ketones, sulfur-containing compounds, acids, furans, and hydrocarbons. The aroma compounds ethyl hexanoate, ethyl butanoate, ethyl 2-methylbutanoate, 2-methylbutyl acetate, hexyl acetate, benzyl acetate, 1,8-cineole, ethyl 2-(methylthio)acetate, ethyl 3-(methylthio)propionate, (E)-2-octenal, (E)-2-nonenal, (E,Z)-2,6-nonadienal, and (Z)-6-nonenal greatly influence the taste and aroma of melons. The total esters and sulfur were high in F-39 from California, aldehydes in TT-DV from Texas, alcohols in TH4 from California, and ketones in TH2 from North Carolina. In summary, the total volatile compound content was highest in TT-DV from Texas and lowest in TH6 from Georgia. Esters and aldehydes were the main factors for discrimination of Texas and North Carolina from Arizona. Partial Least Squares Discriminant Analysis (PLS-DA) showed significant differences among similar varieties of cantaloupes grown in different regions. These results show the impact of location on volatiles and provide useful information for selecting farm location for improving fruit quality.

AGFD011B 3531490 2:05 PM **Transcriptome and metabolome** changes in melon fruits Hisashi Koiwa koiwa@Tamu.edu Melon (*Cucumis melo*) is an important diploid crop with a wide variety of flavors due to its distinct aromatic volatile organic compounds (VOC). To understand the development of VOC profiles during fruit development, we performed metabolomic and transcriptomic analysis of melon samples of two cantaloupe varieties over the course of fruit development. We also expand our analysis by collecting samples from different varieties and various growth locations. RNA-seq analysis were performed in 2 rounds focusing on different aspect of molecular signatures of melon fruit transcriptome. The first round unexpectedly identified frequent asymptomatic infection of tobacco ringspot virus (TRSV) which is seemingly widespread throughout the US. The second round of RNA-seq implemented virus removal procedure to improve the data quality. The 2nd-round samples mainly include time course samples and geographic samples from 7 growth locations using 2 promising varieties. For time course datasets, we collected total of 130 metabolite data and 449014207 RNA-seq reads mapped to the melon genome. A total of 4469 differentially expressed genes in fruits were identified and used to visualize the transition of VOC and transcriptomic profiles during the fruit development. A shift of VOC profiles in both varieties was observed from early-fruit profiles enriched in C5-C8 lipid-derived VOCs to late fruit profiles abundant in C9 lipid-derived VOCs, apocarotenoids, and esters. The shift coincided with the expression of specific isoforms of lipid and carotenoid metabolizing enzymes as well as transcription factors involved in fruit ripening, metabolite regulation, and hormone signaling. This information is being applied to analyze more complex geographic datasets.

AGFD011B 3551078 2:00 PM **Study of potential antimicrobials** from melon (*Cucumis melo* L.) extracts Nitin Dhowlaghar nd288@tamu.edu Cantaloupe ranks first in the per capita consumption as a fresh fruit in the United States due to its sweet taste and potential health-promoting compounds. Cantaloupe rinds can be contaminated with pathogenic bacteria during production and processing. Several cases of food-borne illness were associated with consumption of cantaloupe contaminated with *Salmonella enterica* and *Listeria monocytogenes*. One potential solution to this problem may come from the fruit itself, as fruit secondary metabolites have potential antimicrobial properties. This talk will focus on the antimicrobial effects of various volatiles from cantaloupe flesh and peel extracts towards these foodborne pathogens. Volatile compounds

have been identified in cantaloupe fruits from different breeding and production programs throughout U.S. Using gas chromatography-mass spectrometry (GC-MS), we observed high levels of D-limonene (57.27 µg/kg FW), b-ionone benzaldehyde (1628.10 µg/kg FW), nonanoic acid, octanoic acid (277.78 µg/kg FW), geranyl acetone (454.27 µg/kg FW), and eucalyptol (34.49 µg/kg FW) in extracts of cantaloupe flesh that were previously shown to inhibit foodborne pathogens on different food matrices. The outcome of this study will help growers to improve melon safety. Our future study will examine the effect of individual compounds from cantaloupe to determine their antimicrobial effect on bacteria.

AGFD011B 3551459 2:00 PM **Why we peel melons: A peek into** the prevalence of foodborne pathogens among field-grown melons in Arizona and environmental risk factors for cross-contamination Richard Park RJPARK@EMAIL.ARIZONA.EDU Melons are healthy fruits liked by consumers but have been involved in outbreaks. *Listeria monocytogenes* contaminated cantaloupes caused 33 deaths in a 2001 outbreak. Understanding contamination vehicles and prevalence of foodborne pathogens will assist in risk-analysis. The objective was to investigate soil and dust as pathogen contamination vehicles and prevalence of foodborne pathogens in AZ grown melons and environmental samples. Ten melon cultivars from 5 growing locations were evaluated. Melon rinds were placed on *Salmonella* Newport or *L. monocytogenes* inoculated soil for 1 h. Inoculated dust was sprayed on melon rinds. Melon rinds in Phosphate Buffered Saline (PBS) were sonicated, soil and dust in PBS were vortexed, samples plated on selective media with antibiotics, and enumerated to determine % transfer. 339 cantaloupes, 20 rhizosphere, 20 soil, 20 air and 6 water samples were collected from 4 fields in AZ. Selective enrichment and plating was done to analyze presence/absence of *S. enterica* and *L. monocytogenes* and enumerate indicator bacteria. *S. Newport* % transfer from soil ranged 0.0183±0.0015-0.1227±0.0027, 0.0015±0.00003-0.0542±0.0075, and 0.0029±0.0004-0.704±0.0597 for cantaloupe, honeydew, and hybrid, respectively. *L. monocytogenes* soil % transfer ranged 0.0014±0.00006-0.0448±0.00402, 0.0005±0.0001-0.0092±0.0009, and 0.0207±0.001-0.1112±0.0049, for cantaloupe, honeydew, and hybrid, respectively. *S. Newport* % transfer from dust ranged 0.000007±0.000006, 0.000011±0.000006, and 0.000128±0.000054 for cantaloupe, honeydew, and hybrid, respectively. *L. monocytogenes* dust % transfer ranged 0.00002±0.000004-0.00679±0.001303, 0.00004±0.000036-0.002±0.000159, and 0.00004±0.000013-0.00015±0.000076 for cantaloupe, honeydew, and hybrid, respectively. There was a significant difference for soil having a higher % transfer than dust ($P<0.05$) for all *L. monocytogenes* and most *S. Newport* samples. No pathogens were detected in melons and environmental samples. On cantaloupes, enterococci and coliforms ranged 2.3-2.8 and 3.8-4.1 Logs, respectively. Air samples had the lowest enterococci and coliform counts, <1-3.0 and <1-2.1 Logs, with water samples ranging 1.6-2.2 and 2.1-3.8 Logs, respectively. Two melons were positive for *Escherichia coli*. All fields had signs of wildlife intrusion. Results will help understand pathogen contamination risk in field conditions and provide data for a science-based risk analysis.

AGFD011B 3557934 3:00 PM **Surface texture of honeydew &** cantaloupe melons and its correlation with bacterial attachment Stanislav Vitha vitha@tamu.edu Melons are nutritious fruits with numerous health-promoting properties. Melon varieties include the smooth-skinned honeydews and also cantaloupes which exhibit a network of rougher, suberized tissue, referred to as the "net". Episodes of foodborne illnesses from contamination with *Salmonella* and *Listeria*, associated mostly with netted melons, are of concern to the producers and consumers alike. The surface of the cantaloupe

melon, with its meshwork of netting, provides a large number of attachment sites for bacteria and makes it difficult to remove attached bacteria once in place. The physical characteristics of the surface of fruit, such as roughness and hydrophobicity, and presence of deep fissures in the netting, are believed to play a role in bacterial attachment and resistance of bacteria to the cleaning and sanitization procedures. In this study, the rind in selected cultivars was examined by scanning electron microscopy, and digital elevation models (DEMs) were created from stereo images in order to quantitate the profile roughness and surface texture parameters. The results are compared with results of the *Salmonella* and *Listeria* attachment study performed on adjacent areas on the same individual fruit.

AGFD011B 3556524 3:00 PM **Attachment strength & efficacy** of plant-based antimicrobials against *Salmonella enterica* and *Listeria monocytogenes* on melons grown in different regions of the United States Sadhana Ravishankar sadhravi@email.arizona.edu Foodborne pathogens contaminate melons during production from farm to fork and cause outbreaks. Understanding contamination risks and devising effective decontamination measures are important to prevent foodborne outbreaks. The objective was to investigate a) the attachment strength (AS) of *Salmonella* Newport and *Listeria monocytogenes* to melon rinds and b) efficacy of plant-based antimicrobials against both foodborne pathogens on melon rinds. The AS of *S. Newport* and *L. monocytogenes* and efficacy of antimicrobials on 6-7 melon varieties grown in 7 locations covering 6 US states (AZ, IN, NC, GA, TX-Uvalde, TX-Weslaco, and CA) were investigated. Melon discs or pieces were inoculated with overnight cultures of one of the test pathogens (~6-7 log CFU/mL). Inoculated discs were allowed 30 min for bacterial attachment, then vortexed for 15 sec to recover loosely attached and sonicated for 2 min to recover strongly attached cells, which were enumerated to calculate AS using the formula; $AS = (\text{strongly attached bacteria}) / (\text{loosely attached bacteria} + \text{strongly attached bacteria})$. Melon pieces were immersed in 5% olive extract or 0.5% oregano oil solution for 2 min with gentle agitation, stored at 4°C and survivors enumerated at Days 0 and 3. OC164 and HD150 had the lowest and highest average AS for *Salmonella* (0.24 and 0.31), respectively. HD150 and Infinite Gold had the lowest and highest average AS for *L. monocytogenes* (0.17 and 0.27), respectively. In general, AS of *Salmonella* and *L. monocytogenes* on cantaloupes (0.25-0.28; 0.21-0.27) was higher than on honeydews (0.24-0.31; 0.17-0.23). *Salmonella* showed a stronger AS than *L. monocytogenes*. Plant-based antimicrobials reduced both pathogens on all samples, regardless of melon types, varieties or locations. Compared to control, antimicrobials caused 1.7-3.6 and 1.3-4.0 log reductions in *Salmonella* and *L. monocytogenes*, respectively. In most cases, pathogen populations were below detection levels (1 log CFU/g) at Day 3. In general, oregano oil had better antimicrobial activity than olive extract, and both antimicrobials were more effective on *Salmonella* than *L. monocytogenes* and on honeydews than cantaloupes. Results will help determine a) melon varieties that could pose a food safety risk due to stronger bacterial attachment in case of a contamination event from pathogens and b) antimicrobials that could potentially be used as sanitizers for decontaminating melons.

WEDNESDAY EVENING 4/07/21 start 5:00 PM end 7:40 PM
Beyond Chemistry: Consumer Acceptance of Flavor, Food Safety and Health Benefits of Fruits and Vegetables - Effects of Natural Compounds for Food Safety Interventions

AGFD011C 3552869 5:05 PM **Enhancing the microbial safety of** fresh produce using lactic acid bacteria Kumar Venkitanarayanan kumar.venkitanarayanan@uconn.edu Fruits and vegetables constitute a vital part of a healthy diet, and their consumption has consistently grown over the last several decades. However, fresh produce has been increasingly linked to foodborne disease outbreaks,

and it is estimated that ~ 48% of foodborne illnesses are associated with fresh produce. Although a variety of FDA-approved disinfectants, including chlorine has been employed for inactivating pathogens on produce, their antimicrobial efficacy varies and is compromised in the presence of organic matter. Thus, there is an increasing interest for identifying effective, natural and ecofriendly strategies for controlling pathogens on fresh produce. Lactic acid bacteria (LAB) constitute a heterogeneous group of microorganisms found in diverse environments, including plants, animals and humans. LAB are classified as generally regarded as safe (GRAS) by the FDA and their use in the biological control of pathogens on fresh produce has received attention in recent years. Our research revealed that spraying *Lactobacillus plantarum* (PB9, B-4496, 42-3) reduced *Salmonella* populations on cantaloupe surface by ~ 4.0 log CFU during storage ($p < 0.05$). In another study, we observed that pre-harvest treatment of cantaloupes with LAB cultures of *L. plantarum* and *Pediococcus pentosaceus* reduced *Listeria innocua* by > 2.0 log CFU/cm² on day 5 post inoculation. Additionally, post-harvest treatment with LAB cultures reduced *L. monocytogenes* by > 2.0 log CFU/cm² on cantaloupes after 7 days of storage at 25°C ($P < 0.05$). Similarly, other researchers found that a combination of low oxygen modified atmosphere packaging with *L. plantarum* CICC 6257 significantly inhibited *L. monocytogenes* growth on cabbages. Collectively these results highlight the potential use of LAB as a natural strategy for enhancing the microbiological safety of fresh produce. This presentation will summarize LAB strain selection, modes of application, mechanisms of action and other criteria to be addressed before using LAB as biopreservative agents of fresh produce.

AGFD011C 3531089 5:00 PM **Receptor targeted bioengineered** probiotic promote gut health and prevent enteric disease Arun Bhunia bhunia@purdue.edu Live probiotic bacteria modulate the immune system to improve intestinal microbial balance and protect the host from foodborne pathogens and enteric diseases. The transient nature of probiotic bacteria in the gut prevents them from exerting their full health benefits. Persistence and stable colonization can happen when a probiotic bacterium finds a receptor on the host cells to cling on. The gastrointestinal mucosa represents the critical first site for the dynamic interaction of the enteric pathogens with the host. Therefore, averting this critical pathogen interaction step should help prevent extra-intestinal dissemination of pathogens and the consequent pathology. *Listeria monocytogenes* has been used as a model foodborne pathogen to study bioengineered probiotic approach. *L. monocytogenes* is an invasive human foodborne pathogen infecting primarily the immunocompromised host. The process by which it crosses the epithelial barrier is not fully understood. We show that *Listeria* adhesion protein (LAP; 94 kDa) induces intestinal epithelial barrier dysfunction to promote *L. monocytogenes* translocation. LAP binding to its cognate receptor, Hsp60 activates NF-κB signaling and facilitates myosin light-chain kinase (MLCK)-mediated opening of the epithelial barrier for bacterial translocation. A bioengineered *Lactobacillus casei* probiotic (BLP) expressing LAP helped probiotic interaction with Hsp60 forming a biofilm-like structure on the epithelial surface promoting anti-inflammatory and immunomodulatory responses through activation of Treg cells and improved gut barrier function. BLP protected mice and pregnant guinea pigs from listeriosis by competitive exclusion and immunomodulation, highlighting a novel approach in preventing infectious disease.

AGFD011C 3555085 5:00 PM **Distribution and intraspecific** diversity of lactic acid bacteria in fresh and fermented fruits and vegetables Maria Marco mmarco@ucdavis.edu vegetables Lactic acid bacteria (LAB) have vital roles in plant food safety, quality, and health promotion. Despite their recognized importance in the

production of fermented fruits and vegetables, the prevalence, abundance, and diversity of LAB on those plant foods pre- and post-harvest are not well understood. Our studies have shown that LAB populations on (fermented) fruits and vegetables fluctuate from levels that are below detection to over 10^7 cells per gram tissue and are influenced by environmental conditions, plant species, and microbial succession dynamics. Besides the known, species-level differences among LAB genera, characterization of a collection of 13 strains of *Lactiplantibacillus plantarum* (a LAB formerly known as *Lactobacillus plantarum*) from fresh and fermented plant food sources revealed high levels of intraspecific diversity. *L. plantarum* strains were highly variable with regard to genome content (genome size, enzymatic pathways), the capacity to grow on different carbohydrates (mono- and poly-saccharides), tolerate environmental stresses (high temperature, low water activity, acidic pH, and high alcohol content), form biofilms, and inhibit yeast growth. This variation was associated with the source from which the strain was isolated, indicating that *L. plantarum* is adapted at the strain level for specific (fermented) plant foods. Furthermore, examination of multiple *L. plantarum* strains isolated from the same fermented plant food samples showed that these bacteria have evolved for intraspecies co-existence in food fermentations through gene loss and niche differentiation. The findings provide opportunities to use LAB strain-specific approaches to maximize health and sensory aspects of fruits and vegetables.

AGFD011C 3558376 6:05 PM **Relative risks of poor water quality used in onion production: Drip irrigation vs. foliar spray** Joy Waite-Cusic joy.waite-cusic@oregonstate.edu In the summer of 2020, Canada and the US experienced a large outbreak of *Salmonella* Newport that was epidemiologically linked to onions grown in California. An extensive outbreak investigation failed to yield conclusive evidence to the source or circumstances that led to widespread contamination; however, it is likely that water played a role as either source or dissemination vector. Water is not used in post-harvest onion handling; however, water is commonly applied to the crop via drip irrigation and foliar spray. Dry bulb onion growing regions in the western US have a limited number of water sources, including surface waters of poor microbiological quality. The objective of these studies was to provide field evidence of the risks associated with late season application of contaminated water via drip irrigation and foliar application. In the Oregon study, Vaquero (yellow) onions were irrigated via drip using water inoculated with 0, 1, 2, or 3 log CFU/ml of a cocktail of rifampicin-resistant *Escherichia coli* (TVS 353, TVS 354, TVS 355). In the California study, Ovation (yellow) onions were sprayed with 25 ml of water containing the *E. coli* cocktail (2-3 log CFU/ml). Onions were finished in the field following regional practices and were sampled over the 28-day curing period. Onions ($n = 10\text{-}300/\text{treatment}$) were analyzed for surviving *E. coli* using a combination of standard plate count, filtration, and enrichment methods. A minor percentage (13.3%; 20/150) of onions were contaminated due to drip irrigation with the most contaminated water. The percentage of contaminated onions decreased over time with no contamination detected on any onions from any treatment after lifting (7+ days). Foliar spray resulted in the consistent contamination of 2-3 log CFU/onion; however, die-off occurred rapidly over the first 4 hours. As field curing progressed, the detection of *E. coli* in onions decreased; however, in a small percentage of onions, *E. coli* grew and reached levels as high as 6-7 log CFU/onion on day 4 and remained detectable at these levels after 21 days of field curing. These studies demonstrated that the use of contaminated water via drip irrigation poses very little risk to dry bulb onions; however, the use of contaminated water for foliar sprays leads to significant contamination and can lead to *E. coli* growth in a significant percentage of the crop.

AGFD011C 3542088 6:00 PM **Safety and quality effects of aflatoxin contamination in peanuts** Lisa Oehrli lisa.dean@ars.usda.gov Aflatoxins are metabolites of several species of fungi from the genus, *Aspergillus* and are known to be extremely carcinogenic. Peanuts are one of the commodities that are susceptible to contamination by aflatoxins which renders them unsuitable for human food and animal feedstocks. Regulations in the European Union restrict levels of total aflatoxins in peanuts to 4 ppm and Aflatoxin B₁ (the most common form and the most carcinogenic) to 2 ppm. This is lower than the allowable levels by USA regulations of 20 ppm and affects the value of USA exports. The *Aspergillus* fungi are ubiquitous in soil, but aflatoxin contamination increases with drought stress in peanut crops. In recent years, aflatoxin contamination has become more widespread in peanuts and strategies are being investigated to address the issue. These include both preharvest treatments such as development of more drought resistant peanut varieties and field irrigation procedures and postharvest treatments such as shelling and blanching of peanut kernels. In addition, treatment of peanut kernels by cold plasma and biological treatments have shown promise in the reduction of aflatoxin contamination. Improvement of the safety and quality of peanuts will result from successful treatments against aflatoxin contamination at all stages of peanut production.

AGFD011C 3537649 6:00 PM **Consumer acceptance of food safety-enhancing technologies: From heuristic to consumer communication** Yaohua Feng yfengchi@purdue.edu The food industry witnesses consumers' increased awareness of nutrition, discriminating palate that seeks appealing flavor, and demand for easy, convenient preparation. To address consumers' needs, many safety-enhancing technologies were developed and applied in food processing. Acceptance of products processed by those technologies depends on the consumers' perception of benefits and risks, which are influenced by consumers' heuristics of the technology, worldview and previous experience of novel technology, the perceived credibility of information, demonstrated food safety, and environmental responsibility of industry. This presentation will showcase consumer acceptance of three safety-enhancing food technologies to explore the effect of individual characteristics and consumer communication on technology acceptance. The label used for technology can have a large impact on how a technology is perceived. Many consumers rely on affect heuristic, instead of science-based information, to make decisions. This can lead to a biased and may result in lower acceptance of food technology. The speaker will describe research which reveals how messaging and technology neophobia affects technology use by contrasting the limited application of food irradiation and the more widely used high-pressure processing (HPP). This technology is used in many food processing facilities, including juice, avocado puree, and tree nuts. The third case study is adding safety-enhancing processing aid, Dimethyl dicarbonate (DMDC), to freshly squeezed juice. DMDC can be used to reduce microbiological levels in juice. The United States does not require mandatory labeling of juice with DMDC. Food processors who value transparency need to balance communicating their processing methods without raising concerns about chemical use. The presenter will share findings from a focus group study to identify consumer responses to and preferred communication approaches about the use of DMDC in juice. This presentation will be uniquely positioned to address the consumer acceptance of food safety-enhancing technologies that were developed to improve the quality and safety of fruit and vegetables. At the end of the presentations, the speaker will identify strategies to improve consumer acceptance through more effective communication and education.

AGFD011C 3551800 7:00 PM **Sensory scale use in berries: How do the 9-pt, labeled affective magnitude, and unstructured visual analog scales differentiate real product sets of fresh berries?** Jacob Lahne jlahne@vt.edu When measuring consumer sensory responses for fresh fruit, what type of response scale should the analyst select? In contrast to instrumental food-analysis research, in which data can be measured objectively, in consumer testing data is by-nature subjective. There is still no real consensus on which scale a sensory scientist working in industry should use to measure actual hedonic responses to food products, especially highly variable and rapidly changing products like fresh berries. A key criterion for a hedonic scale are whether it sensitively and efficiently discriminates among consumer responses to products. Therefore, the key question this study investigates is whether the use of different scales by the same subjects on the same products in a real-world situation would provide different results for the sensory analyst. This study comprises the evaluation of 6 for-market varieties each of 4 berries—raspberry, strawberry, blackberry, and blueberry—by the same N = 147 untrained subjects using 3 popular scales—the 9-pt hedonic scale, the Labeled Affective Magnitude Scale (LAM), and the unstructured Visual Analog Scale (VAS). Data were analyzed by mixed-effects ANOVA with subsequent scale-performance and post-hoc measures, and by bootstrapping simulation studies to estimate the empirical power of each scale to detect differences. For each berry type, significant differences in liking were detected by at least one scale, but scale performance differed. The 9-pt scale was the only one of the three to detect differences among the blueberry samples, and examination of ANOVA and post-hoc results for all berries showed that the 9-pt scale consistently discriminated among samples as well or better than the other two scales. In simulation studies, the 9-pt scale showed reliable detection of differences at sample sizes smaller or equal to the other two scales. Alignment between instrumental (chemistry) and subjective (consumer) data has significant impact in the world of fruit breeding and product development. As the 9-pt scale discriminates consumer liking for different products as well or better than two continuous scales it can be retained in industry research programs for this purpose

THURSDAY MORNING 4/08/21 start 9:00 AM end 11:40 AM
Beyond Chemistry: Consumer Acceptance of Flavor, Food Safety and Health Benefits of Fruits and Vegetables - Crop Improvement/Bioactive Compounds and Health Benefits of Fruits and Vegetables

AGFD011D 3531205 9:05 AM **Metabolomics-based identification of new alkaloids as urinary biomarkers for dietary tomato intake** Hans-Ulrich Humpf humpf@uni-muenster.de The goal of this study was the identification of potential urinary biomarkers for the consumption of tomatoes and tomato products. During a dietary intervention study, the human urinary metabolome of a study cohort receiving either a tomato-free diet or tomato juice was compared by application of an HPLC-HRMS-based metabolomics approach. Statistical analysis showed several unique features which were detectable after the intake of tomato juice. The most discriminating markers were identified as metabolites of the steroidal glycoalkaloid esculeoside B recently found in tomato juice. Hydroxylated and sulfonated metabolites of the corresponding aglycone esculeogenin B were detected in urine samples. In addition the β -carboline alkaloids tangutorid E/F and a series of new imidazole alkaloids as well as glucuronidated derivatives thereof were identified in urine. The structures of all mentioned biomarkers were fully elucidated by MS and NMR. For the quantitative assessment of the tomato biomarker intake a two-week crossover dietary intervention study was performed. Fourteen volunteers obtained a low and high dose of tomato juice after a 3-day washout period and urine samples were analyzed by HPLC MS/MS. Several imidazole alkaloids were shown to specifically indicate the tomato juice consumption for 24 h

and partly >24 h. The hydroxylated and sulfonated metabolites of esculeogenin B were detectable for at least 48 h after consumption and serve as long-term biomarkers for tomato juice. The β carboline alkaloids were identified as supporting, but non-specific dietary biomarkers for tomato juice intake. As β carboline alkaloids are formed during thermal processing they are not detectable in fresh tomatoes and can be used to distinguish between fresh and processed tomato intake. In summary the results show that the dietary intake of tomato juice is detectable based on the urinary excretion of multiple β -carboline, imidazole and steroidal alkaloids, and can be determined for a period of up to 48 h after consumption. Furthermore, low and high doses of tomato intake can clearly be differentiated based on the urinary excretion of biomarkers.

AGFD011D 3551695 9:00 AM **Developing a biochemical understanding of the health benefits of consuming tomato-rich diets** Jessica Cooperstone cooperstone.1@osu.edu Tomatoes are the most commonly consumed non-starchy vegetable by Americans, and their consumption is associated with a decreased risk for a variety of chronic diseases. Lycopene, the red pigment in tomatoes, has been studied for its putative bioactivity, though numerous studies have demonstrated an enhanced benefit of whole tomato vs. purified lycopene, suggesting other phytochemicals are at play. The Cooperstone lab aims to understand the phytochemicals responsible for the benefits of tomato-rich diets. Working at the intersection of plant, food, and nutritional sciences, here she will present data towards 1) a better understanding of the phytochemicals within tomato that may impart benefits and their genetic control in fruits, 2) ways to assess tomato intake in humans, and 3) how tomato consumption can alter the microbiome. Together, these data contribute towards a bigger understanding of how tomato consumption can impact human health.

AGFD011D 3557668 9:00 AM **Nanoparticle-mediated seed priming: An effective technique to improve germination, growth, yield while maintaining the quality of watermelon** Pratibha Acharya acharyapratibha977@gmail.com Rapid and uniform seed germination is important for adequate crop establishment to ensure economic sustainability in commercial agriculture. In the present study, turmeric oil nanoemulsions (TNE) and silver nanoparticles (AgNPs) synthesized from agro-industrial byproducts were used as nanopriming agents to improve germination, yield, and quality of diploid (Riverside) and triploid (Maxima) watermelon seeds. Internalization of nanomaterials was confirmed by neutron activation analysis, transmission electron microscopy, and gas chromatography-mass spectrometry. The seedling emergence rate was significantly higher in AgNP-treated triploid seeds compared to other treatments. Soluble sugar (glucose and fructose) contents were enhanced during germination in the AgNP-treated seeds at 96 h. Seedlings grown in the greenhouse were transplanted at four locations in Texas: Edinburg, Pecos, Grapeland, and Snook in the first year and at Weslaco in the second year. A significantly higher yield was observed in AgNP- treated Riverside and Maxima watermelons grown at Snook. Physico-chemical properties and phytochemical profiles were assessed after mature fruits were harvested and stored at 23°C for 0, 10, and 20 d. While seed emergence and stand establishments were enhanced by seed priming, total phenolics radical-scavenging activities, and macro-and microelements in the watermelon fruits were not significantly different from the control. Combined analysis across all locations demonstrated a non-significant treatment effect on the levels of health-promoting compounds such as carotenoids, ascorbic acid, and citrulline. The results of the present study demonstrated that seed priming with AgNPs can enhance seed germination, growth, and yield while maintaining fruit quality through an eco-friendly and sustainable nanotechnological approach.

AGFD011D 3550647 10:05 AM **Influence of varietal selection** and pasteurization on raw almond flavor, quality and consumer acceptance Alyson Mitchell aemitchell@ucdavis.edu Almonds, botanically a fruit, are the most widely produced and consumed tree nut in the world. Almonds are a good source of protein in vegetarian and vegan diets and consumption is linked with numerous health benefits. Raw almonds produced in California are required by law (since 2007) to undergo pasteurization to reduce the potential for foodborne illness. Thermal moist air pasteurization (TMA) involves exposing almonds to hot moist air for a short time, followed by a cooling/drying step. Propylene oxide (PO) is a fumigant used on raw agricultural products for pasteurization. In almonds, the approved process involves exposing kernels to PO for 4 hours in a heated chamber (47-51 °C), followed by ventilation at 38-43 °C for 2 days or 15 °C for 5 days. Because almonds are 50-60 % lipid by weight, of which is 95 % are unsaturated fatty acids, they are susceptible to lipid oxidation during storage. During either pasteurization process, almonds are exposed to heat and/or moisture, which can influence the activity of enzymes related to fatty acid hydrolysis and lipid oxidation. Fumigation agents such as PO, also have the potential to deactivate enzyme through protein alkylation. This talk will describe the main sensory and chemical characteristics of raw almond flavor and discuss how varietal selection and pasteurization influence raw almond flavor and quality as it relates to consumer liking and acceptance. Main results indicate that pasteurization protects almonds by decreasing lipid oxidation during storage. Chemical measurements demonstrate lower amounts of free fatty acids and lower levels of headspace volatiles related to lipid oxidation in pasteurized almonds as compared to controls. Descriptive analysis indicates that PO and TMA pasteurized samples have significantly lower total oxidized flavor and painty/solvent flavor over storage relative to controls.

AGFD011D 3555425 10:00 AM **Characterization of volatile** profiles in 28 melon breeding lines using headspace solid-phase microextraction gas chromatography-mass spectrometry Drishti Majithia drishtimajithia@tamu.edu The sweetness and aroma of melons (*Cucumis melo* L.) are the two most important attributes of the fruit for consumer acceptance. Volatile organic compounds (VOCs) play a major role in improved fruit flavor, odor and aroma. The present study identified 113 volatile compounds from 28 melon breeding lines (BL) using HS-SPME-GC-MS. Physicochemical parameters like color, sugars and brix° were also determined. Volatile compounds were grouped according to their chemical classes; esters, aldehydes, alcohols, ketones, acids, hydrocarbons, sulfurs and other compounds were identified. The major volatile compounds identified were benzaldehyde, geranylacetone and beta-ionone. BL-30 had the highest concentration of VOCs whereas the lowest was found in BL-22 as compared to the other lines. BL-7, BL-12, BL-4, BL-30 and BL-20 contained volatiles which were found to be associated with antimicrobial, antifungal and antiviral properties. BL-22 and BL-14 had the highest and the lowest total sugar concentrations, respectively. The highest sucrose contents were found in BL-4 and BL-24 as compared to others. The color results indicated that the melon samples were rich in beta-carotene. Principal component analysis was used to separate the breeding lines into different clusters based on their volatile content. This study was an effort towards identifying potentially healthier melon breeding lines with improved flavor and aroma that could be used for future breeding purposes to better suit consumer preferences and demands

AGFD011D 3553137 10:00 AM **Anti-colitic effects of** anthocyanins: Role of gut bacteria Lavanya Reddivari Lrediva@purdue.edu Ulcerative colitis (UC), a form of inflammatory bowel disease (IBD), is rising worldwide. Gut bacterial dysbiosis plays an essential role in UC. We have recently shown that

anthocyanin-rich foods exert anti-inflammatory activity and improve barrier function in colitic mice. However, limited information is available on the extent to which gut bacteria play a role in the anti-colitic activity of anthocyanin foods and whether different anthocyanins differ in their anti-colitic activity. This study investigated the anti-inflammatory effects of anthocyanins within a whole-food matrix against dextran sulfate sodium (DSS)-induced colitis using red/purple-fleshed potatoes that differ in the composition of anthocyanins in mice with the intact and antibiotic-ablated microbiome. We used the DSS-induced murine (C57BL6) colitis model with and without the administration of antibiotics in drinking water for nine weeks. Mice were randomly assigned to the control (AIN-93G diet), 20% red- and purple-fleshed potato supplemented diets. After eight weeks, mice were treated with 2% DSS in their drinking water for five days to induce colitis. Intestinal permeability was measured using FITC-dextran. Serum myeloperoxidase (MPO) levels were measured using ELISA. RT-PCR was used to analyze the relative gene expression levels of pro- and anti-inflammatory cytokines and bacterial abundance. Administration of antibiotics resulted in a 95% reduction in gut bacterial load. Antibiotics administration did not alter food intake, water intake, and weight gain. However, antibiotic-treated mice had five times greater cecum weight, a hallmark of germ-free mice, compared to no-antibiotic mice. In antibiotic mice, DSS-induced splenomegaly, elevated gut permeability (serum levels of FITC-dextran), and reduced colon length and weight were more pronounced compared to no antibiotic mice. Purple- or red-fleshed potato supplementation (20% w/w) ameliorated ($P < 0.05$) DSS-induced suppression in colon length, elevation in spleen weight, intestinal permeability, and colonic MPO levels in no antibiotic mice only. Moreover, purple-fleshed potato supplementation alone improved the ZO-1 and MUC-2 gene expression levels related to gut permeability in no-antibiotic mice, but not in microbiota-ablated mice. In summary, these results suggest that the gut microbiome is critical for the anti-colitic activity of anthocyanin-containing potatoes and anthocyanin composition does play a role in anti-colitic activity.

AGFD011D 3558248 11:00 AM **Bitter melon (*Momordica* charantia)** : An exotic vegetable with a treasure of health-promoting compounds Siddanagouda Shivanagoudra siddu4191@gmail.com Plants and herbal preparations have been used as medicine throughout the world since ancient times. Most plants contain a diverse range of bioactive compounds and provide a multitude of health benefits. *Momordica charantia* L., also known as bitter melon, belongs to the Cucurbitaceae family. This vegetable has potential health-promoting and nutritional properties, and currently, this vegetable is widely consumed as a healthy vegetable in several countries. Numerous bioactive compounds have been isolated from the various plant parts of the bitter gourd, including leaves, stems, roots, fruits, and veins. Bioactive compounds, including proteins, polysaccharides, flavonoids, triterpenes, saponins, ascorbic acid, and steroids, have shown promising potent biological activities. In recent years, bitter melon has been used to treat different diseases, mainly diabetes, and related conditions. Additionally, various extracts demonstrated a significant anticancer and antitumor activity, glucose reducing effect, and AMP-activated protein kinase activities. In our previous study, we isolated 17 compounds from the Chinese cultivar of *M. charantia*, including two novel compounds, and structures of the purified compounds were elucidated by HR-ESIMS, 1D, and 2D NMR experiments. Additionally, isolated compounds were evaluated for *in vitro* antidiabetic and antiinflammatory activities, where compounds showed significant biological activities. However, most reported studies on bitter melon bioactive compounds were performed on cell lines and animal models. A limited number of clinical and pre-clinical studies have been documented on the antidiabetic and hypoglycemic effects of *M. charantia* through

various postulated mechanisms. This review addresses a comprehensive overview of our previous research work and phytochemistry. It also discusses their pharmacological activities and their adverse effects, aimed at providing and biological activities of M. charantia

THURSDAY AFTERNOON 4/08/21 start 1:00 PM end 3:40 PM
Beyond Chemistry: Consumer Acceptance of Flavor, Food Safety and Health Benefits of Fruits and Vegetables - Food Processing-impacts on Quality Sensory

AGFD011E 3549738 1:05 PM **Effects of high pressure processing (HPP) on the physicochemical properties, bioactive compounds, antioxidant capacities, microbial safety, and shelf-life of aronia berry puree** Mei Lu mlu4@unl.edu Aronia (Aronia melanocarpa) berry possesses a high level of health-beneficial polyphenols. This study aimed to characterize the impact of non-thermal high pressure processing (HPP) on the quality, nutrition, microbial safety, and the shelf-life of aronia berry puree. The effects of HPP (200 - 600 MPa/2.5 or 5 min) on the physicochemical properties (color, pH, titratable acidity, total soluble solids content/TSSC, pulp content, particle size distribution, and viscosity), bioactive compounds (total phenolic and anthocyanin contents), antioxidant capacities (DPPH radical scavenging capacity and ferric reducing antioxidant power), and microbial counts (aerobic plate counts/APC, yeast and mold counts) of aronia berry puree were investigated. All results were compared between HPP treated and untreated purees. TSSC decreased significantly when pressurized above 400 MPa/2.5 min. Viscosity reduced significantly at all HPP conditions. Other physicochemical properties changed insignificantly after HPP. No significant reduction in phenolic contents or antioxidant capacities was observed in the pressurized puree. Pressurization at 400 and 600 MPa effectively reduced yeast and mold counts to below 1 log CFU/g. It reduced APC to below 2 log CFU/g only when pressurized for 5 min. In the shelf-life study, aronia berry puree was subjected to HPP (400 MPa and 600 MPa/5 min) and then stored at refrigerated temperature for 8 weeks. The microbial shelf-life and quality changes of aronia puree during 8-week refrigerated storage were evaluated. Similar results were observed in both HPP conditions. After the initial significant reduction of APC by HPP, APC changed insignificantly during the 8-week refrigerated storage. HPP completely inactivated yeasts and molds, and no regrowth was observed during storage. In contrast, yeasts in untreated puree increased from 4.7 to 6.1 log CFU/g. Physicochemical properties, total phenolic contents, and antioxidant capacities of aronia puree had insignificant changes right after HPP and during storage. Total anthocyanin content of untreated samples and those treated at 400 MPa decreased continuously during the storage. In conclusion, HPP (400 MPa/5 min and 600 MPa/5 min) significantly reduced microbial load, retained the physicochemical properties and nutritional values of aronia berry puree. HPP (600 MPa/5 min) could be an effective preservation technique for microbial reduction, quality retention, and shelf-life extension of aronia puree.

AGFD011E 3542140 1:00 PM **Utilization of byproducts from the fruit processing industry in extruded puffed products** Girish Ganjyal girish.ganjyal@wsu.edu Over the past few years, significant work on the exploration of the utilization of fruit processing byproducts has been reported. The majority of the byproducts carry significant nutritional value, along with unique functional characteristics. Extrusion is a versatile processing technology that is widely used for the manufacturing of numerous food products. If we can understand the extrudability of these byproducts, they can be utilized to a great extent and enhance the nutritional quality of the many starch heavy extruded products. This presentation will make an effort to review the current information on the fruit processing byproducts and their

utilization in extrusion processing. An effort will also be made to identify the technical gaps that exist in the utilization of these byproducts.

AGFD011E 3553433 1:00 PM **Exploration of Prachyrhizus erosus (Yam bean) tubers as potential source of inulin, a potent prebiotic for development of functional products: An approach towards nutraceutical advancement** Rohn Sarkar rohan1994sarkar@gmail.com Prebiotic compounds play a major role in proliferating human gut microbiome thus helps to prevent severe gastric problems and facilitate boosting immune system. Being an under-utilised crop, Prachyrhizus erosus (Yam bean) tubers have been utilised as a source of prebiotic substance, inulin. The inulin was extracted using conventional hot water method (yield of 9% w/w) that showed around 48.86% higher prebiotic potential over Lactobacillus fermentum compared to glucose. To understand the interaction between oligomers and the target site, in-silico analysis was conducted that showed inulin with monomer units of 3 and 7 had better binding efficiency towards inulinase enzyme than compared to entire polymer chain. This docking study was validated under laboratory condition by enzymatic hydrolysis followed by activity of hydrolysates over target microorganism. About 14.28% and 28.57% increase in activity was observed for oligomers having monomer units of 3 and 7 compared to inulin polymer respectively. Further the inulin was used to encapsulate β -carotene through emulsification by homogenisation process. Confocal laser scanning microscopic image and XRD spectrum confirmed formation of encapsulated product. Encapsulation efficiency and loading capacity were achieved about 66% and 1.2% respectively. Higher antioxidant activity was observed for the developed product compared to their ingredients. Cumulative release of β -carotene from the formulation was around 49.65% and 75.23% under simulated gastric and intestinal fluid conditions respectively. Fitting release data into korsmeyer peppas model, similar kind of release pattern (non-fickian diffusion, 0.5<n<1) were found for both the conditions. This study helps to visualise the utilization of inulin in order to obtain its prebiotic potential at its best possible way.

AGFD011E 3558212 2:05 PM **Investigation of biochemical and structural mechanisms for the release of phytochemicals from cell-based carriers** Rewa Rai rewarai.iitd@gmail.com Delivery of bioactives using cell based carriers provides an alternative to engineered micro-carriers for both the food and pharmaceutical industries. This study was focused on understanding the role of intracellular compositions and structure in modulating the release and bio-accessibility of encapsulated phytochemicals during simulated gastrointestinal digestion of cell-based carriers. Conventionally, changes in the structure of the micro-carriers during digestion is correlated with the release of encapsulated bioactives, however the cell based carriers are significantly complex and has diverse biochemical composition that can modulate the release of encapsulated bioactives. Yeast was selected as a model cell-based carrier and trans-resveratrol (trans-Res) as a model encapsulated phytochemical. The release of encapsulated trans-Res was evaluated during the simulated gastric, intestinal (at low and high bile salt concentration), and sequential (gastric followed by intestinal) conditions. A combination of vibrational spectroscopy (FTIR) and principal component analysis (PCA) were used for characterizing biochemical changes in cellular composition during gastric and sequential digestions. Transmission electron microscopy (TEM) was used for characterizing structural changes in the cells. The results illustrate the role of gastric treatment in influencing the intracellular protein secondary structures and aggregation and the significant role of these biochemical changes in accelerating the release of encapsulated phytochemical during gastric as well as during sequential digestions. In contrast, limited changes in structural

properties of cells were observed using TEM. Bile salts solubilizes the intracellular lipids and improve partitioning of phytochemical to the intestinal fluid during sequential digestions. The gastrointestinal treatments have no significant effect on the intracellular nucleic acid confirmations. Overall, the results highlight significant role of the gastric treatment and bile salts in the release and bio-accessibility of encapsulated phytochemicals from cell based carriers based on biochemical changes while limited effect was observed on structural properties of these carriers during gastro-intestinal digestion.

AGFD011E 3530227 2:00 PM **Binding studies for the interaction** between hazardous organophosphorous compound phosmet and lysozyme: Spectroscopic and In-silico analyses Lajpreet Kaur hanzra0003@gmail.com Organophosphorus compounds are generally toxic compounds that are used profoundly in agriculture, medicines and various other industries. Various organophosphorus compounds are hazardous and result in mortalities on acute exposure. Some of these are potential chemical warfare agents owing to their toxic nature. Phosmet is one such organophosphorus compound with moderate nerve toxicity on prolonged exposure. The present study investigated the binding of phosmet with lysozyme to understand the transportation and metabolism of phosmet. The U.V-Visible spectroscopy revealed the interaction between the phosmet and lysozyme. The fluorescence quenching further clearly indicates the formation of the lysozyme-phosmet complex. The collisional or dynamic binding nature of lysozyme and phosmet was reported from the analysis of Stern-Volmer plots. The binding constant (K_a) and the number of binding sites (n) were calculated from the double logarithmic regression curve. Finally, from the Molecular docking analysis with glide score -5.273 kJ/mol in consistent with all the experiments confirms the interaction of lysozyme and phosmet.

AGFD011E 3551965 2:00 PM **Developing a fresh berry lexicon:** Adapted descriptive analysis and consumer validation Katherine Phetxumphou katphet@vt.edu A challenge that the fresh berry industry faces is the lack of uniform sensory lexicon to characterize berries and communicate with retailers and ultimately, consumers. Fresh berries have varying sensory properties due to berry type, genetics, seasonality, and growing locations. This research aimed to adapt descriptive analysis (DA) methodologies to develop berry lexicon that accounts for these factors. Strawberries, blueberries, raspberries, and blackberries were evaluated from February to November 2020 using revolving trained DA panels over 13 "session-blocks." Each session-block consisted of six total hours, split over four consecutive days (due to limited self-life of berries). Panelists ($N=5-10$) were trained in DA and evaluated one berry type (e.g., strawberries) with multiple genetics per session-block. A total of 110 berry genetics were evaluated (30 for strawberries, 27 each for both raspberries and blackberries, and 26 for blueberries). A typical DA protocol was adapted for berry availability and spoilage for each session-block. Day 1 focused on sensory evaluation methods and DA training. Day 2 involved initial sensory evaluation (appearance, aroma, flavor, taste, and texture) of available genetics, preliminary consensus lexicon development, and recommendations for reference standards. Day 3 finalized the aroma, flavor, and taste terms and respective reference standards using typical DA methodology and a Check-All-That-Apply (CATA) tool. Day 4 allowed time for further revision as well as defining texture terms and respective reference standards. Day 4 also included visual evaluations and photographing berries for relevant appearance terms. An optional Day 5 was occasionally required for defining terms or reference standards that were not finalized during the typical four-day session-block. Following the conclusion of all berry session-blocks, consumer validation using an online relevance survey (target $N=175$ per berry type) was conducted to evaluate consumer recognition and use of attributes developed during the DA. An online hierarchical sorting

study (target $N=50$) was conducted to define the lexicon taxonomy with the terms retained after the relevance survey. Overall, the combination of adapted DA methodology, consumer relevance surveying, and hierarchical sorting revealed lexicons that could be used to consensually characterize berries and describe differences stemming from berry type, genetics, seasonality, and growing locations.

AGFD011E 3557130 3:00 PM **Comparison of anthocyanins,** organic acids, and antioxidant capacity of different commercial blueberry products Jayashan Adhikari jadhikari@tamu.edu Blueberries (*Vaccinium corymbosum* L.) are a good source of dietary bioactive components and recognized for their potential health benefits. Among the various health-promoting compounds, anthocyanins and organic acids have a major effect on blueberry's antioxidant capacity and nutritional quality. The concentrations of health-promoting compounds are influenced by crop management practices, processing, and storage conditions. Therefore, to improve the quality of fruits and/or their commercial products, it is important to understand the role of these factors. In the current study, we developed a sensitive and rapid analytical method to analyze the influence of pre- and post-harvest factors on blueberry's anthocyanins and organic acids. A total of 11 blueberry products of different commercial brands (freshly harvested berries, processed juice, and freezer stored berries) were selected for the study. The antioxidant activities were evaluated by DPPH and ABTS assays. We tentatively identified and characterized 19 anthocyanins and 6 organic acids using liquid chromatography-mass spectrometry. We observed a wide variation in anthocyanin and total organic acid content in different clean-label blueberry products. The total anthocyanin content had a positive correlation with antioxidant capacity, but the total organic acid contents had an inverse relationship with antioxidant capacity. Blueberries stored in the freezer had lower concentrations of citric, shikimic acid, and total organic acids compared to fresh blueberries. Overall, processing and storage conditions had a significant impact on the accumulation of anthocyanins and organic acids in different blueberry products.

THURSDAY EVENING 4/08/21 start 5:00 PM end 8:00 PM
Beyond Chemistry: Consumer Acceptance of Flavor, Food Safety and Health Benefits of Fruits and Vegetables - Innovative Approaches in Horticulture Technology

AGFD011F 3556710 5:05 PM **Non-destructive methods to** determine the maturity of specific fruits and vegetables Tushar Dhanani tushareign@tamu.edu Fruits and vegetables such as watermelon (*Citrullus lanatus*) contain health-promoting bioactive compounds, but the levels of these compounds and other key quality parameters vary at different stages of fruit maturity. Establishing a relationship between optimum maturity and quality parameters including health-promoting compounds is critical to increase consumption and provide nutritional security. However, many chemical assays require destructive sampling of the fruit. Recently, non-destructive methods such as Raman and near-infrared spectroscopy (NIR) have attained increasing interest due to advances in instrumentation and chemometric applications. In the case of Raman spectroscopy, narrow and highly resolved bands allow non-destructive extraction of chemical and physical information from the samples. Similarly, NIR has been extensively used for non-destructive measurement of internal quality of fruits and vegetables. The presentation will focus on Raman and NIR and the application of different techniques to detect changes in quality parameters during the ripening of watermelon fruits. We evaluated the external maturity of watermelon using a non-invasive Raman spectroscopy. Spectral acquisition from the fruit surface was carried out at wavelength range 400–2000 cm^{-1} using a handheld Raman spectrometer equipped with 830 nm laser excitation source. The changes in the

intensity of three Raman peaks (1002, 1156, and 1525 cm^{-1}) assigned to the carotenoids were evaluated using chemometric analysis. The level of carotenoids decreased as the watermelons ripened, and the spectral signatures obtained from carotenoids can be used to evaluate the external maturity of watermelon. Furthermore, internal quality attributes (soluble solid contents) were predicted non-destructively using NIR and Soft Independent Modelling and Class of Analogy. Our results demonstrated that the developed model had good predictive power with high sensitivity. Therefore, these novel techniques have enormous potential to replace time-consuming, destructive and labor-intensive conventional techniques for monitoring quality indicators of fruits and vegetables.

AGFD011F 3534397 5:00 PM **Exploring native diversity of** fruits and spices in Andaman and Nicobar Islands, India for nutritional and livelihood security Ajit Waman ajit.hort595@gmail.com Andaman and Nicobar Islands are a group of 572 humid tropical islands and isles distributed in the Bay of Bengal. These islands are home to about 2,600 species of flowering plants of which 300 taxa are endemic in nature. The aboriginal tribes and settler communities of these remotely situated islands have been dependent on many of these native species for food, medicine, fodder, timber and other purposes. Systematic studies were undertaken to explore the horticultural potential of selected native plant genetic resources and to prioritize them for domestication based on their prospects in providing nutritional and livelihood security. Blood fruit (*Haematocarpus validus*, Menispermaceae) was identified as novel tropical fruit crop and a source of Pelargonidin and Cyanidin. Endemic species viz. *Garcinia dhanikhariensis* and *Garcinia andamanica* (Clusiaceae) were recommended for commercial exploitation as nutritious fruits, acidulants and processed products. FAME analysis of seed fats of six native *Garcinia* species revealed industrial potential of these species. For *Curcuma mangga* (Zingiberaceae), a medicinal spice, suitable agro-techniques and micropropagation protocols were developed. GC-MS profiling of rhizome essential oil revealed presence of β -Myrcene and Cyclofenchene as dominant compounds. Woody pepper (Piperaceae) was identified as a novel spice in which stem pieces of the vines were employed as spice. Woody pepper based cropping system models for cultivation are being evaluated for their commercial feasibility. Semi-intensive models for commercial cultivation of a minor spice-Culantro (*Eryngium foetidum*, Apiaceae) were developed. These interventions involving sustainable exploitation of native genetic resources of vulnerable tropical islands could not only provide livelihood opportunities but also offer nutritional security to the dwellers of these far-flung tropical islands

AGFD011F 3552844 5:00 PM **Effect of jackfruit seed starch on** physico-chemical and sensorial analysis of pasta P Azoubel pazoubel@gmail.com Despite the growth for gluten-free products, its inclusion in the diet, such as pasta, can impact more than 50% of the family food budget. Therefore, the use of non-conventional raw materials and by-products can be alternatives to reduce this impact. In this context, jackfruit (*Artocarpus heterophyllus* L.) seed can represent up to 15% of the weight of the fruit, with starch as its main component. Thus, the objective of this work was to produce a gluten-free pasta with jackfruit seed starch (JSS) extracted with ultrasound. Jackfruits were collected, and the seeds were removed, peeled, crushed, and the starch was extracted using ultrasound (25 kHz) for 15 min. The yield of unpurified starch was approximately 18%, which was dried at 50 °C for 310 min. JSS was used as the basis for two gluten-free pasta formulations, both being added by 25% of pregelatinized tapioca gum, and one of them added with spices dried at 60 °C. The obtained pastas were evaluated for physical-chemical composition and sensory evaluation. JSS could be considered a

nutritional source, especially of carbohydrates and proteins. The results of the sensory analysis showed acceptance of the elaborated products, being the aroma attribute the only one that presented significant difference. The jackfruit seed starch may become a raw material of wide commercial use, promoting greater diversification of ingredients.

AGFD011F 3557521 6:05 PM **Amino-acid profiling of resistant** and susceptible watermelon plants during gummy stem blight (*Stagonosporopsis cucurbitacearum*) infection Kishan Biradar kishanbiradar@tamu.edu Gummy stem blight (GSB) is a major disease of watermelon (*Citrullus lanatus*) caused by the fungal pathogen *Stagonosporopsis cucurbitacearum*, found in the majority of production areas of the United States, including Texas. The use of fungicide and crop rotation is usually advisable to control GSB. However, the pathogen that causes GSB has developed resistance to many fungicides; therefore, genetic resistance to GSB in watermelon may provide a useful alternative. Currently, there are no GSB-resistant watermelon cultivars commercially available to growers in the U.S. Moreover, very limited information is available about molecular interactions between *S. cucurbitacearum* and watermelon germplasm regarding pathogenic infection. Therefore, the main objective of this research was to screen GSB-resistant lines and commercial cultivars of watermelon using metabolomic approaches. We collected symptomatic plants from commercial watermelon fields around Texas. A strain of pathogen was isolated from lesions on stems and leaves of symptomatic plants by single spore isolation and identified based on morphological features of the colonies. Pathogenicity tests of the obtained isolate were conducted on susceptible cultivars. Seeds of five moderately resistant lines acquired from the Germplasm Resources Information Network (GRIN-USDA) and two susceptible cultivars were inoculated with the isolated pathogen. Seedlings from control and inoculated plants were collected at different times (0, 7, 14 and 21 days post inoculation, dpi) for metabolite profiling. The amino acid profile was analyzed using HPLC-FLD, which showed that amino acids such as γ -amino butyric acid (GABA), β -alanine and aspartic acid were significantly increased in seedlings at 14 dpi. Therefore, our findings indicate that free amino acids are involved in the watermelon plant's defense response to the pathogen. Further studies are required to establish the key metabolites such as hormones and phenolic acids that mount defense responses and identify key biomarkers for infection.

AGFD011F 3554446 6:00 PM **Chemometric study of post-harvest** storage effects on bioactive compounds in melon cultivars Varsha Ravindranath varsharavindranath@tamu.edu Melon (*Cucumis melo* L.) is a sweet, aromatic and flavorful important horticultural crop that is a rich source of bioactive compounds. Understanding how these phytonutrients change during post-harvest storage provides critical information for preserving the health-promoting properties of these popular fruits. Three cantaloupes (Western shipper, Infinite Gold, and Da Vinci) and three honeydew varieties (Orange Casaba, HD-150, and HD-252) grown in Uvalde, Texas were used for testing. Harvested fruits were stored at 10 °C and processed for analysis at 5-day intervals (0, 5, 10, 15 and 20 day) for carotenoids, amino acids and ascorbic acid using high performance liquid chromatography. The Tuscan type (Da Vinci) variety showed high levels of β -carotene on day 0 of storage. Total ascorbic acid content decreased from day 0 to day 20 in Western Shipper and Da Vinci melons. Honeydew variety HD252 showed the highest total ascorbic acid levels at day 5, which then gradually decreased to day 20. All six cantaloupe and honeydew melon varieties showed an overall increase in the total amino acid level by day 20 among which Da Vinci and Infinite Gold showed the highest content. Total phenolic content was the highest for the Tuscan type

(Da Vinci) melon on day 0 and for Western Shipper on day 5. The volatile profile, analyzed by HS-SPME-GC-MS, identified alcohols, aldehydes, esters, monoterpenoids, and norisoprenoids. These results indicate that the changes in bioactive compounds during post-harvest storage study are influenced by melon variety and storage period.

AGFD011F 3531083 6:00 PM **Food safety research at Virginia State University** Chyer Kim ckim@vsu.edu Recognizing the importance of food safety education toward students and stakeholders, the Food Safety and Microbiology program at Virginia State University (VSU) works continually to improve the safety and quality of our nation's food supply through research, teaching and outreach. The program's research is designed to increase knowledge of microbial ecology with regard to the routes of contamination from on-farm investigations to food distribution. The program also evaluates methods and approaches to better prevent, intervene and verify the presence of foodborne pathogens from farm to fork. Program resources are utilized to teach and train students on current and emerging food safety issues. The program provides students conventional and advanced techniques in food safety analysis, empowering them to meet global societal needs. The program works closely with Cooperative Extension specialists to benefit small-scale farmers and processors with limited resources. The program endeavors to develop a regional educational and training initiative for stakeholders on safe food production and handling. In keeping with the vision of the program, active collaborations with intra- and extramural institutions and government agencies are sought to promote multidisciplinary approaches and to strengthen research and education capacity related to current and developing issues in food safety. Therefore, my presentation will include an overview on the importance of food safety research and a summary of ongoing projects

AGFD011F 3557066 7:10 PM **Bitter melon: Exploring the nutritional potential of an underutilized cucurbit** Jose Perez jose.perez@usda.gov Bitter melon (Momordica charantia) is a vegetable that is underutilized in the United States (likely due to its characteristic bitterness), yet it is widely used in many other countries. Bitter melon is known in traditional medicine to have anti-diabetic activities among various other health benefiting properties. Several reports have identified potential bioactives in bitter melon, but the characteristics of many of its bioactives remain to be explored. Here, using various chromatographic and mass spectral techniques, we measured and/or isolated several bioactive compounds from bitter melon. In this study, we observed high levels of vitamin C in various bitter melon cultivars and high levels of various carotenoids and carotenoid esters, showing that bitter melon is a rich source of carotenoids, especially lycopene. Finally, bitter melon extracts and isolated triterpenoids displayed potent anti-inflammatory activities in RAW 264.7 cells. The results presented in this study provide vital information that can potentially be used to promote the incorporation of bitter melon in Western diets.

AGFD011F 3555484 7:00 PM **Production maximization of high-quality food additives utilizing citrus peels** Supradip Saha s_supradip@yahoo.com With the aim to fulfill the sustainable development goals (SDGs) concerted efforts have been made with the purpose of valorization utilizing citrus peel. Essential oil from three different sources (Mosambi, Kinnow and Orange) of citrus peels were extracted, characterised and found to possess dl-limonene as the major constituent. Nanoemulsion were prepared using three different technique i.e. ultrasonic bath sonicator, ultrasonic probe sonicator and high speed homogenization and characterised. Particle size analyser showed mean particle diameter of different nanoemulsions (33.42-48.83 nm, 34.56-47.32 nm and 33.87-48.25 nm for mosambi, kinnow and orange peel oil, respectively. Further

confirmation was done using TEM, which showed clear differences between two emulsions. Stability study (thermodynamic and dispersibility study) confirmed that out of these nine nanoemulsions, seven were proved to be stable and evaluated for bioefficacy study against Candida albicans . The study revealed that nanoemulsion is 3 times more efficacious than conventional emulsion. Phenolics were also extracted from the de-oiled peel, characterized and evaluated for antioxidant activity. Naringin was found to be the major component in the extract. Antioxidant activity followed mosambi peel> orange peel>kinnow peel sequence. Pectin was extracted and after characterization it was found that in general all the pectins comprised of >6% methoxyl content, >65% of anhydrouronic acid content with >50% of degree of acetyl value. FTIR showed characteristic peaks present in pectins and XRD data showed crystalline nature. Order of crystallinity followed the order was Orange>kinnow>mosambi. Rheological study of different pectins depicted their comparative flow behaviour. Prebiotic activity of three different pectins showed 2-2.5 times higher activity compared to sugar. Cellulose and hemicellulose content was determined after extracting all functional components from three peels and bioethanol potential was evaluated using yeast culture. All three citrus peels produced ethanol with >70% fermentation efficiency. Orange peel showed better result (8.77 g L⁻¹ ethanol with 84.21% efficiency) compared to kinnow (41.86 g L⁻¹, 82.07%) and mosambi peel (38.06 g L⁻¹, 74.62%). Comparative evaluation of these three peels for the production of essential oil, phenolics, pectin and bioethanol produced significant data for its further utilization.

FRIDAY EVENING 4/09/21 start 5:30 PM end 7:30 PM Sci-Mix

AGFD099A 3554033 5:00 PM **Lifetime and fate of hop (Humulus lupulus) acids in craft brewing cultivars by HPLC analysis** Celina Paoletta celina.paoletta.18@cnu.edu There are many chemical changes that take place during wort boiling, to include the oxidation of polyphenols, production of melanoidins via Maillard reactions, protein precipitation, enzyme inactivation, and isomerization of hop acids. Hops are one of the most important raw materials used in the production of beer as it is responsible for the bitter flavor and aroma of beer. The metabolites in hops also provide beer with other qualities like flavor stability, foam stability, microbial stability, color, and mouthfeel. During the wort boiling, the α -acids are isomerized to iso- α -acids. These products can lead to various ratios of the cis/trans -iso- α -acids, which can affect the kinetics of oxidative degradation as well as the bitter taste development in the final product. Environmental changes to the terroir can lead to alterations in the acid profiles of individual hop cultivars. Therefore an accurate assessment of initial α -acid components is clearly important for brewers in determining a consistent product. Additionally, determination of the fate of these compounds throughout the brewing process is of interest for studies focused on the stability and shelf life of the product. Here we present our initial findings of acid profiles from hop pellets and the corresponding isomerization and degradation products as a function of wort boiling at a local craft brewery.

AGFD099A 3549441 5:00 PM **Physical and chemical properties of edamame over bean development and application of spectroscopy-based machine learning methods to predict optimal harvest time** Dajun Yu dajunyu@vt.edu Edamame has been widely consumed in China and Japan for centuries as a snack or side dish. In the US, the consumption of edamame has been increasing, and edamame has become the second most highly consumed soy-food after soymilk because it is nutritious and has potential health benefits. The edamame harvest window is narrow but critical for producing high-quality beans. Current methods for determining the optimal harvest

time of edamame rely on the ability of experienced edamame growers to detect these changes visually, by touch or taste. These determination methods can be quite subjective and pose a major obstacle for inexperienced growers in the US. Therefore, to foster growth of the domestic edamame industry, a rapid, consistent, and standardized method for determining optimal harvest time is desired. This study aims to understand the physical and chemical property changes of edamame over bean development (R5 to R7 stages) and develop a spectroscopy-based machine learning technique to rapidly predict optimal harvest time. The results showed that pod weight, bean weight, and pod thickness peaked at R6 and remained stable for the remainder of bean development. Sugar, starch, alanine, and glycine contents also peaked at R6 but proceeded to decline thereafter. Meanwhile, fat, fiber and ash contents remained low at the R6 stage. Based on the physical and chemical properties, the harvested edamame samples was labeled as 'early', 'ready' or 'late' to indicate early, ready or late to harvest. The machine learning method based on the spectral reflectance of pods had a high accuracy of 0.95 for classifying "early" and "late" harvested edamame and 0.87 for classifying "early" and "ready" harvested edamame. This work would provide a platform technology for developing rapid and accurate prediction of optimum harvest time of edamame, which is essential to ensure to produce consistent and high-quality edamame for the market.

AGFD099A 3554996 5:00 PM **Comparison of aflatoxin and ochratoxin A levels in home-style and commercial Doenjangs** (soybean paste) prepared with traditional and modified methods Seung Yoon Kang tmddb1457@naver.com Doenjang is known as a traditional fermented soybean-based food in Korea, but safety concerns have been raised as it can be contaminated with fungi that produce aflatoxin (AF) and/or ochratoxin A (OTA) during the fermentation process. To address this, the modified method of adding selected microorganisms to starter (meju) or soybean, is sometimes used in homes and factories. The purpose of this study is to optimize and validate the method of analyzing AF and OTA in doenjang matrix, and to compare the levels of AF and OTA in home-style and commercial doenjangs prepared with traditional and modified methods. The optimized method was validated in terms of linearity ($R^2 \geq 0.9999$), limit of detection (0.015-0.173 $\mu\text{g/kg}$), limit of quantification (0.047-0.526 $\mu\text{g/kg}$), recovery (intra-day: 84.5-98.3%, inter-day: 84.0-100.0%), and precision (intra-day: 2.72-6.25%, inter-day: 2.93-7.44%). Using the method, we analyzed AF and OTA levels of a total of 60 (15 each) home-style and commercial doenjang samples prepared with traditional and modified methods. AF and OTA were detected in 11 out of 30 home-style doenjangs and in 7 out of 30 commercial doenjangs. All mycotoxins (AFB1, AFB2, AFG1 and OTA) except AFG2 were detected in doenjang prepared with traditional method, but only trace amounts of AFB1 were detected in doenjang prepared with modified method. In the commercially available traditional and modified doenjangs, total AF (sum of AFB1, AFB2, AFG1 and AFG2) was in the range of 0.54-37.89 $\mu\text{g/kg}$ and 0.18-0.39 $\mu\text{g/kg}$, respectively. On the other hand, in homemade traditional and modified doenjangs, total AF was 1.72-281.92 $\mu\text{g/kg}$ and 0.23 $\mu\text{g/kg}$, respectively. OTA was in the range of 1.25-32.64 $\mu\text{g/kg}$ in traditional doenjang, but was not detected in modified doenjang. These findings suggest that the AF and OTA levels of modified doenjang are lower than those of traditionally prepared doenjang.

AGFD099A 3552337 5:00 PM **Simple chromatographic determination of aflatoxins in Korean fermented soybean products** Doenjang, Ganjang, and Gochujang with comparison of derivatization methods So Young Woo mochalatte9@naver.com Some fungal contamination in the production of the common Korean fermented soybean products Doenjang, Ganjang, and Gochujang

saucers can produce harmful aflatoxins (AFs); therefore, there is a need for simple and effective methods for AF determination in these complex food matrices. AFs in three commercially available Korean fermented soybean sauces were analyzed by HPLC with fluorescence detection. The best AF extraction efficiency from Doenjang, Ganjang, and Gochujang sauces was achieved using methanol:water (70:30, v/v) as the solvent, and polyethylene glycol as the extraction additive. Pre-column derivatization of the AF extracts was performed using trifluoroacetic acid (TFA), and post-column derivatization was performed in a photochemical reactor for enhanced detection (PHRED). Both derivatization methods resulted in acceptable performances with suitable linearity ($R^2 \geq 0.999$), recovery (71-118%), and precision ($\leq 10.6\%$) values. The mean recovery and precision obtained with pre- and post-column derivatization were similar, but the limit of detection and limit of quantification were superior with post-column derivatization. The procedures based on TFA or PHRED described herein can therefore be implemented for the routine AF analysis of Korean Jang products and but also various types of fermented soybean products, such as Japanese Miso and Shoyu, Chinese Dajiang, Doubanjiang and Chiangyu, and Nepal Kinema. The validated method was applied in the analysis of commercial Doenjang, Ganjang and Gochujang, which showed that their contamination levels were extremely low. Among the 42 tested samples, 26% were contaminated with at least one AF in the concentration range of 0.08-0.41 $\mu\text{g/kg}$, which are significantly lower values than those of current regulatory limits

MONDAY MORNING 4/12/21 start 9:00 AM end noon
Overviews of Sustainability

AGFD003A 3552933 9:00 AM **ACS initiatives to advance the U.N. Sustainable Development Goals** Mary Kirchhoff m_kirchhoff@acs.org The U.N. Sustainable Development Goals (SDGs) provide a framework for protecting the planet, ending poverty, and ensuring that all people enjoy peace and prosperity by 2030. The chemical sciences play a key role in meeting the ambitious targets detailed within the 17 SDGs by creating therapeutics and vaccines to treat emerging diseases; producing effective fertilizers and targeted pesticides to feed the almost 8 billion inhabitants of planet Earth; and developing affordable sources of clean energy that do not contribute to climate change. This presentation will outline the American Chemical Society's (ACS) initiatives to address the SDGs in three areas: Research, innovation, and translation; sustainable manufacturing and chemicals management; and transforming chemistry education.

AGFD003A 3555289 9:00 AM **Nanotechnology for agriculture and food system: Recent advances in application research** Hongda Chen hongda.chen@usda.gov Agriculture and food systems are facing multiple daunting challenges including ensuring global food and nutrition security, the resources for advanced industrial manufacturing, consumer products, and bioeconomy toward sustainable future. Finite land, water and other natural resources of the Earth used for agricultural and food production and processing have already largely been exploited. Climate change and variability further exacerbate global agricultural production. Current practices, products and applications need to be much improved in terms of resource use efficiency to protect the environment, ensure safe and nutritious food supply, and sustain long term development. User-inspired ideas and transformative solutions emerged from multidisciplinary and transdisciplinary approaches will likely be better positioned to address system-framed challenging research questions and to lead successful inquiry. Nanoscale science, engineering and technology have enabled numerous advances that provide promises for sustainable agriculture and food system by the convergency of physical and biological sciences, biotechnology, information sciences, and other frontiers. The presentation will

provide an overview of recent research advances in nanotechnology applications for agriculture, food, and the environment. It will highlight some examples and considerations of nanotechnology R&D supported by USDA/National Institute of Food and Agriculture that address sustainability, vulnerability, health, and joy of living of society relevant to food and agricultural production, processing, and consumption.

AGFD003A 3557195 9:00 AM **The intersection of Green Chemistry and synthetic biology** Zach Serber zserber@zymergen.com John Warner jwarner@zymergen.com Through approximately 300 years of modern chemistry, humans have developed a toolbox to drive chemical transformations. With this toolbox we have been able to create medicines to cure the sick, foods to feed the hungry, and materials to house and protect our families. Biological evolution has had 3.8 billion years to design and deploy complex materials that have unique and specialized properties based on precise molecular transformations within cells. These cellular processes serve to provide the foundation of the field of synthetic biology. When considering the intersection of green chemistry and synthetic biology, there are a number of exciting opportunities to drive massive material innovation in a safer, more sustainable way. However, like chemistry itself, there are also some cautions. This presentation will explore the intersection of Green Chemistry and Synthetic Biology

AGFD003A 3551573 10:00 AM **Environmentally responsible synthetic organic chemistry catalyst formation:** Sculpted by, and used at the ppm level in water Bruce Lipshutz lipshutz@chem.ucsb.edu The facility in which Nature carries out complex organic synthesis is truly astounding, especially from the standpoint of environmental responsibility. Bonds are made in water, under mild conditions, and oftentimes using trace metal-containing catalysts. Indeed, with millions of years of “experience” to its credit, Nature is the perfect model. But since modern organic synthesis continues to be practiced, for the most part, in organic solvents, the “new rules” associated with doing chemistry in water are only recently starting to be uncovered. Processes are accumulating, indicating that real synthetic advances are to be anticipated, in addition to the payoff that such chemistry is minimizing waste generation, minimizing the need for energy to be invested (in the form of heating or cooling), and minimizing our reliance on unsustainable amounts of endangered transition metals. Taking advantage of the “nano-to-nano” effect (i.e., nano micelles delivered to nano metal catalysts), shown below (top), a new nanoparticle catalyst formed under the influence of water (bottom), mediates Pd-catalyzed Mizoroki-Heck couplings using ppm levels of precious metal in recyclable water under mild conditions.

AGFD003A 3552553 10:00 AM **Insights of chemistry in water:** metal-micelle cooperativity for sustainable catalysis Sachin Handa sachin.handa@louisville.edu Water is a safe, stable, inexpensive, and naturally abundant solvent. However, it is predominantly used for reaction work-ups in organic synthesis rather than as an alternative solvent. Nonetheless, it has many exciting features to offer better and cleaner chemistry for green chemical synthesis and catalysis, such as enhancing catalysis and controlling the reaction selectivity via metal-micelle cooperativity. Therefore, in the big picture, the use of water in syntheses enables powerful catalysis, saves toxic organic solvents, boosts the workers' and environmental safety, and adds economic value. In this talk, the focus will be on: (i) the fundamental understanding of how nanomicellar catalysis work; (ii) the design of sustainable nanocatalysts via synergy between water, metal, and micelle; (iii) reaction selectivity arising from metal-micelle cooperativity

AGFD003A 3557451 11:05 AM **Using waste carbon to produce chemicals and biofuels for a circular economy** Elizabeth Nesbitt elizabeth.nesbitt@usitc.gov Manufacturers are increasingly using emerging carbon capture utilization (CCU) technologies to capture waste carbon—in the form of carbon monoxide (CO) and/or carbon dioxide (CO₂)—from industrial emissions and process it into sustainable, value-added biofuels and chemicals. These new CCU technologies can not only benefit the environment, potentially allowing companies to meet emissions goals, but can also cut production costs and monetize industrial emissions. This working paper describes new CCU technologies stemming from advances in fields such as industrial biotechnology and electrolysis; identifies sectors and geographical locales in which these technologies are being adopted, as well as factors driving adoption; and examines potential implications for U.S. and global industrial competitiveness within one sector with high emissions, the steel industry. This paper concludes that these CCU technologies are promoting a paradigm shift that has the potential to increase firm-level competitiveness for manufacturers that adopt these processes, while also reducing the environmental impact of these manufacturers. To the extent that these technologies become widely adopted, they could result in substantial increases in supply of such chemicals globally, with potential disruptive impacts on trade and prices

MONDAY AFTERNOON 4/12/21 start 1:00 PM end 4:00 PM Biobased Polymers

AGFD003B 3556127 1:00 PM **Enzyme polymerized polysaccharides** Helen Lu helen-s.m.lu@dupont.com Polysaccharides are important biopolymers with established industrial applications, including coatings, paper, home and personal care. With the ever-increasing market demand for sustainable products, there is a renewed interest in polysaccharides materials. DuPont Nutrition & Biosciences have been developing enzyme polymerized polysaccharide technology. The enzyme polymerized technology offers the advantage of the ability to engineer the polysaccharide structure and properties based on the enzyme catalyst, the substrate, and the processing conditions. This presentation will give an overview of DuPont's enzyme polymerized polysaccharide platform. The properties and applications of representative enzyme polymerized polysaccharides will be presented.

AGFD003B 3551971 1:00 PM **Super-Hydrophobic biocoatings** of interest in food packing applications Jose Maria Lagaron Lagaron@iata.csic.es In this study, super-hydrophobic coatings suitable for the functionalization of conventional packaging paper and bioplastic films were developed. To do so, three different kinds of compostable/biodegradable biopolymers, i.e. polylactide, poly(ϵ -caprolactone), and biowaste derived poly(3-hydroxybutyrate-co-3-hydroxyvalerate) were used, processed by electrohydrodynamic processing (EDHP). As a first step, the ultrathin biopolymer fibers were deposited onto the substrates by electrospinning and, thereafter, functionalized silica nanoparticles were sequentially electrosprayed. The materials were finally optimized by low temperature annealing to further promote substrate adhesion. The films were characterised in terms of morphology, contact angle, thermal, barrier and interlayer adhesion in order to shed some light into the relationship between structure, processing and properties. The resultant materials presented a hierarchical micro/nanostructured surface with an apparent contact angle (WCA) higher than 155° and sliding angle (SA) lower than 10°. It was observed that PHA nanostructured coatings showed the best performance in terms of the overall water vapor permeance in the case of the paper substrate, and, interestingly, the super-repellent properties remained high when some foodstuffs were used instead of water. These biocoatings can have significant interest in packaging applications, where fully compostable/biodegradable packaging structures, compatible with circular bioeconomy strategies, are put

forward to, among other necessary functions, help the necessary reduction in food waste.

AGFD003B 3549516 1:00 PM **Diazonium-based chemical approach to fabricate hemp fiber composites for hydroponic application** Chin Cheung ccheung2@unl.edu This presentation describes our approach for making chemically reactive forms of lignin and lignin-containing materials and applying these materials to fabricate growing media for hydroponics. Lignin is an abundant, under-utilized, and cheap bio-resource. Our strategy is to couple lignin with a bifunctional linker molecule containing an aromatic amine and a protected vinyl sulfone. The chemical process starts with converting the aniline nitrogen of this linker to an electrophilic diazonium salt, which then reacts with the electron-rich naphthalene rings of the lignin to form the chemically reactive lignin. The other functional end of the linker is deprotected under basic conditions and slightly elevated temperatures (pH~8 and 60 °C) to yield the vinyl sulfone for forming covalent bonds to the hydroxyl groups of substrates via the Michael reaction. The process is eco-friendly because it is performed in water without organic solvents and harmless inorganic salts are the only major byproducts. Our chemical approach was demonstrated to activate lignin within hemp materials in the fabrication of hemp fiber composites. The recent increase in the cultivation of hemp in the U.S. has led to a large supply of hemp fibers. The lignin of hemp fibers was functionalized using the diazonium bifunctional linkers to make chemically reactive hemp. The anchored vinyl sulfonate groups were applied to crosslink hemp fibers with polyvinyl alcohol to yield hemp fiber composites. The hemp composites did not easily crumble under compressive mechanical tests. However, they became soft upon soaking in water. Properties of this hemp composite such as carbon/nitrogen ratio, water retention capacity values, and salinity were investigated to determine their suitability for hydroponics applications. The hemp fiber composites were evaluated as hydroponic growing media for model plant systems. Our results showed that the hemp composite can be successfully applied as other organic growing media such as peat moss for hydroponics

AGFD003B 3553222 2:00 PM **Leveraging the native properties of lignin via polymer grafting** Newell Washburn washburn@andrew.cmu.edu Lignin is an important component of plants and is the second most-abundant terrestrial biopolymer. It is the main coproduct of paper production but is underutilized in chemical and materials technologies. Polymer grafting of lignin using living polymerization chemistries has been explored to leverage the mechanical and interfacial properties of lignin through the synthesis of hybrid organic nanomaterials based on a lignin core and a polymer corona. High-strength nanocomposites can be formed through grafting thermoplastics from a kraft lignin macroinitiator while high-performance dispersants can be designed by grafting water-soluble polymers onto kraft lignin or lignosulfonate. Synergies between lignin and polymer-graft variables have been elucidated through experimental and computational methods. A machine learning algorithm has been developed to model the competing forces in complex physical systems, and this has been adopted for both molecular design as well as formulation design. Large-scale applications of lignin-based dispersants have been explored in agriculture and hydraulic cement, and the prospects for commercial translation will be discussed.

AGFD003B 3533302 2:00 PM **Toward more sustainable high-performance CFRPs via pairing bio-based resins with recycled carbon fibers** Joseph Stanzone stanzone@rowan.edu The purpose of the presented work is to provide a short yet concise update on our work related to the development of new bio-based polymeric composites that are derived from xylochemicals (wood-derived

building blocks). Short carbon fiber reinforced polymers (SCFRPs) have been produced by coupling bio-based resins and recycled carbon fibers reclaimed by the pyro-gasification of CFRP scraps. SCFRPs containing commercial, washed commercial, and recycled carbon fibers and commercial matrices were synthesized. Additionally, formulated matrices that contain polyphenolic molecules, monomers, oligomers, and resins derived, or have the potential to be derived from biomass, were utilized to generate bio-based SCFRPs. Testing of the manufactured SCFRPs has included spectroscopic, rheological, thermomechanical, thermogravimetric, and mechanical measurements to fundamentally understand the structure-processing-property relationships of our SCFRPs. Similar to nature, we strive to engineer materials that aid in sustaining life, withstand environmental stress factors, and serve multiple needs. As a result of this work, we are generating a valuable library of new bio-based polymeric composites containing recycled carbon fiber that are potentially and initially suitable for non-structural applications where relatively high performance, lightweight, and low-cost material is desired and required.

AGFD003B 3550109 3:05 PM **Macromolecular materials from various biomass feedstocks: a contribution to bioeconomy development** Elisabete Frollini elisabete@iqsc.usp.br Macromolecular materials from various biomass feedstocks: a contribution to the bioeconomy Macromolecular materials have been prepared using raw material mostly from lignocellulosic, oilseed, and forest biorefineries. Methodologies of relatively easy application have been sought to increase the possibility of scaling. In this context, hydrogels have been obtained via the deconstruction of sisal lignocellulosic fibers, using LiCl and dimethylacetamide as a solvent system (which can be recovered with a yield above 95%). The hydrogels have shown high water absorption capacity (up to approximately 7500% absorbed water content). Microcrystalline cellulose (MCC) and castor oil (CO) have been used as polyols, together with polymeric diphenylmethane-4,4'-diisocyanate (pMDI), to synthesize polyurethanes with simultaneous film formation. The polyurethane-type films have shown transparency; the ratio cellulose/CO tuned other properties. The glass transition temperature (T_g, from tan delta peak) ranged from sub-ambient, 6°C, to 75°C, for 0% and 100% MCC, respectively. The tensile strength at break increased to approximately 800%, and the modulus to approximately 15 000%, from 0% to 100% MCC. Hydrogels and polyurethane-type films were evaluated for cell viability and proved to be non-cytotoxic. Sodium lignosulfonate and CO (polyols), and pMDI were used to synthesize polyurethanes (in a mold, under temperature and pressure). The reagents were mixed and distributed below and above sisal or rayon blankets, with or without 20% MCC, and composites were formed simultaneously with the synthesis of polyurethanes-type matrices. The materials proved to be unbreakable under flexure, and did not fracture under impact when MCC was one of the composite reinforcements. These studies have added value to renewable raw materials. They have also contributed to decreased fossil feedstock use considerably, thus collaborating with both the development of the bioeconomy and to pave the way to reach sustainability

MONDAY EVENING 4/12/21 start 5:00 PM end 7:40 PM
Chemistry and Health Benefits of Fermented Foods

AGFD008A 3548324 5:05 PM **Biochemical conversion and flavor chemistry of Congou black tea: From fresh leaves to tea infusions** Jia Li jiali1986@tricaas.com Tea, brewed from leaves of *Camellia sinensis*, is the most popular beverage worldwide. Congou black tea is the orthodox Chinese black tea known for its elaborate manufacturing procedures, from plucking of fresh leaves, to the processing (withering, rolling, fermentation, firing, refinement), and to the brewing. Thus it is of significance to investigate biochemical

conversion and flavor chemistry of congou black tea at different stages. This report will summarize our recent efforts in this context, from fresh leaves to the processing and tea infusions. To explore the features of tea cultivars suited for black tea processing, nontargeted metabolomics, combined with comprehensive pathway mapping, were performed on fresh leaves of different tea cultivars. Cultivars suited for black tea manufacturing had significantly higher catechins, condensed products and phenolic acids, and lower contents of flavone C-glycosides, free sugars, and amino acids. Unique glycosylation patterns of flavonol glycosides were also identified. Further, a novel method for wide-scale tea lipids profiling was established, enabling simultaneous analysis of 200-300 tea lipids. This method was used to study the dynamic changes of tea lipids during black tea processing. The significantly differential lipids and related metabolic pathways have been identified, involved with chlorophylls degradation, glycolipids degradation, and other extraplastidial membrane lipids' metabolic pathways. Particularly, the glycolipids enriched with acyl chain 18:3, e.g., monogalactosyldiacylglycerol (MGDG) (18:3/18:3), showed the most significant decrease during the rolling phase, which may contribute to aroma formation during black tea manufacture. In addition, we investigated the key compounds that influence the sweet-mellow taste of congou black tea infusions, employing an integrated approach consisting of quantitative analysis of taste-active compounds, taste contribution analysis, taste supplementation experiments and human sensory evaluation. It was found that caffeine, γ -aminobutyric acid, rutin, succinic acid, citric acid, and gallic acid negatively affect the sweet-mellow taste. In contrast, glucose, sucrose, and ornithine positively contribute to the sweet-mellow taste. Particularly, rutin, γ -aminobutyric acid, gallic acid, and caffeine, which impart a significant inhibitory effect to the manifestation of the sweet-mellow taste, were identified as the key impact components.

AGFD008A 3553503 5:00 PM **Plant-based compounds improve** the antifungal and antiaflatoxigenic efficiency of strobilurins against *Aspergillus flavus* Fei Tian tianfei_real@163.com Aflatoxins are a group of carcinogenic and mutagenic fungal secondary metabolites that have threatened human health and global food security. Aflatoxin contamination can be controlled by applying fungicides, such as strobilurins. Although these compounds have been effective, they may be risky to the environment and human health due to their wide usage. In this study, a total of 68 plant-based compounds were tested to promote the performance of strobilurins (azoxystrobin and pyraclostrobin) against aflatoxigenic *Aspergillus flavus*; six natural compounds, including flavonoids ($n = 2$), lignans ($n = 3$) and terpenoid ($n = 1$), were found to exhibit synergistic antifungal effects with strobilurins with fractional inhibitory concentration index < 0.5 . Multiple natural compounds showed no inhibitory effects against *A. flavus* growth, but strongly suppressed aflatoxin production. This kind of activity would be greatly useful for removing aflatoxin from fermented foods without altering their original microbial community. Some of them also greatly enhanced the *in vitro* and *in situ* antifungal and antiaflatoxigenic efficacy of strobilurins and transformed them from fungistatic to fungicidal agents. These plant-based compounds may be used as effective natural chemosensitizing agents to improve the performance of strobilurins against *A. flavus*. These findings provide novel insights for the development of safer and more effective strategies for the control of aflatoxin contamination in food cereals and fermented foods.

AGFD008A 3555607 5:00 PM **Fermented and cooked vegetables** as a source of bioactive compounds with potential ability to inhibit *in vitro* glycation process Malgorzata Starowicz m.starowicz@pan.olsztyn.pl The aim of the research was to analyze the anti-glycation activity of vegetable-based products and to

determine its relationship with the profile and content of their bioactive molecules. The material used in the research was beetroot *Beta vulgaris* (raw, fermented, cooked) and red cabbage *Brassica oleracea* (raw and fermented). Experiments of advanced glycation end-products formation (AGEs) were carried out in the *in vitro* model systems of bovine serum albumin-glucose (BSA-glucose) and albumin-methylglyoxal (BSA-MGO). The spectrophotometrical measurement of the total content of phenols (TPC) and flavonoids (TF) was determined. Moreover, the profile of bioactive compounds (phenolic acids, flavonoids, anthocyanins and betalains) in extracts from selected products was also analyzed using the LC/MS-MS method. The fermentation process of red cabbage showed an increase of TPC at 10% and 14% in TF in comparison to raw material. The fermentation and cooking process decreases the TPC and TF values for beetroot. In turn, the fermentation of both beetroot and red cabbage increased the ability to inhibit AGEs. Fermented red cabbage extracts showed a higher level of AGEs inhibition by 17% (BSA-MGO) and 25% (BSA-glucose), while fermented beetroot extracts by 23% and 18%, respectively, compared to raw materials. The cooking of red beetroot reduced its anti-glycation abilities by 13% in the BSA-MGO model and by 16% in BSA-glucose, compared to fresh material. The dominant bioactive compounds in fermented red cabbage are 3-(sinapoyl)(sinapoyl)-diglucoside-5-glucoside and cyanidin-3-diglucoside-5-glucoside, as well as sinapic acid and epicatechin. In contrast, compounds such as syringic acid and epicatechin dominate in fermented beetroot, and isoferulic acid in cooked. 2.17-bidecarboxy-betainin, and 2.5.17-tridecarboxy-betainin were noticed as the dominant compounds of betalains, both in fermented and cooked red beetroot. The fermentation process of red cabbage and beetroot can have a positive effect on the health-promoting properties of the designed food. The tested products can be a rich source of bioactive compounds. At the same time, they can be effective inhibitors of the formation of AGEs and probably decrease AGEs accumulation in the human body, and thus can be a part in the broadly understood prevention of diet-related diseases

AGFD008A 3554930 6:00 PM **Improving the safety of Queso Fresco** Michael Miller mille216@illinois.edu *Listeria monocytogenes* is an opportunistic and zero-tolerance foodborne pathogen that causes listeriosis, a rare illness but with a high fatality rate. Listeriosis outbreaks have often been linked to the consumption of Hispanic-style cheeses (HSC), accounting for 17% of total outbreaks in the U.S. in the past ten years. In particular, Queso Fresco (QF), the most common HSC in the U.S., is characterized by a near neutral pH, high fat ($> 20\%$) and low salt ($< 3\%$) content, and a short shelf-life requiring refrigeration. In addition, QF is known to support the growth of *L. monocytogenes*. For the last five plus years, my group has focused on improving the safety of QF. Initially, we developed a miniaturized laboratory-scale queso fresco (MLQF) that accurately replicates the composition of commercial QF while enabling the incorporation and testing of novel antilisterials. The *Listeria* phage endolysin PlyP100, a lytic enzyme from the GRAS phage P100, is listeriastatic for 28 days in QF. Evaluation of endolysins from different *Listeria* phages has confirmed that PlyP100 is currently the best endolysin for QF. While nisin A by itself is completely ineffective, combining PlyP100 with nisin A can reduce the *L. monocytogenes* population by 5-log over 28 days of refrigerated storage. We have improved the antilisterial efficacy of nisin A by creating a targeted mutant, H27/31K, with improved biochemical characteristics (decreased hydrophobicity and increased solubility at pH 7) that are suitable for its application into QF. Combining PlyP100 and H27/31K is the most effective antilisterial treatment we have discovered for QF. Our work highlights that there are listeriastatic and listeriacidal antimicrobials that can be added to QF and dramatically improve the safety of QF

AGFD008A 3558802 6:00 PM **Characterization of aroma-active compounds in chardonnay marc** John Munafo jmunafa@utk.edu Chardonnay is the most abundant grape varietal in California wine production. Chardonnay marc, also referred to as chardonnay pomace, is the main by-product in the production of the juice that is fermented into chardonnay wine. The marc is comprised primarily of grape skins, seeds, and stems. Initiatives to decrease waste and uncover alternative uses of agricultural by-products have led to the discovery that chardonnay marc contains a rich source of health promoting molecules. Studies suggest that marc, including chardonnay, has the potential to significantly benefit human health, including improvements in cardiovascular health, gastrointestinal health via modulation of the microbiome, and modulation of inflammatory response. In addition to the health benefits, chardonnay marc has recently gained popularity as a flavorful new superfood ingredient with its mild velvety astringency, slightly tart taste, and subtle floral and fruit-like aroma attributes. To gain the first insights into the aroma contribution of the individual components, dried grape skin clusters, manually separated from WellVineTM chardonnay marc, were subjected to aroma extract dilution analysis (AEDA). Thirty-five odorants were identified, including 13 with flavor dilution (FD) factors ≥ 64 . Odorants with high FD factors (FD 1024) included β -ionone (floral, violets), (2E,4E)-nona-2,4-dienal (fatty), and (2E,4E)-deca-2,4-dienal (fatty). Odorants with FD factors of 256 included 3-methylnonane-2,4-dione (hay-like) and 2,5-dimethyl-4-hydroxy-3[2H]-furanone (caramel). Some odorants with FD factors of 64 included ethyl octanoate (fruity), β -damascenone (cooked apple), hexanal (green), linalool (floral, citrus), and 2-phenylethanol (floral, rose). As a result of these findings, a collection of odorants was identified that contribute to the complex aroma of chardonnay marc. Our present investigation establishes a foundation for future studies aimed at determining the contribution of individual components (skin, seeds, and stems) to the aroma profile of chardonnay marc.

AGFD008A 3548570 7:00 PM **Activity of endogenous and exogenous amylases in wheat bread** Katharina Scherf katharina.anne.scherf@gmail.com The use of exogenous microbial enzymes is common in wheat bread making to help standardize dough and bread quality, reduce dough stickiness, increase mixing stability, improve bread volume and prolong shelf-life. While endogenous enzymes from wheat and yeast are also active in the dough, their activities are lost during baking due to heat-induced irreversible denaturation. In contrast, some exogenous enzymes, especially maltogenic α -amylases, are known to be heat-resistant, so that their activities may partially persist in the final product. According to legislation in the European Union, enzymes used as processing aids do not have to be labeled, because they are not classified as food ingredients of technological relevance in the final product. However, in case residual enzyme activity persists and this causes a functional effect in the product, the enzyme would have to be labeled. To clarify which exogenous amylases still have detectable residual activity in bread crumb, we added one selected α -amylase, maltogenic or maltotetraogenic amylase each to a model toast bread. Residual amylase activities were analyzed using standard test kits and starch hydrolysis products including glucose, maltose and oligosaccharides were quantitated by high-performance anion exchange chromatography with pulsed amperometric detection. Discovery-driven proteomics revealed the identities and relative proportions of the amylases in each preparation. The addition of each exogenous amylase led to characteristic changes in saccharide concentrations in bread crumb compared to the control. As expected, the main starch hydrolysis product was maltose, followed by glucose, maltotriose, maltotetraose and other oligosaccharides with up to eight glucose units. Five out of six α -amylases had no detectable residual activity in bread crumb 22 h after baking, whereas one α -amylase and

both maltotetraogenic amylases had very low residual activity amounting to less than 4% of the applied activity. All five maltogenic α -amylases showed detectable residual activities ranging from 14-45% of the applied activity and the maltose concentrations also increased in these breads during storage for up to 96 h. All amylase preparations contained the main enzyme next to variable percentages of wheat flour or starch as carrier material. Overall, the changes in saccharide concentrations over longer storage periods might eventually result in a functional effect due to starch degradation.

TUESDAY MORNING 4/13/21 start 9:00 AM end 11:50 AM

Food Processing

AGFD002A 3549792 9:05 AM **A new nanocarrier prepared by ultrasonic self-emulsification method for mitochondrion-targeted astaxanthin delivery** Mingqian Tan 2468750030@qq.com Oil in water (O/W) nanocarriers for mitochondrion-targeted astaxanthin delivery were constructed by using (3-carboxypropyl) triphenylphosphonium bromide (TPP) modified casein emulsion through the method of ultrasonic self-emulsification. The morphology of nanocarriers was characterized by TEM and SEM. The results showed that the nanocarriers of casein emulsion loaded with astaxanthin and casein emulsion modified by TPP encapsulated with astaxanthin had spherical structure and the average particle size was 300.6 and 615.2 nm, respectively, with an encapsulation efficiency of $88.51\% \pm 1.85\%$ and $80.51\% \pm 6.29\%$. After encapsulation, the thermal stability and resistance to UV radiation of astaxanthin were significantly improved and the ability of astaxanthin to scavenge DPPH was well protected. The results of fluorescence co-localization imaging proved specific targeting effect of casein emulsion modified by TPP toward cellular mitochondria. Meanwhile, after modification by TPP, the nanoemulsion on cellular reactive oxygen species, mitochondrial membrane potential, and cell viability of normal rat kidney (NRK) and RAW264.7 (leukemia cells in mouse macrophage) cells were evaluated, and the results showed that the nanoemulsion could significantly protect the function of mitochondria and promote the growth of cells. After modification with TPP, the nanoemulsion improved the bioavailability and biocompatibility of astaxanthin, which provided a strategy for efficient utilization and absorption of astaxanthin.

AGFD002A 3551873 9:00 AM **Development of a model for espresso extraction** Christopher Hendon chendon@uoregon.edu Typical espresso is a small (< 50 mL), concentrated (~10% w/w coffee solubles), beverage made using high pressure and temperature water. However, the variability in flavor between two seemingly identical shots of espresso highlights a more fundamental challenge with its production — the complex interplay between several independent variables. To overcome this variability, we have developed a numerical model¹ that enables the isolation of each variable (e.g. grind size, mass of coffee, mass of water, temperature, etc.), and provides a blueprint to access reproducible flavor profiles for any particular coffee prepared on an espresso machine. To parameterize the extraction, we develop a rate law based on diffusivity of coffee solubles within the particles, as well as a rate constant that broadly encompasses the extraction of "coffee" (treated as one collection of equally soluble molecules). Our model highlights key areas of variability in espresso extraction, and emphasizes the importance of particle size.

AGFD002A 3554583 9:00 AM **Pasteurization and alternatives applied to extend safety and shelf-lives of novel beverages** Jaime Jurado j2jurado@aol.com Pasteurization represents our oldest established and proven food safety technology applied to beverages. Novel alcoholic and non-alcoholic beverages have emerged which benefit from the stability of pasteurization, and today there are other means available (either chemical, or mechanical) to preserve and

stabilize novel beverages. A review of application of various options available currently, accompanied by notes on relative levels of treatment are shared and influences on resulting flavors

AGFD002A 3555519 10:05 AM **Distribution and antioxidant efficiency of theaflavins in stripped soybean oil/ Tween 20** Lu Chegn lc894@scarletmail.rutgers.edu Efforts to minimize the lipid oxidation in oil-in-water (O/W) emulsions have been made for many years. One of the most effective, economical and convenient employed strategies for food system is addition of antioxidants (AOs). Theaflavins (TFs) as an important group of AOs are reported to effectively inhibit lipid oxidation. The AOs efficiency in O/W emulsions depends not only on their rate constants of scavenging free radicals but also on their distributions. However, determining TFs distributions in intact O/W emulsions is not an easy task because of the physical impossibility of separating the interfacial region from the oil and aqueous regions. In this study, we employed a well-established pseudophase kinetic method on the basis of reactions between a hydrophobic 4-hexadecylbenzenediazonium ions (16-ArN₂⁺) and the selected / water based oil-in-water emulsions: application of a novel pseudophase kinetic method.

AGFD002A 3556792 10:00 AM **Developing analytical grade chemical digestion procedures for beer** Jason Farmer jcf257@nau.edu The Food Safety and Modernization Act has led to increased oversight of beer production. Throughout history, commercially available beer has remained unregulated relative to other food and beverage products. At present, the brewing industry is transitioning from minimal oversight to regulations more in line with other commercial beverages. Mounting pressure from regulatory bodies and industry rivals has created considerable demand for better QA/QC procedures pertaining to beer. One topic of growing interest and concern is the heavy metal content of finished beer. There are currently no impactful regulations on the heavy metal content of commercially available beer. Recent research has indicated the presence of previously unknown heavy metal contaminant exposure routes in the industry. Two areas of particular concern are: 1) diatomaceous earth filter-aids facilitate the transfer of arsenic. 2) low grade or incorrectly graded stainless steel is suspected of leaching chromium into process water and beer in progress. This is worrisome, as it is the responsibility of brewers to ensure that consumers are not chronically ingesting trace metals. The industry needs methods that ensure quality control. An optimized sample digest procedure would be a significant boon to this effort. Inadequate chemical digest leads to analyte losses and subsequent false negatives. An adequate digestion protocol would prepare a sample for elemental analysis, without losing analyte or introducing heavy metal contaminants. Applying such methods to beer is a difficult task. Beer is a loose term that applies to a complex organic sample matrix with distinct compositions and infinite varieties. Even consecutive executions of the same brewing processes can produce batches with significant chemical differences. The focus of this presentation is the development of analytical sample digest methods; these methods will enable brewers and chemists alike to probe their beer with rigor and reproducibility

AGFD002A 3554559 10:00 AM **Separation of fusel oils by distillation** Farley Chicilo chicilo@gmail.com As a result of the Covid-19 pandemic, biofuel ethanol production has become a vital source of higher grades of ethanol used in producing disinfectants and hand sanitizers like United States Pharmacopeia (USP) grade. Fusel oils, which accumulate in yeast fermented solutions through the action of the Ehrlich pathway, can be included in biofuel. However, the mixture of higher alcohols present in fusel oils, including amyl, n-propyl, and isobutyl alcohols are only allowed in small concentrations in USP ethanol. During fractional distillation fusel oils

can accumulate in the rectifier and are removed in a fraction that contains ethanol and water to improve distillation performance. The resulting fusel oil/ethanol/water mixture can be further distilled, separating recovered ethanol from fusel oils. Fusel oils can be recovered for industrial applications such as burning the oils to supply energy for a plant, or be used in fuel additives. In this project, the components of a mixture of fusel oils procured from local and sustainable sources, are performed using multiple high resolution distillation techniques (ex: fractional, spinning band distillation) in both laboratory and larger scale applications. The distilled materials obtained using these various techniques are evaluated using gas chromatography, and the efficacy of each method is compared. Using high resolution distillation techniques, technical grade ethanol is produced with the potential to be used as a disinfectant for hand sanitizer applications. Additionally, this process separates the higher alcohols present in fusel oil, allowing for the materials to be repurposed and reducing the cost for manufacturers.

AGFD002A 3530952 11:10 AM **Selecting effective drying strategies for small-scale hop growers: aroma and quality considerations** Xueqian Su xueqians@vt.edu Hop (*Humulus lupulus L.*) is known as an indispensable raw material for beer brewing and is usually added in the form of dried cones. As a result, drying has become an important postharvest practice for hops, with kiln or belt drying being the most common practices to achieve mass production in industrial scale. However, there has been a significant increase in the number of microbreweries and home growers in recent years, suggesting the needs for effective drying techniques for small-scale hop handlers. This study aimed for selecting an efficient small-scale drying method to appropriately preserve aroma and quality of hops from oven, dehydrator and freeze-drying approaches. Fresh Cascade and Chinook hops that harvested from different regions in Virginia were dried to 8.5 to 10% moisture content (wet basis) by oven, dehydrator and freeze-drying techniques, respectively. Aroma profiles of dried hops were characterized by headspace solid phase microextraction-gas chromatography-mass spectrometry-olfaction (HS-SPME-GC-MS-O). Stable isotope dilution analysis (SIDA) and standard addition method (SAM) were applied to quantify predominant aroma-active compounds. Principal component analysis (PCA) and hierarchical cluster analysis (HCA) were employed to indicate the volatile variation among hops obtained from different drying techniques. Total essential oil content and bittering acids panel were analyzed following ASBC standard methods 13 and 14, respectively. Color quality of dried hop cones was measured using colorimeter with L, a, b scales. A total of 36 aroma-active compounds were identified in all dried hop samples, with β -myrcene and α -humulene dominating the profiles. In general, the contents of both individual aroma compound and total essential oil were always the highest in dehydrator-dried hops especially when comparing to oven-dried hops. PCA and HCA results revealed the distinctive aroma profiles for hops from different drying approaches. Additionally, the α -acid and β -acid contents in hop cones were not significantly affected by different drying methods in most of the hop samples. Freeze-drying approach provided the most desirable color for all hop samples. In conclusion, dehydrator drying was a realistic and effective drying practice for small-scale hop handling due to the low equipment investment and the advantages on aroma and quality retention. The findings of this study will help improve the quality and value for local hop and brewing products

AGFD002A 3554238 11:00 AM **Utilizing the diverse hydrogen sulfide release properties of dialkylthiophosphates for applications in agriculture** Eric Brown eric-m-brown@uiowa.edu Hydrogen sulfide is an important gasotransmitter in plants that has been shown to aid in the survival of plants during environmental stressors such as

droughts and high levels of salt in soil. Because hydrogen sulfide is a gas and toxic at high concentrations, delivery of hydrogen sulfide to plants is achieved by using chemicals that degrade to release hydrogen sulfide. The common chemicals used for this include sodium sulfide and GYY-4137. Sodium sulfide releases hydrogen sulfide too quickly to be applicable, and although GYY-4137 offers a more sustained release, the byproducts are not naturally found in the environment. Additionally, these chemicals are not easily tuned to control the rate of release of hydrogen sulfide. A series of dialkyldithiophosphates were synthesized using different alkyl alcohols or thiols. Upon addition to water, these chemicals had a sustained and slow release of hydrogen sulfide. The rate of release of hydrogen sulfide was easily tuned by changing the alkyl group. Degradation products from these chemicals included phosphoric acid and the corresponding alcohols, which are both natural chemicals depending on the alcohol used. Rate constants of the degradation of each chemical were obtained at elevated temperatures. The rates varied by four orders of magnitude, giving rise to easily accessible chemicals with vastly different hydrogen sulfide releasing properties, an important characteristic for the future of hydrogen sulfide releasing chemicals in the field of agriculture. To show the potential of these dialkyldithiophosphates in agriculture, peas were treated with dibutyldithiophosphate and the weight of the pea plant increased by 43% at a small loading of 1 mg per plant.

TUESDAY MORNING 4/13/21 start 9:00 AM end noon
Biobased Molecules

AGFD003C 3530507 9:00 AM **Combining solid dispersion-based spray drying with co-spray drying agents to improve the functionality and flavor profile of pea protein isolate.** Jiajia Rao jiajia.rao@ndsu.edu The common method used in the food industry to manufacture pea protein isolate (PPI) is extracted by alkaline extraction-isoelectric point precipitation, followed by spray drying. In this study, the effect of adding a different type of co-spraying agent (cyclodextrin, disaccharides, emulsifying salt) to PPI at a ratio of 10:90, on the structure, functionality and aromatic profile of spray-dried PPI was studied. Results showed that the addition of co-spray drying agent induced protein conformational changes in accordance to FTIR spectrum and quantification of free sulfhydryl and disulfide groups. The surface charge (ζ -potential) and surface hydrophobicity of co-spray dried PPI was also modified substantially. Such structural changes exhibited significant impacts on the functionalities of co-spray dried PPI, including solubility, water/oil binding capacity, thermal property, emulsifying capacity and stability, and foaming capacity and stability. In general, co-spray dried PPI with emulsifying salt (e.g., sodium hexametaphosphate) had better functionalities. For example, the better foaming properties of co-spray dried PPI with sodium hexametaphosphate was also supported by measuring their ability to reduce air-water surface tension. In addition, the impact of co-spraying agents on the aromatic profile of PPI was investigated. Heat map analysis also showed a remarkable beany odor mitigation effect upon the addition of cyclodextrin, which was further proved to be due to cyclodextrin entrapping aroma compounds during spray drying. The developed technique could potentially increase the functionality and aromatic profile of PPI, thus providing commercial available tools for quickly adapting to the food industry.

AGFD003C 3542307 9:00 AM **Highly compostable high oleic soy-based impact-modifiers via reactive extrusion with polyesters** Eric Cochran ecochran76@gmail.com In this talk I share recent progress we have made with the application of poly(acrylated epoxidized high oleic soybean oil) (PAEHOSO) as a biobased and biodegradable impact modifier for polyesters. With proper modification, polyesters like poly(L-lactic acid) (PLLA) and poly(butylene terephthalate) (PBT) can serve as high performance

engineering thermoplastics. To date, the most effective impact modifiers have been rubber-filled core-shell particles. While composites bearing these particles have excellent performance, the cost and sustainability are drawbacks, especially in materials like PLLA that are often chosen for their renewable carbon and biodegradability. PAEHOSO and related copolymers comprise a family of biobased and highly compostable thermoplastic rubbers from high oleic soybean oil. These polymers contain a rich variety of residual functionality—epoxy, vinyl, ester, and alcohol—that can be exploited in the extruder barrel to yield interface-stabilizing graft copolymers with a chemically complementary matrix component. By tuning the PAEHOSO architecture and compounding parameters, we can design extrudates with rubbery PAEHOSO micelles encapsulated by a robust interfacial region. These micelles effectively blunt crack propagation and dissipate energy through cavitation, increasing the impact strength by up to two orders of magnitude with minimal deterioration in modulus.

AGFD003C 3559078 9:00 AM **Benign by Design Bioproducts** William Hart-Cooper william.hart-cooper@usda.gov Environmental persistence can amplify toxic effects of chemicals, exacerbating antibiotic resistance, aquatic toxicity and hazards to human health. Agriculturally-derived bioproducts are being increasingly sought as low-toxicity, biodegradable alternatives to hazardous substances. Inspired by nature, the principles of green chemistry and self-assembly were used to develop low-hazard ingredients for agricultural, industrial and consumer use. Design principles used to develop safer pesticides, packaging and cleaning ingredients are described. These examples attest to the power of fundamental chemical properties, including reversible bonding, charge, and lipophilicity, to reduce human and environmental hazard.

AGFD003C 3558264 10:00 AM **High-performance sustainable aviation fuels from bio-based terpenes** Benjamin Harvey benjamin.g.harvey@navy.mil Terpenes are ubiquitous natural products that can be obtained from sources including crude sulfate turpentine (byproduct of paper production), gum turpentine, and plant extracts. More recently, these molecules have been prepared by fermentation of biomass sugars with metabolically engineered organisms. This latter approach opens the way to the utilization of wood, agricultural waste, and lignocellulose as abundant sustainable feedstocks that can be leveraged for the production of terpene-based platform chemicals, polymers, and advanced sustainable aviation fuels (SAFs). Terpene-based SAFs offer a number of benefits compared to conventional jet fuel including, higher densities, higher gravimetric and volumetric heats of combustion, as well as lower viscosities and freezing points. These properties allow for the formulation of designer biosynthetic fuels that outperform petroleum-based jet fuel. This presentation will discuss various sources of terpenes (wood drying operations, production of isoprenol and isoprene via fermentation), catalytic methods for the conversion of terpenes to advanced jet fuels, and structure/property relationships for terpene-based fuels. Finally, a roadmap for exploitation of this technology in commercial and military aviation will be outlined.

AGFD003C 3551779 10:00 AM **Production and purification of natural phenylpropenoids** David Compton david.compton@ars.usda.gov Ethyl ferulate was transesterified with a soy-based vegetable oil containing 80 – 85 % diacylglycerol using Novozym 435 at 60 °C. The resultant feruloylated vegetable oil reaction product produced a precipitate (96.4 g, 4.02 wt%) after 7 d of standing at room temperature. Preliminary characterization of the precipitate identified the natural phenylpropenoids 1,3-Diferuloyl-sn-glycerol (F₂G) and 1-Feruloyl-sn-glycerol (FG) as the major components. A flash chromatography method was developed and optimized (e.g., mass of sample load, flow rate, binary solvent

gradient slope, separation run length) using a binary gradient of hexane and acetone mobile phase and silica gel stationary phase to separate and isolate F₂G and FG. The optimized parameters afforded F₂G (1.188 ± 0.052 g, 39.6 ± 1.7 %) and FG (0.313 ± 0.038 g, 10.4 ± 1.3 %) from 3.0 g of the transesterification precipitate, n = 10 trials. Overall, all flash chromatography separations combined, F₂G (39.1 g, 40.6 %) and FG (9.4 g, 9.8 %) were isolated in a combined yield of 48.5 g (51.4 %), relative to the 96.4 g of transesterification precipitate collected. The optimized flash chromatography method was a necessary improvement over previously reported preparative HPLC and column chromatography methods used to purify milligram to low gram quantities of F₂G and FG to be able to process ~ 100 g of material in a timely, efficient manner.

AGFD003C 3555016 11:05 AM **Flavonoids: diverse functions and values as nutraceuticals, drug leads and wastewater treatment catalysts** Qing Li qingl@hawaii.edu Flavonoids are a large family of plant secondary metabolites. Three flavonoids – cyanidin, dihydromyricetin and isoorientin – are discussed here. Cyanidin is a common type of anthocyanin. Our recent studies showed that cyanidin promotes photoreductive degradation of the fungicide chlorothalonil and the herbicide dichlobenil via hydrogen radical. The photosensitization efficiency is apparently related to flavonoid structures and likely to their hydrogen donation ability. Obesity is one of the most serious public health problems, due to accumulation of excessive adipose tissue. Therefore, the discovery of inhibitors against adipose tissue accretion contributes to developing anti-obesity therapies. We recently found that dihydromyricetin can dramatically reduce intracellular oil droplet formation in 3T3-L1 adipocytes. We performed the drug affinity responsive target stability and surface plasmon resonance experiments and demonstrated the direct interactions between dihydromyricetin and the 78-kDa glucose regulated protein, having a dissociation constant of 22 μM. The results suggest new understanding of dihydromyricetin in the modulation of obesity and hold promise for anti-obesity applications. Structural modifications of dihydromyricetin may be worthwhile for anti-obesity drug discovery. Alzheimer's disease (AD) is a progressive neurodegenerative disorder and the most common dementia. The three main hallmarks of AD are clear: Aβ plaques, tau tangles and neuroinflammation, although the mechanisms involved in AD pathology are not well understood. Our recent results showed that isoorientin alleviates all the three AD hallmarks in vivo mouse models and in vitro. Isoorientin selectively inhibits glycogen synthase kinase 3β (GSK-3β) in vitro and alleviates tau hyperphosphorylation, neuronal cytotoxicity, neuroinflammation and/or inflammation in neuron cells, microglia, macrophages, APP/PS1 model mice and endotoxemia mice, in addition to cognitive and memory enhancement in AD-like mouse model. GSK-3β is a putative action target of isoorientin and its semi-synthetic analogs. Isoorientin may serve well as a nutraceutical and as a drug lead to develop GSK-3β inhibitors as AD drugs.

TUESDAY AFTERNOON 4/13/21 start 1:00 PM end 4:00 PM
Byproduct Utilization

AGFD003D 3559081 1:00 PM **New uses for crop coproducts toward zero waste agricultural processing** William Orts bill.orts@usda.gov The Western U.S. is among the world's leaders in production of a wide array of specialty crops, including almonds, walnuts, pistachios, table grapes, wine grapes, olives, lettuce, artichokes, avocados and, most recently, hemp. This presentation outlines recent strategies by our USDA research team to optimize the value of crop coproducts toward “zero waste” processing. In one project we apply torrefaction, a thermal treatment in which feedstocks are heat-treated between 200-300°C in limited oxygen to create “torrefied” fibrils and nanoparticles. Results

are presented in which torrefied almond shells (TAS) were evaluated as fillers in industrial natural rubber compounds for full and partial replacement of petroleum-derived carbon black. TAS altered thermomechanical properties including curing time, dynamic modulus, and tensile strength compared with industrial carbon black., most likely a result of particle size; particles derived from almond shells were larger than the petroleum-derived particles. Subsequently, TAS were tested in the rubber bumpers used in tree shakers to harvest almonds. Tree shakers employ large rubber shaker pads as vibration transmission/dampening elements. A proprietary natural rubber formulation was developed and employed that utilized TAS as a potential carbon black substitute. In a related project composites were made from landfill-diverted plastic compounded with TAS. We will describe a multi-million dollar project with CalRecycle and several industrial partners to build a first of its kind processing line to add torrefied almond shells to landfill-recycled plastics as part of a statewide initiative to reduce greenhouse gases, lower pollution, and create financial incentives for building industries in disadvantaged communities. The addition of torrefied almond shells to degraded plastics acts as mechanical reinforcement and can be customizable for specific applications

AGFD003D 3558172 1:00 PM **Comprehensively sustainable circular materials by natural fiber welding** Luke Haverhals luke.haverhals@gmail.com The problems associated with extraction of finite fossil resources to produce energy and materials are substantial. Presently, trillions of dollars per year of high carbon footprint plastics are produced for fashion, accessories, footwear, automobile interiors, et cetera for about 1/5th of the world's population that can afford luxuries such as a new car or couch. Comprehensive definitions for ‘sustainable’ footwear or ‘circular’ fashion have not been agreed upon. Moreover, data sets to measure the impacts of plastics are noticeably lacking and, as a result, the true cost of plastics to the environment and societies is not acknowledged. Add to this that unit economics, chemistry, product design, and logistics conspire to severely limit that amount of plastic recycled globally. Meanwhile, plastics pollute the environment in a number of ways including microfiber from washing 100's of billions of pounds of plastic clothing. In contrast, nature – and, in particular, photosynthesis – is the most abundant, versatile, sustainable, and ‘circular’ production system in the known universe. Plants are amazingly diverse and grow in nearly every part of the biosphere. Using solar power, nature upcycles, downcycles, and recycles nutrients into complex materials that are interchangeable and that are balanced across orders of magnitude of scale and multiple dimensions (e.g., space and time). We will explore examples of how complex natural composites, produced from abundant natural ‘waste’, can be the genesis for a comprehensively sustainable and circular materials economy. In particular, we describe materials that use biomass ‘as is’ and/or with minimal derivatization so that natural structural motifs are retained to enhance performance while eliminating waste, dramatically lowering carbon footprints, and providing new options for recycling.

AGFD003D 3551007 1:00 PM **Biodegradable mulch films** produced from soy-filled polymer resins Wan-Ting Chen WanTing_Chen@ucl.edu Plastic waste disposal has become an area of increasing interest throughout the world in recent years, as accumulations of plastic which have been improperly disposed of accrue throughout the environment. A solution to this issue, which has been implemented by many companies in recent years is by using biodegradable polymers. In this study, several byproducts from the soy protein isolate production (provided by ADM and DuPont/Solae) were filled with biodegradable polymer resins, including poly(lactic acid) (PLA), polybutylene adipate terephthalate (PBAT), and biobased linear low-density polyethylene (B-LLDPE). Based on prior

studies, a 20 wt.% of soy waste was compounded with PLA, PBAT, and B-LLDPE and then cast extruded into mono-layered films. Thermal analyses (thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC)), mechanical property testing, and material processability were used to down-select promising formulations for a biodegradation study and pilot-scale production. Ultimately, a combination of ADM-Superb soy waste/PBAT was down-selected for further investigation. A 6-week soil biodegradation was carried out to evaluate if the soy-filled mulch film can degrade faster than conventional plastic mulch films. Kraft paper, neat PBAT film, and conventional plastic mulch films made of LDPE were included for comparison. The biodegradation characteristics (surface morphology, TGA, DSC, and chemical compositions) shows that the down-selected Superb/PBAT started to biodegrade in a week while neat PBAT remained unchanged (Figures 1 and 2). Finally, a pilot-scale mulch film was manufactured using a 10 wt.% of Superb/PBAT as a preliminary study. The worldwide market for plastic mulch films is approximately 2 million tons annually, with the North American (NA) market making up about 180,000 tons. Based on 0% additional and 20% market share, this represents 1.2 million and 13.5 million for NA and global markets respectively. With promising results obtained from this study, the mulch industry would be able to supply potentially less expensive films that do not require collection post-harvesting.

AGFD003D 3556453 2:00 PM **Converting okara to superabsorbent hydrogel for enhancing vegetable growth under water-limited conditions** Jun Li jun-li@nus.edu.sg Okara is a food waste produced from the soybean milk and soybean curd industries and has been identified as a suitable candidate for development of bio-based functional materials. Here we report the design, synthesis, and characterization of superabsorbent hydrogels through graft copolymerization of okara with acrylic acid (AA) and acrylamide (AAM). The suspension of okara fine particles was activated with ammonium persulfate, which then initiate the free radical polymerization to randomly graft poly(acrylic acid) (PAA) and polyacrylamide (PAAM) onto okara particles in the presence of small amount of N,N'-methylenebisacrylamide (MBA) as crosslinker, producing okara-based superabsorbent hydrogels. The properties of the hydrogels, including their water absorbency, water holding and retention capacities in potting mix, were studied for application as soil supplement. The hydrogels were evaluated for plant growth using choy sum (Brassica rapa subsp. chinensis var. parachinensis), a common green Asian leafy vegetable. We demonstrated that the crop growing in potting mix supplemented with the hydrogels showed more advanced growth stage, significantly higher shoot fresh weight, and larger leaf areas. Seedlings grown in potting mix containing the hydrogels survived better than those without the hydrogels under extreme water-stressed condition. More than 80% growth enhancement was observed in crop under water-limited conditions in hydrogel-enhanced potting mix. Therefore, the okara-based superabsorbent hydrogels hold promise for potential agricultural and farming applications. Through converting the food waste okara to high value-added hydrogels, it has been demonstrated that upcycling waste materials contributes to sustainability and saves water.

AGFD003D 3530051 2:00 PM **Improved utilization of commodity agricultural byproducts** H.N. Cheng hncheng100@gmail.com Agricultural production can generate many byproducts or residues, which are often disposed of or used in low-value applications. It would be desirable to convert these materials to potential products of higher value. Earlier we have taken cottonseed hull, cotton burr, wheat straw, barley straw and rice hull and produced CMC, methyl cellulose, cellulose acetate, and mixed cellulose esters. More recently we have worked with cotton gin trash, xylan (a type of hemicellulose found in many plants, such as wood,

grasses, and cotton) and cashew gum (a high-molecular weight complex heteropolysaccharide, obtained from the bark of the cashew tree). Thus, we have converted xylan to xylan acetate and succinate using a mild process involving Lewis acid catalysis. A similar study has also been done with starch. The degree of substitution obtained depends on the choice of the Lewis acid used and the reaction conditions. Cashew gum has been converted to carboxymethyl cashew gum and hydrophobically modified polymers. Other studies include polysaccharide blends and the potential uses of polysaccharides in packaging films.

AGFD003D 3530930 3:05 PM **Development of a new catalyst applied to biogas treatment: From the laboratory to the farm** Vitor Almeida vitor.falmeida20@gmail.com In Brazil, the number of pig farms that produce biogas has grown rapidly in recent years. This has been happening due to the possibility of producing electricity using biogas as fuel to power electric generators. Nowadays Brazil produces 1.4 billion Nm³/year, and this represents about 1.5% of the production potential. Although 1.5% seems to be a small share, it represents 8.3% of the electric energy produced in Brazil in 2019. One of the main drawbacks in this process is the corrosion of the gas pipelines, engine, and turbine, caused by hydrogen sulfide (H₂S) present in the biogas causing a high maintenance cost. Recently, we have developed a new efficient and low-cost process to remove the H₂S, based on a new carbon catalyst on a lab-scale (efficiency of 94% in the H₂S oxidation). In this work, we describe the scaleup of this technology. The first step was to produce an active catalyst replacing the high purity chemicals with commercially available industrial raw materials. A new series of catalysts were produced using industrial grade silica, quaternary ammonium salt, and Fe₃⁺ salt with an important change, replacement of acetonitrile (more expensive and toxic carbon source) to bioethanol with performances similar (92% H₂S conversion) to the original catalyst (94%). Working with non-analytical reactants brings lots of new challenges to the research. To improve this rate and produce a catalyst that can be synthesized in large amounts a wide variety of tests have been done. After running through 15 synthesis a catalyst capable of oxidizing 92% of the H₂S present in a solution. The second step was to design and built a reactor to carry out a continuous CVD to produce 15 kg_{catalyst}/h. This reactor was installed, and the first reactions carried out and are currently under optimization. The third step is to test the catalyst production and validate the application in a local farm.

TUESDAY AFTERNOON 4/13/21 start 1:00 PM end 4:00 PM
Food Authentication and Adulteration Detection
 AGFD006A 3549264 1:05 PM **Tools to fight food fraud: Gap analysis** Franz Ulberth franz.ulberth@ec.europa.eu Fraud in the food chain has shattered the confidence consumers have in their food supply and has serious effects on the reputation of honest food business operators. Prevention of fraud and promotion of authentic agri-food products is key to assure the commercial success of high-value agri-food products on international markets. International collaboration on food safety is already well established, while for food authenticity this is not yet the case. There is a great need for international harmonization in order to be able to detect and, what is more important, prevent or at least minimize fraud. Therefore, the fight against food fraud calls for an international and systemic approach involving cooperation and consultation among all stakeholders at all levels of the food chain. Early warning systems, horizon scans, vulnerability assessment tools and appropriate analytical methods are among the critical elements for equipping regulatory agencies as well as industry in the fight against food fraud.

AGFD006A 3536647 1:28 PM **Bona fide or bogus - the importance of analytical instrumentation for detecting food fraud** Eberhardt Kuhn erkuhn@shimadzu.com Food has been adulterated for thousands of years. Examples include adding water to wine, saw dust to spices, and corn sugar to honey. The primary motivation for food adulteration is economic gain. Diluting an expensive premium food, like extra virgin olive oil, with a less expensive food, like canola oil, can increase profits of the manufacturer. Since the foods are typically adulterated with other foods, there is usually no threat to the health of the consumer. In some cases, however, the fraudsters use toxic chemicals. For example, when adulterating milk with melamine. The increasingly sophisticated techniques used by the food fraud criminals present a challenge for regulatory agencies that are tasked with monitoring food safety and food quality, like the US Food & Drug Administration (FDA), US Department of Agriculture (USDA), and US Customs and Border Protection (CBP). This talk provides an overview of the most advanced tools available to fight food fraud. It describes the analytical detection methods and state-of-the-art instrumentation for the most frequently adulterated foods, including olive oil, coconut oil, palm oil, milk, meat, and honey. Specific techniques covered include GCMS, LCMS/MS, UV/vis, FTIR, and MALDI-TOF and the presented data compare pure and adulterated foods.

AGFD006A 3532080 1:51 PM **Detection of undeclared sweeteners in steviol glycosides by LC/MS** Tongtong Xu TONGTONG.XU@USP.ORG Because of growing concerns about the need for added sugar reduction in food products and consumer's preferences for "clean label" products, the food and beverage industry are taking their efforts towards calorie reduction through product reformulation using low- and no-calorie sweeteners from natural sources. Steviol glycosides, which are obtained from the leaves of *Stevia rebaudiana* Bertoni using various processing techniques, consist of a mixture of compounds containing a steviol backbone conjugated to sugar moieties. These products have been used globally as sweeteners in recent years, and the availability of various formulations created to suit the needs of a range of food manufacturers, as well as their consumer desirability have led to increased usage. In fact, the worldwide market for stevia extracts is expected to reach 700 million US dollars in 2024. The price of steviol glycosides is considerably higher than many other low- and no-calorie sweeteners, therefore making them vulnerable to adulteration with less expensive and less desirable high-intensity sweeteners. As a part of ongoing efforts to assist the food industry and regulators in combating economically motivated adulteration, the Food Chemicals Codex (FCC) has developed, validated and published a proposed LC-MS method to detect the presence of nine potentially undeclared low- and no-calorie sweeteners in steviol glycosides. As a source of global food standards, the FCC seeks to increase the role of public standards and guidance methods, including this publication, to protect consumers and food manufacturers from the growing trend of food adulteration.

AGFD006A 3534745 2:14 PM **Advancement of techniques for fruit juice authentication – the last barrier to prevent food fraud** Yaxi Hu huyaxi2004@gmail.com Fruit juice adulteration has been a long-standing concern since the morphological and physical properties of the original ingredients are removed completely during processing. Various traceability and risk assessment systems have been developed to prevent general food fraud. With rapid globalization and complex supply chain, functions of those systems have been inevitably hindered. Serving as the last barrier to ensure food authenticity, reliable techniques to identify fraudulent fruit juice are indispensable. Techniques for fruit juice authentication can be categorized into nucleic acid-based and metabolite-based, utilizing polymerase chain reaction and gas/liquid chromatography-

hyphenated tools, respectively. These traditional techniques suffer from time-consuming and labor-intensive experimental procedures and/or with low accuracy, sensitivity and/or specificity, hindering their application by inspection agencies and the food industry. To address these issues, two novel authentication tools were developed. One method combines isothermal DNA amplification technique and microfluidic platform to authenticate pure pomegranate juice and identify the potential adulterants of apple and grape juice. The multi-channel microfluidic platform enabled an instrumental-free sample-to-answer analysis of pomegranate juice within 1 h with high sensitivity and specificity. Another novel technique was developed using comprehensive two-dimensional gas chromatography-mass spectrometry to authenticate orange juice. With substantially improved separation efficiency and molecular resolution, this metabolite-based technique achieved accurate identification of the biological species, geographical origin and harvesting year of orange juice. These novel techniques have high potential to be adapted by inspection agencies, the food industry, and even consumers to authenticate fruit juice products in a simple and reliable manner.

AGFD006A 3556914 2:47 PM **Authentication of coconut water** Dana Krueger dkrueger@kfl.com Coconut water is a fast-growing category of fruit juice beverage products in the US market. Relatively little information has been published regarding the composition of coconut water that can be used for purity evaluation of commercial products. The author's laboratory has produced data from the analysis of nearly a thousand coconut water samples. The samples derive from various, mostly commercial sources and include both raw materials and retail finished products. The data were reviewed and summarized to produce a profile of coconut water composition to facilitate the detection of problems of coconut water adulteration. Coconut water composition is not statistically uniform. Young coconut water produced from immature coconuts harvested principally for water production has a very different compositional profile from mature coconut water produced as a secondary product from mature coconuts harvested for coconut meat production. The data indicates that mislabeled or fraudulent coconut water is widespread in the marketplace. The principal problems observed are the undeclared addition of nutritive sweeteners to coconut water and the dilution of coconut water by substitution of sugar and water for coconut water.

AGFD006A 3551508 3:10 PM **Amino acid fingerprints of authentic skim milk and whey protein products** Sneha Bhandari sdbhandari1@gmail.com The dairy products are most widely used sources of good quality dietary proteins. Consumers have acknowledged the health benefits of dairy proteins in various formulations leading to their increased demand. Dairy products including milk and whey ingredients are sold at premium prices and are traded in large volumes. This makes them vulnerable to fraudulent activities and these products are prone to adulteration. There is an immediate need to establish comprehensive and meaningful authenticity testing of dairy ingredients based on their identity and purity. The authenticity verification of dairy ingredients will be very helpful to reduce risk of their economically motivated adulteration (EMA) and in improving consumer confidence in these type of premium products. Studies were undertaken to develop a method to verify authenticity of milk and whey proteins by analysis of their amino acid fingerprints. Amino acid composition of authentic skim milk and whey protein samples was determined not only in the authentic samples but also those spiked with selected potential adulterants. The results led to the development of the standard amino acid fingerprints of authentic skim milk powder and whey proteins samples in Food Chemicals Codex. Different amino acids of the dairy proteins samples are affected to different extent by different adulterants. Some amino acids are more sensitive to adulteration and

are very helpful in establishing authenticity of whey protein and milk powder samples.

AGFD006A 3550523 3:33 PM **Analytical methods to detect undeclared synthetic colorants in spices** Eric Schwartz eric.schwartz@usp.org The global spice market, currently a 12 billion-dollar industry, continues to grow at a rapid rate and is highly prone to adulteration. Spice adulteration is a crime that generates significant profits for fraudsters. Some spice adulterants, including undeclared synthetic colorants, pose a serious threat to public health and confidence. The Food Chemicals Codex, an internationally recognized compendium of standards for the identity, purity, and quality of food ingredients, is involved in the development of multiple analytical tests to address the challenge of spice fraud. One approach includes a simple, inexpensive thin-layer chromatographic technique, involving optimized solvent systems, to visualize abnormal colorant spots and detect adulteration with undeclared synthetic colorants through comparison to authentic samples. This method can be used early in the supply chain to detect colorants at higher limits. The other approach involves liquid chromatography and mass spectrometry to screen for 39 synthetic colorants in spices to detect colorants at lower levels. This sophisticated approach can be used further downstream in the supply chain to accurately identify adulteration with undeclared synthetic colorants. The use of these tests to combat spice fraud will be discussed.

TUESDAY EVENING 4/13/21 start 5:00 PM end 8:00 PM Waste Product Utilization

AGFD003E 3530888 5:00 PM **Circular economy of polyolefins and super absorbent polymers** Dimitris Collias collias.di@pg.com Recycling of high-volume polymers is a top priority for all companies around the world, and necessary to achieve their sustainability goals. In addition to such goals, high-volume recycling benefits the environment, stimulates the economy, improves people's health and water quality, and generates energy needed by consumers in developing regions of the world. Two examples of high-volume polymers are polyolefins, such as polypropylene and polyethylene, and acrylate-based superabsorbent polymers. The vision for this work is to eliminate polymer waste going to landfills or incineration via introducing recycling and circularity. The objectives of the work are to develop cost- and energy-effective recycling technologies which can: 1) provide circular solutions, via replacing parts of virgin polymers; 2) recycle waste polymers into other products; and 3) be re-applied to other polymers, as appropriate. More specifically, we will present the examples of a dissolution recycling technology we developed for polypropylene waste and a degradation recycling technology we developed for superabsorbent polymers. The dissolution recycling technology is based on the use of a solvent which causes the polypropylene to be purified from the contaminants associated with its life and recycling journey. Key parameters of the dissolution technology that we will discuss are solvent type; extraction, dissolution, and purification conditions; and product properties. The dissolution technology is currently at the pilot stage. The degradation recycling technology is based on breaking down the crosslinked network of acrylic acid of the superabsorbent polymer waste into smaller fragments which are then purified and can be used in other products, such as coatings or adhesives, or incorporated back into the superabsorbent polymer. Key parameters of the degradation technology are degradation and incorporation conditions and product properties. The degradation technology is currently at the lab scale

AGFD003E 3557918 5:00 PM **Sustainable green composites: A circular bioeconomy driven advances and applications** Amar Mohanty mohanty@uoguelph.ca Sustainable green composites from renewable, recycled, and waste sources are gaining more

attraction recently in the manufacturing sectors with applications ranging from lightweight automotive parts to green packaging. The whole world looks toward a low-carbon and decarbonized economy through an innovative circular bioeconomy unlike through a linear approach to mitigate the dangers of climate change. The issue of plastic waste is making headlines on a daily basis, where several countries are restricting/banning single-use plastic. Currently, the world produces around 450 million tons of plastic annually, which is expected to surpass one billion by 2050. As per a UN report, the world makes 300 metric tons/year of plastic waste which is nearly equivalent to the weight of the entire human population. It is expected that the sea will have more plastic than fish. Similarly, it is estimated that billions upon billions of tons in food waste including agro-/forestry residues and by-products and coproducts from various industrial processes are created. The philosophy of "Nothing is waste – wastes are resources" supports the concept of a circular economy. The renewable nature of bioplastics is not enough to claim them as sustainable from a commercial perspective. A group of researchers at the Bioproducts Discovery and Development Centre, University of Guelph are working on developing cost-competitive biocomposites and green composites for uses in eco-friendly auto-parts, consumer products, and compostable packaging. This presentation will highlight the research on waste valorization and how innovation can be garnered through a unique circular bioeconomy approach, which is made possible from University-Industry-Government collaborations.

AGFD003E 3532434 5:00 PM **Bacterial polyesters – a sustainable material with an innate potential** Carmen Scholz cscholz@chemistry.uah.edu Bacterial polyesters continue on an exciting academic and industrial journey, from their "re-discovery" during the 1970's oil-crisis to iconic shampoo bottles and Target gift cards, they have been produced from a multitude of carbon sources, their structures have been tweaked to carry side chains of various lengths and broadly faceted functional groups and they were even synthesized in microgravity. As a sustainable plastic that can be synthesized from a variety of agricultural surplus as well petrochemical sources, this material has now found its place in the realm of biodegradable polymers for the packaging industry and as implant material in biomedicine. In addition to looking briefly at the history of this sustainable material, and the factors that guarantee its sustainability, this presentation will address polymer-analogous conversions of functionalized poly(b-hydroxyalkanoate)s, PHAs, that will ready the material for more advanced biomedical applications. Specifically, the potential of PHAs in the delivery of nucleic acids and as pro-drugs will be discussed. Observations on the behavior of PHAs in click-reactions using novel catalysts as well as metal-free coupling reactions will be presented. An outlook will be given on potential future research that could provide bacterial polyesters with more omnipresence

AGFD003E 3549689 6:00 PM **CO₂: Waste to value via facile chemistry towards creating feedstock chemicals** Hunaid Nulwala nulwala@liq-ion.com Developing ways to convert carbon dioxide from an energy and industrial sector waste product to a feedstock will spur the development of new technologies, products, and industries while limiting emissions to the atmosphere. CO₂ is a stable molecule and there is an energy penalty associated with the conversion of CO₂ to other substances. There has been quite a work which is being done in breaking the CO₂ bonds through a chemical or catalytic method that often requires a large amount of energy and affects the lifecycle analysis of emissions reduction. Many Innovators and scientists have been exploring the use of various catalyst systems to convert CO₂ via using renewable energy. However, the problems which remains are the geological constraints i.e. the cost of transport and re-use of CO₂ to take place near sources of captured CO₂. Local concentrations of CO₂ at a

particular place is a function of multi-component variables such as human population in that area, industrialization, various applications from which it is produced etc. Hence, the CO₂ use needs to be flexible so it can be implemented in varied climates and at different scale. In this talk, we will present our work on the direct conversion of CO₂ in water based systems to produce cyclic carbonates in high yields and selectivity. The system is robust and amendable to a number of substrates.

AGFD003E 3555338 6:00 PM **Versatile, valuable materials from waste products of petroleum and agriculture industries** Andy Tennyson atennys@clermson.edu Hydrodesulfurization (HDS) processes are essential to petroleum refining as they remove S-atoms from sulfur-containing molecules from petroleum streams before they can poison precious metal catalysts employed in later steps. The resulting S-atoms are separated from the petroleum streams in H₂S, an extremely toxic gas that cannot be released into the environment or conveniently stored as waste. The H₂S(g) is oxidized to cyclo-octasulfur (S₈), a non-toxic solid that can be readily manipulated under a wide variety of environmental conditions. In this manner, petroleum refineries generate nearly 7 million metric tons of S₈ that find no productive use and are discarded in solid-waste storage sites. Elemental sulfur is a remarkably unreactive compound, but at temperatures >160 °C, the cyclo-S₈ form ring-opens to generate oligo- and poly-sulfur chains comprising sulfur-radical termini. These radical termini can then react with alkenes to form highly-crosslinked polymers and networks. Research in our group has emphasized alkene-containing carbon feedstocks derived from agricultural wastes. Unsaturated free fatty acids (FFAs) are particularly promising feedstocks given that they are generally discarded as unusable wastes following rendering processes and that they comprise C=C bonds without requiring any additional chemical functionalization. Our findings on FFA/S₈ thermoplastics and cements will be presented.

AGFD003E 3537406 7:05 PM **Dairy sustainability: Balancing nutrient production and environmental impact** Michael Tunick mht39@drexel.edu Dairy foods are noteworthy for supplying high-quality protein and various essential vitamins and dietary elements. However, a cow expels around 100 kg CH₄/yr through enteric fermentation in her rumen. The atmospheric warming potential of CH₄ is 28 times that of CO₂, and cows are responsible for more than 35 percent of the CH₄ emissions resulting from human activity. Therefore, decreasing the CH₄ generation from cows while maintaining the high level of nutrients in milk would aid the reduction of global warming without affecting the diet of people who consume dairy products. Specific changes in feed, such as supplementation with long-chain fatty acids, have been shown to reduce CH₄ production without materially affecting the nutritional content of the milk. Research has also shown that the microbiome of the rumen consists in part of heritable microbes, with nearly 40 species correlating with the genotype of the animal. Breeding with the goal of reducing CH₄-generating microbes would presumably reduce greenhouse gas emissions. The environmental impact of the dairy industry may be decreased by incorporating feed and genetics when raising cows.

TUESDAY EVENING 4/13/21 start 5:00 PM end 7:45 PM
Food Authentication and Adulteration Detection

AGFD006B 3552793 5:00 PM **Analysis of influencing factors of adulterated extra virgin olive oils by UV-Vis spectroscopy with ANOVA derived multivariate modelling techniques** Jingyao Zhang 18390940914@163.com The pooled-analysis of variance (pooled-ANOVA), ANOVA-principal component analysis (ANOVA-PCA)

and projected difference resolution (ANOVA-PDR) were applied to analyze multiple influencing factors by UV-Vis spectra toward extra virgin olive oil (EVOO) adulteration detection. Three factors including the EVOO origin, adulteration level, and adulteration type, and the interaction of factors were studied. The pooled-ANOVA showed the significance level of each factor. ANOVA-PCA and ANOVA-PDR mutually verify and complement each other, and detailed separation of the internal classes of the three main factors. Partial least-squares-discriminant analysis (PLS-DA) and PLS regression (PLSR) were used to further verify the results. It was demonstrated that pooled-ANOVA, ANOVA-PCA, and ANOVA-PDR could effectively identify the sources of changes in complex sample sets. The sums of the squares of the same matrices were used to show that origin, level, and type contributed 80.66, 11.05, and 0.5% of the variance, respectively. Since the three main factors and their interactions were all important sources of spectral changes, the EVOO adulteration detection model established by the use of UV-Vis spectroscopy combined with PLS should be used under appropriate validation and model transfer.

AGFD006B 3562133 5:00 PM **Geographical origin discrimination of Chinese wheat based on multi-small-molecular-profile analysis** Wenhao Zheng zhengwenhao@sjtu.edu.cn Boyan Gao zjy1002@sjtu.edu.cn Wheat is the staple food of an enormous number of people around the world. Aiming at geographical origin discrimination of wheat, analytical methods need to be established. A total of 94 wheat samples originating from 8 provinces of China was studied. Based on the optimization of extraction method, ultra-high-performance-liquid-chromatography tandem time-of-flight mass spectrometry (UPLC-QTOF MS) was used mainly for the determination of non-volatile components. Volatile components of wheat were analyzed using headspace gas chromatography together with mass spectrometry (headspace-GC-MS). Multivariate data analysis techniques were associated and compared in different provenances. As the results, both UPLC-MS and headspace-GC-MS along with principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA) were able to distinguish wheats from different origins. The results indicated that wheat in Henan Province distributed in the center of the PCA scores plot, which is consistent with its actual location of China. On the other hand, the results of UPLC-MS and headspace-GC-MS complemented each other to construct a contour profile of the small molecules in wheat

AGFD006B 3562086 5:00 PM **Image classification by deep learning to the quality control of chrysanthemum teas** Weiyang Lu weiyang.lu@sjtu.edu.cn Seven commercial Chinese chrysanthemum tea products were classified by computer vision combined with deep learning. Without the need of building any specific hardware, the image acquisition and deep learning was achieved by both a bench top gel imager and a regular smartphone. The deep neural network was applied directly on the raw image, yielded 96% and 89% correct identifications when classifying flowering stage and tea type, respectively. In comparison, multivariate classification models including k-nearest neighbor, multiple linear perceptron and support vector machine were built after morphological feature extraction of the image. The best prediction accuracies when classifying flowering stages and tea types were only 90% and 63%, respectively. The result indicated that computer vision, especially when combined with deep learning or other machine learning techniques can be a convenient and versatile method in the evaluation of food quality. The model can be applied for rapid and automatic quality determination of other related foods.

AGFD006B 3564834 6:00 PM **Discovery of Marker Compounds for Botanical Based Dietary Supplements Authentication-A Case**

Study for Black Cohosh Jianghao Sun Jianghao.sun@usda.gov
Botanical based dietary supplements are regulated as foods in United States under the Dietary Supplement Health and Education Act of 1994 (DSHEA) act. Black cohosh is a plant native to eastern North America with a long history of medicinal use for the treatment of menopausal symptoms. However, the misuse of raw materials is still a problem in black cohosh based dietary supplements. Due to the complexity and variation of the chemical constituents in authentic black cohosh (*Actaea racemosa*) and its potential adulterant species, it is in urgent needs for accurate and feasible methods for black cohosh authentication. LC-MS fingerprinting method combined with chemometric approach was employed to discover new marker compounds. Hydroxycinnamic acid amide (HCAA) glycosides are proposed as potential marker compounds for differentiation of black cohosh from related species, including two Asian species (*A. foetida*, *A. dahurica*) and two American species (*A. pachypoda*, *A. podocarpa*). Partial least square-discriminant analysis (PLS-DA) model was established and validated for the classification of *A. racemosa* and other *Actaea* plant samples.

AGFD006B 3553457 6:00 PM **Detection of adulteration in botanical dietary supplements:** Analytical strategies for finished product/ingredient quality control Hong You hongyou@eurofinsus.com Botanical dietary supplement (BDS) industry is a fast-growing multi-billion-dollar industry that faces many quality-related challenges in ensuring product safety in the marketplace. BDSs are advertised as being more "natural" and "safer" than isolated or synthesized chemicals and therefore fit the modern lifestyle trend. However, because BDSs are legally considered as foods in many territories such as India, the European Union, New Zealand, and the USA, they do not require, as with drugs, premarket approval and safety/effectiveness assessment in these areas. Due to the development of globalization and online trading platforms, economically motivated adulteration in BDSs has a great chance to occur when the products are transported between different countries. Because of the complexity and continuous development of BDS products, the detection of adulteration is often accomplished using an orthogonal approach via multiple analytical technologies, ranging from macro-microscopic examination to DNA-based, spectroscopic, and chromatographic testing. This presentation will overview adulteration detection strategies by demonstrating real case studies in an industrial setting.

AGFD006B 3557198 7:00 PM **Development of USP standards for cranberry dietary ingredients** Maria Monagas mjm@usp.org The large and widespread use of cranberry dietary supplements among the female population to alleviate symptoms associated with urinary tract infection demands the creation of robust public standards to assure the quality of these products. Proanthocyanins (PACs), oligomers and polymers of flavan-3-ols, are claimed to be the active components in cranberry dietary ingredients. Cranberry PACs are heteropolymers composed of epi(catechins) units linked by two different type of interflavan bonds (A-type and B-type). Challenging in setting compendial specifications for cranberry dietary ingredients include: the diversity of commercial ingredients, complex phytochemical profile, polymeric nature of cranberry PACs, and differentiation from other dietary sources of PACs (i.e. grape seed, maritime pine bark and peanut skin extracts). Due to the limitations and lack of specificity of current analytical methods to characterize the high molecular PAC fraction, cranberry dietary ingredients are usually under risk of economically motivated adulteration. Cranberry dietary ingredients are derived from: (i) whole fruit, (ii) fruit juice concentrate, or (iii) by-products of the juice processing (i.e. pomace). Juice can be further purified into cranberry juice extracts or spray dried over a carrier to produce cranberry dry juice. In addition, pomace material can be further

extracted to produce cranberry pomace extract. Traditional standards inherited from the cranberry juice industry, including sugar profile and ratio of organic acids, play an important role in complementing the requirements for identity and authenticity some juice-derived ingredients. However, as ingredients are further processed or purified, juice specifications become less important or are lost, while the phytochemical profile (i.e. polyphenols) of fruit becomes more important for the characterization of the ingredient. The present abstracts summarize the work carried out by the United States Pharmacopeia (USP) in the development of the cranberry standards. The application of HPTLC and RP-HPLC tests for the analysis of the low molecular weight polyphenol profile of cranberry (i.e., anthocyanins, flavonol glycosides, and flavan-3-ols) as new compendial ID tests will be presented. Other analytical approaches for the characterization of the polymeric PAC fraction of dietary ingredients using advanced techniques (i.e., HILIC-MS) currently under development by USP, will also be discussed.

WEDNESDAY MORNING 4/14/21 start 9:00 AM end 11:35 AM

Food-Energy-Water Nexus 1

AGFD003F 3552296 9:00 AM **Changes in climate influence the food-energy-water nexus** and consequently impact human health John Finley JFINLE5@LSU.EDU The changing climate results in dynamic alterations of the Food Energy Nexus, including fluctuations in crop yields, quality and nutritional value. Furthermore, the uncertainties associated with increases in global and regional temperatures impacts commodity production, and energy and water inputs. Regional changes in climate requires adaptations of lifestyles, energy needs and resources, which influences regional food and water availability, air quality, and human health. Several mitigation strategies have been proposed and modeled. This presentation provides a critical assessment of the merits and limitations of implementing integrated solutions to the emerging challenges of delivering food energy and water under the influences of a changing climate with respect to an increasing population and impacts on human health. Addressing these challenges would help enable sustainable production of safe and nutritious food, while being integrated to optimize energy and water utilization.

AGFD003F 3558644 9:00 AM **Prolonging and stabilizing the release of 2-heptanone as mite repellent for the protection of honey bees** Massoud Miri mjmsch@rit.edu 2-Heptanone is an effective mite-repellant to protect honey bees and helps to reduce bee collapse. An efficient way to prolong and stabilize the release of 2-heptanone is by deketalization of its ketals with either glycerol (Gly-Ket) or polyvinyl alcohol (PVAI-Ket). The synthesized ketals were characterized by ^1H and ^{13}C NMR spectroscopy, and for PVAI-Ket also DSC. Two set ups were used for monitoring the concentration of the 2-heptanone: a 1.5 L environmental chamber and a miniaturized set up for up to 10 vials, each having a 20 mL volume. Deketalizations were catalyzed by phosphoric acid with the temperature and relative humidity of 30 $^{\circ}\text{C}$ and about 80 %, resp., resembling bee hive conditions. The deketalizations were optimal between pH values of 2.0 and 2.5 for Glyc-Ket and 2.0 and 3.5 for PVAI-Ket. Headspace gas chromatography was applied to monitor 2-heptanone vapor released by the ketals. For Gly-Ket, the 2-heptanone concentration could also be directly monitored from the liquid emulsion containing the ketal using ^1H NMR spectroscopy. The measurements indicated that the 2-heptanone release lasted at reasonably high levels for at least 23 days with PVAI-Ket and 42 days with Gly-Ket (i.e. 2 brood cycles with the latter). In contrast to the pure ketone, which evaporates rapidly, the concentration of 2-heptanone released from the ketals remained relatively stable. An

alternative physicochemical approach to release the 2-heptanone will also be briefly discussed.

AGFD003F 3534122 9:00 AM **Climate change adaptation and planning** V. Rao Kotamarthi vrkotamarthi@anl.gov We will discuss some of the changes in climate that have occurred over the past 100 years and the continuing trends in temperature and precipitation changes. The need for climate models and basic principles of building climate models that are used for projecting climate change for the next 100 years and beyond, the uncertainties involved in the process, will also be presented. We will discuss the process for calculating the projected changes in climate at regional and local scales and use of these projections for developing adaptation strategies. Examples of the application of regional and local scale climate projections for estimating risk from changing climate over the Southeastern USA will be presented.

AGFD003F 3548623 10:00 AM **Nanoscale micronutrients as a sustainable approach to manage crop disease** Jason White jason.white@ct.gov Low use and delivery efficiency of conventional agrichemicals is a significant impediment to maintaining global food security, particularly given that a 60-70% increase in global food production is needed by 2050. Thus, novel and sustainable strategies for enhancing food production are needed all along the “farm-to-fork” continuum. Given the known role of micronutrients in plant growth and defense against both abiotic and biotic stresses, we began mechanistic investigations into the potential of nanoscale micronutrient platforms for disease management. In a number of studies, foliar amendment of nanoscale materials such as CuO, CuS, and SiO₂ have been shown to significantly alleviate damage caused by the fungal pathogens, resulting in enhanced growth and yield. Importantly, disease suppression is largely a function of modulated plant nutrition and disease resistance and not direct toxicity against the pathogen. However, it is clear that the ability to effectively tune nanoscale material function and composition will enable optimization of positive impacts, including tolerance to pathogen activity, as well as allow for potentially significantly reduced amounts of agrichemical use. Results will be presented from several studies where manipulation of nanoparticle synthesis resulted in tunable materials that yielded greater disease management potential and plant health by a range of agronomic endpoints.

AGFD003F 3555701 10:00 AM **Polymer encapsulated nanoscale urea for sustainable and precision agriculture** Ramesh Raliya rameshraliya@iffco.in Nitrogen is one of the key major nutrients required for plant growth and development. It is a major component of chlorophyll, energy-transfer compounds, amino acids, and genetic materials. Therefore, it is critical to maintaining the required nitrogen content often 3 to 4% in the plant's above-ground tissues. Among other nitrogenous fertilizers, urea is a predominant compound, used as nitrogen fertilizer across the globe. Urea has the highest nitrogen content (45-46%) in all the commonly used dry-solid nitrogenous fertilizers. It is applied to plants as basal (just below the ground in rhizosphere zone), side-dressing, and top dressing. The chemical transformation of urea nitrogen to plant-available/uptake form of nitrogen takes up to a week and depends on various factors in the soil such as the quantity of enzymes, temperature, pH, humidity, type of microbial population and plant residues/extracellular secrets, etc. Because of the variability in these environmental factors, the nitrogen use efficiency from applied urea fertilizer is often less than 30%. A majority of urea fertilizer gets runoff, volatilize, or leach to the environment. Agricultural nitrogen emission and runoff are one of the major contributors to greenhouse gas and eutrophication, respectively. Nanotechnology deals with the particle size of less than 100 nanometers, offers the potential to minimize environmental loss

by precision delivery and controlled release. In this investigation, nanoscale urea or nano urea was developed by the formation of its stable particles using a bottom-up fabrication approach. The resultant particles were in the physical size range of 18 to 30 nanometer (nm) and the hydrodynamic diameter was also less than 100 nm. The synthesized nano urea particles were tested for their efficacy on the wheat crop, both in the pot and field experiments under various agroclimatic conditions. Efficacy parameters such as plant growth, development, yield, chlorophyll, protein contents were quantified. It was observed that nano urea is able to fulfill the demand for nitrogen and increase an average plant yield up to 8% when compared to control. Interestingly, in the wheat, the optimum dose requirement of nano urea was 10% less than conventional urea. This study offers the insight that nanotechnology may help to provide the major nutrients such as nitrogen precisely to plants, but also save the environment by minimizing nitrogen leaching/volatilization.

WEDNESDAY MORNING 4/14/21 start 9:00 AM end noon
Recent Trends in Food Analysis

AGFD002B 3552876 9:00 AM **Systemic evaluation of chiral fungicide pydiflumetofen: Stereoselective bioactivity, aquatic toxicity, and environmental fate** Zhen Wang 2020202059@stu.njau.edu.cn Pydiflumetofen, as a new succinate dehydrogenase inhibitor (SDHI) chiral fungicide, has been used in crop production because of its broad-spectrum and high-efficiency antifungal activity. However, little literature is known about pydiflumetofen at the chiral level. In the present study, a sensitive enantioselective determination method based on UHPLC-MS/MS coupled with Lux Cellulose-2 chiral column for pydiflumetofen enantiomers, and quantitative determination in food and environmental samples, was successfully developed and validated. And the absolute configuration of the first eluted peak was confirmed as S-(-)-pydiflumetofen and the second peak was R-(+)-pydiflumetofen by comparing the calculated ECD spectra and experimental as well as measuring the optical rotation. Then, the stereoselective bioactivity against the seven targeted phytopathogens, the acute toxicity to different life stages of zebrafish (embryo, larva, and adult), and degradation of pydiflumetofen in different vegetables (cucumber, eggplant, and cowpea) and soil were investigated. Pydiflumetofen presented effective bioactivity against the tested phytopathogens. Moreover, the bioactivities of R-pydiflumetofen were 49.4-958.8 times higher than that of S-pydiflumetofen and nearly twice than that of Rac-pydiflumetofen. According to the molecular docking study, R-enantiomer could bind more tightly to the target protein (SDH) with the shorter binding distance (TRP B-230 and TRY D-144, with the distance of 2.2 Å and 1.8 Å, respectively) and lower energy affinity (-7.0 kcal mol⁻¹) than S-enantiomer, which could illuminate the reason for the stereoselective activity. Otherwise, the toxicity results showed that pydiflumetofen has high toxicity to different life stages of zebrafish, while the embryo constitutes the most sensitive period of zebrafish to pydiflumetofen. And the toxicity of R-enantiomers was nearly 10 times higher than S-enantiomers in the 96-h acute toxicity test. Nevertheless, there was no significant difference between R-pydiflumetofen and Rac-pydiflumetofen. Besides, the results of field degradation experiments revealed that R-(+)-pydiflumetofen was preferential degradation in vegetables and soil. Consequently, R-pydiflumetofen not only exhibited a higher bactericidal activity with less dose but also had fewer environmental risks in the environment, which can provide scientific guidance and assertive evidence for developing the high-efficiency and low-risks fungicide.

AGFD002B 3552926 9:00 AM **Systematic analysis of toxic acrylamide protein targets using covalent docking** Mercedes Alfonso-Prieto malfonsoprieto@gmail.com Acrylamide is formed by Maillard reaction between sugars and proteins during baking, frying

or roasting. Cumulative exposure to acrylamide may result in neurotoxicity. Such toxic effects could result from covalent modification of proteins via Michael addition reaction of acrylamide with cysteine residues. The determinants of acrylamide adduct formation and its effects on protein function are not completely understood at the molecular level. As a follow-up of previous computational studies by Carloni and coworkers, here we have performed a systematic study of known acrylamide protein targets using covalent docking. Analysis of these acrylamide-protein complexes provides insights into the determinants of cysteine reactivity, as well as the residue composition of acrylamide binding sites. Moreover, it sheds light into the molecular mechanisms by which acrylamide impairs protein function. This information could potentially be used to predict additional protein targets mediating acrylamide neurotoxicity. This project was inspired by the late Dr. Ernesto Illy.

AGFD002B 3554359 9:00 AM **Portable sensing platforms for hypoxanthine detection in fresh and deteriorated fish** Fatima Mustafa iltbe@yahoo.com Food freshness sensors provide valuable information about food quality that enable easy and affordable monitoring. In this presentation, we will discuss the development of enzyme-based portable sensing platforms that utilize nanomaterials or dyes. These substances are integrated on paper. The functionalized paper sensors are capable of selectively detecting hypoxanthine, a freshness marker that is originated from the degradation of the adenosine triphosphate in fish meat. The sensing mechanism enables a colorimetric response that can be observed by naked eyes and moreover evaluated by imaging software. The design, fabrication, and characterization of these enzymatic sensors will be described as a representative example of a potentially deployable biosensor for large-scale monitoring of food quality and safety.

AGFD002B 3551254 10:00 AM **NMR spectroscopy as a powerful tool for identification of polymers and other oxidation products in frying oil** Hong-Sik Hwang hongsik.hwang@usda.gov Although polymers are the major oxidation products accumulating in oil during frying, mechanisms of polymerization have not been well understood. Polymers along with aldehydes in frying oil are known to be associated with adverse health effects. Understanding mechanisms of polymerization and structures of polymers is critical to understand their toxicity and to develop methods to prevent their formation. An earlier study reported that Diels–Alder reaction, a long-believed mechanism for the polymerization of oil, was not the major reaction to produce polymers. In this study, we found that ester bonds are one of the chemical bonds forming polymers during frying using NMR spectroscopy. Ester value increased as soybean oil oxidized and ¹³C NMR spectrum showed new ester carbonyl carbon signals evidencing the formation of ester bonds. The NMR spectroscopy after the reaction of oxidized soybean oil with acetyl chloride was also employed to verify NMR signals corresponding to alcohol. By this method, proton signals at 3.61 and at 3.71 ppm, which were reported to be ether bonds forming polymers, were found to be those of alcohols produced in oil. Some uncertain assignments of proton signals of oxidized oil were clarified as signals of alcohols, several previously assigned signals as alcohols were confirmed, and a new proton NMR signal was assigned to be an alcohol. There are so many oxidation products that were not yet identified, and this study indicates that the NMR spectroscopy can be a great tool to identify oxidation products formed in oil.

AGFD002B 3557465 10:00 AM **GC-FID analyses of alcohol-based hand rubs** Timothy Tse timothy.tse@usask.ca The global transmission of COVID-19 led to panic-buying of alcohol-based hand rubs (ABHRs). In response, governmental agencies (e.g. Health Canada) relaxed regulations for production of ABHR enabling many

microbreweries and industrial ethanol plants to include “technical-grade” alcohol formulations. The relaxed regulations quickly increased availability of these alcohol-based products with approximately 3700 different products being introduced by June 2020. ABHRs formulated with technical-grade ethanol contain elevated concentrations of contaminants (e.g. acetaldehyde, ethyl acetate, etc.), which may exhibit dose-dependent toxicity. In this study, 26 liquid and 16 gelled ABHRs were analyzed via gas chromatography flame ionization detection (GC-FID) to determine compliance with United States Pharmacopeia (pharmaceutical-grade), and Health Canada interim guidelines on the use of technical-grade ethanol in ABHRs. Of the 42 samples analyzed only six ABHRs appeared to be compliant with the United States Pharmacopeia monograph on organic contaminants in ethanol. Most ABHRs analyzed were compliant with the interim guidelines stated by Health Canada. However, those that were non-compliant exhibited elevated concentrations of acetaldehyde, with a maximal concentration observed of $251.05 \pm 10.24 \text{ mL L}^{-1}$; 3.3X higher than currently permitted. Altogether, frequent testing of ABHRs should be conducted to ensure compliance with interim guidelines that ensure consumer safety. Risk of consumer exposure to ethanol contaminants increased with the number of products available in the market.

AGFD002B 3558629 11:10 AM **Monitoring plant health with nIR fluorescent H₂O₂ nanosensors** Juan Pablo Giraldo juanpablo.giraldo@ucr.edu Near-infrared (nIR) fluorescent single-walled carbon nanotubes (SWCNTs) were designed and interfaced with leaves of Arabidopsis thaliana plants to report hydrogen peroxide (H₂O₂), a key signaling molecule associated with the onset of plant stress. The sensor nIR fluorescence response is quenched by H₂O₂ with selectivity against other stress-associated signaling molecules and within the plant physiological range. In vivo remote nIR imaging of H₂O₂ sensors enabled optical monitoring of plant health in response to stresses including UV-B light, high light, and a pathogen-related peptide (flg22), but not mechanical leaf wounding. The sensor's high biocompatibility was reflected on similar leaf cell death and photosynthetic rates to controls without SWCNT. These optical nanosensors report early signs of stress and will improve our understanding of plant stress communication, provide novel tools for precision agriculture, and optimize the use of agrochemicals in the environment

AGFD002B 3551213 11:00 AM **SERS detection of aflatoxin B1 in amaranth using an optical nanosensor based on gold nanotriangles** Mary Licuona mary.licuona@pucc.edu.pe Aflatoxin B1 (AFB1) is a mycotoxin produced as a secondary metabolite by filamentous fungi such as Aspergillus flavus and Aspergillus parasiticus. Among other illness-related issues attributed to AFB1, according to the International Agency for Research on Cancer, there is evidence that it is carcinogenic. This mycotoxin proliferates mainly in nuts, spices, milk, and cereals, such as corn, rice, and amaranth. For that reason, many countries have set rules about the maximum AFB1 levels allowed in different food items (around the ppb range). The standard mycotoxin detection protocols rely on liquid or gas chromatography methods, in many cases coupled to mass spectrometry. These methods can detect AFB1 concentrations in the range of 1-20 ppt, but they are not very accessible, require tedious sample preparation, highly trained personnel, and expensive equipment. These requirements narrow their applicability in quality control by farmers and small to medium businesses, so novel sensors that overcome these drawbacks are needed. Herein, we present the development of a detection system based on gold nanotriangles (AuNTs) functionalized with mercaptopropionic acid (MPA) to induce the adsorption of the mycotoxin. Once the AFB1 is close to the AuNTs, these nanostructures' excellent optical properties make them act as nanoantennas capable of enhancing the mycotoxin's

Raman signals in solution without the need of any additional reporter. A multivariate analysis method based on partial least squares (PLS) regression has also been implemented to process the surface-enhanced Raman scattering (SERS) spectra. Very promising results have been obtained, being able to selectively discriminate AFB1 content in amaranth extract solutions down to the ppb level.

**WEDNESDAY AFTERNOON 4/14/21 start 1:00 PM end 3:40 PM
Upcoming Topics in Food Analysis**

AGFD002C 3555344 1:05 PM **Using mass spectrometry to detect the presence of and dissect the structure of prions** Christopher Silva christopher.silva@usda.gov A prion's (PrP^{Sc}) distinct pathogenic character is enciphered solely in its conformation. Prions replicate by inducing a natively expressed prion protein (PrP^C) to adopt the PrP^{Sc} conformation. Although distinguishing between protein conformations is challenging, PrP^{Sc} can be purified from PrP^C using proteinase K (PK) digestion and ultracentrifugation. The resulting characteristic protein (PrP 27-30) can, after denaturation, be detected by mass spectrometry using the multiple reaction monitoring method (MRM). MRM employs a triple quadrupole mass spectrometer's mass filters to isolate and detect specific peptides derived from the tryptic digestion of PrP 27-30. We used the MRM method to quantitate the temporal increase of PrP 27-30 in hamsters following a peripheral (intra-peritoneal) challenge using Sc237 prions. PrP 27-30 increased in a log linear relationship over time and was detectable at a time comparable to its earliest detection by bioassay. We adapted our MRM method to detect and quantify the oxidation of a methionine at position 213 (Met213) of the prion protein. Oxidation of Met213 has been proposed as a covalent signature of prions. We quantitated the change in Met213 oxidation over time and demonstrated that it decreased, indicating that its oxidation is not a covalent prion signature. 1.8% of the amino acids in a typical mammalian protein are methionines. In contrast, methionines comprise 4.3% of the amino acids in the hamster prion protein, suggesting the possibility that, in the prion protein, methionines serve another purpose. We optimized the MRM parameters for a set of methionine containing peptides, which allowed us to quantify the extent of methionine oxidation of all nine methionines in the hamster prion protein. After reaction with oxidants, such information can provide invaluable structural information for the prion conformation.

AGFD002C 3556960 1:00 PM **Detection & quantitation of trace level pesticides in commercial baby foods** Todd Richards todd_richards@leco.com In order to mitigate developmental risks to infants various regulatory agencies have begun to lower the maximum residue limits (MRL) of various pesticides in commercially prepared baby foods. While the foods themselves may be fairly basic the pigments, sugars and other matrix compounds they contain often interfere with the pesticide analysis. As the MRLs are lowered the matrix interferences can have an outsized impact and make it harder to achieve accurate detection and quantitation of the pesticides on a consistent basis. This presentation will focus on pesticide quantitation in several baby food products using traditional split/splitless injections paired with time of flight mass spectrometry (TOF-MS). Also explored are as well as less commonly applied techniques like large volume injections (LVI) and comprehensive, two-dimensional (GCxGC) chromatography to increase quantitation accuracy and alleviate matrix interference while achieving detection limits well below the currently established MRLs.

AGFD002C 3530234 1:00 PM **Coin-operated water vending machines: Bacterial contamination analysis** Stephen Bryan Asenjo brainasenjo@yahoo.com Coin-operated water vending machines (locally known as A utomatic T ubig M achines) have been an

instant and cheap source of drinking water around Cebu City, Philippines. They are mostly located along the sides of roads and streets making them prone to contamination. With the high risk of contamination of these ATMs, this study aimed to determine the bacteriological quality of potable water from coin-operated water vending machines around Cebu Normal University. Bacteriological analysis was done on water samples collected from 5 ATMs around CNU. Various quality parameters were analyzed including total coliform, fecal coliform and heterotrophic plate count (HPC). The results showed that 100% of the samples analyzed has high concentration of total coliform, fecal coliform and heterotrophic bacteria. The level of total and fecal coliforms contamination and heterotrophic plate count have failed to meet the standards of Philippine National Standards for Drinking Water (PNSDW) and Dialysis Water Standard (DWS). By the result of the analysis, it was concluded that ATMs cannot ensure safe water public consumption as bacteriological concentration exceeded the minimum standards set by PNSDW and DWS. It is necessary to maintain cleanliness of the machines, the surrounding environment and help secure reliable water source

AGFD002C 3549759 2:00 PM **Determining the absorption & tissue incorporation kinetics of linoleic acid-derived 13-hydroxyoctadecadienoic acid in rats** Zhichao Zhang yntzhang@ucdavis.edu 13-Hydroxyoctadecadienoic acid (13-HODE) is a bioactive product of linoleic acid oxidation (LA) that regulates multiple signaling processes in vivo. 13-HODE is also produced when dietary LA is oxidized during food processing. It is not known, however, whether dietary 13-HODE is bioavailable and incorporates into tissues. The present study measured the absorption and disposition of unesterified d4-13-HODE into rat liver, visceral adipose, heart and brain following gavage or intravenous injection (n=3 per group). Mass-spectrometry analysis revealed that d4-13-HODE was absorbed within 20 minutes of gavage, and continued to incorporate into plasma esterified lipid fractions containing lipoproteins throughout the 90-minute monitoring period. Intravenously-injected d4-13-HODE was rapidly taken up from plasma, with a half-life of 58.3 seconds. Analysis of liver, visceral adipose, heart and brain collected at 90 minutes post-administration, revealed that the tracer incorporated into liver, adipose and heart, but not brain. Liver and heart incorporation coefficients were significantly higher for esterified d4-13-HODE (calculated from esterified plasma levels in the gavaged group) compared to unesterified d4-13-HODE provided intravenously (P<0.05), suggesting preferential incorporation of esterified d4-13-HODE into these tissues. Free d4-13-HODE entered adipose tissue at a similar rate to esterified d4-13-HODE (P>0.05). Tissue half-life of d4-13-HODE in visceral adipose, liver, and heart was 0.5, 4.5, and 3.7 days, respectively, which is greater than published values for dietary fatty acids such as eicosapentaenoic acid (4.6 hours in liver and 2.7 hours in heart). This study provides new evidence that dietary 13-HODE is absorbed, and incorporated into peripheral tissues but not the brain. The prolonged effects of dietary 13-HODE exposure on tissue levels and physiology remain to be determined.

AGFD002C 3558838 2:00 PM **Characterization of odorants in culinary sage, *Salvia officinalis*** Nancy Chiang nancy.chiang@effem.com Culinary sage, *Salvia officinalis* L., is a common spice plant in the mint family (Lamiaceae) that has been utilized since ancient times for culinary, medicinal, and cosmetic purposes. It is native to the northern coastal region of the Mediterranean and predominantly grows in the mountains of northern Spain, southern France, and the Adriatic belt of the Balkan Peninsula. Today, culinary sage has been naturalized and cultivated throughout the world. Teas prepared from sage are purported to aid in gastrointestinal discomfort, mental disorders, menstrual and fertility

issues, as well as for soothing coughs and sore throats. The leaves of culinary sage are consumed in various forms, whole or ground, fresh or dried, and added as a flavoring to food dishes such as stuffing for turkeys, sausages, salads, marinades, and sauces. Although the volatiles present in culinary sage have been reported, the odorants responsible for its distinct aroma profile have, thus far, remained unknown. In the present study, a total of twenty-six odorants were identified employing solvent assisted flavor evaporation (SAFE) and aroma extract dilution analysis (AEDA). Odorants with high flavor dilution (FD) factors of 1024 included 1,8-cineole (eucalyptus), α -thujone (camphorous), and camphor (camphorous). Odorants with FD factors of 512 included α -pinene (pine) and β -thujone (camphorous). Odorants with FD factors of 256 included (2E,6Z)-nona-2,6-dienal (cucumber), isoborneol (earthy), and (E)- β -damascenone (cooked apple). As a result of this study, a collection of odorants was identified that contribute to the pleasant aroma profile of culinary sage. This study provided a foundation for future quantitative and sensory evaluations on culinary sage aroma

AGFD002C 3557263 3:00 PM Predicting uranium
concentrations in sheep kidneys using mixed effect models Andee Lister arl87@nau.edu During the Cold War, uranium ore was mined on the Colorado Plateau, which overlaps the majority of the Navajo Nation. Additionally, there were various mining sites all across the Navajo Nation including Cameron, AZ where open pit mining occurred. The legacy mining has led to community concerns of exposure from uranium, arsenic, and other contaminants. Research at Northern Arizona University is focused on health risks and community impacts (e.g., consumption issues, threats to cultural values, spiritual concerns, and public health impacts) from exposure to environmental uranium contamination. The purpose of this project is to use mixed effect models to predict uranium concentrations in sheep kidneys based on grazing distances from abandoned uranium mine sites. The sheep kidney tissue samples were collected, dried, homogenized, powdered, acidified, filtered, diluted, and analyzed using an inductively coupled plasma mass spectrometer (ICPMS). The statistical analysis suggests that distance from an abandoned uranium mine site is an influential aspect as far as uranium accumulating in sheep kidneys. Consequently, for every mile that a sheep grazes away from an abandoned uranium mine site there is a decrease in uranium concentration in the kidney. The results of this analysis will inform policy with respect to traditional foods and uranium contamination and inform community members on the Navajo Nation.

WEDNESDAY AFTERNOON 4/14/21 start 1:00 PM end 4:00 PM Food-Energy-Water Nexus 2

AGFD003G 3557816 1:00 PM Dynamic functionality of the Food-Energy-Water Nexus: Efforts to help agriculture meet global needs. James Seiber jseiber@ucdavis.edu Developing environmentally stable energy processes and sources can have a positive impact on the Food-Energy-Water (FEW) Nexus paradigm. Much progress has been made over the utilization of solar, wind, and nuclear sources of energy. More efficient carbon economy and air quality practices will benefit from improved energy storage technology and uses of biofuels. Other areas to improve the FEW Nexus include reducing HCFCs refrigerants through more environmentally favorable substitutes. Current agricultural practices rely on unsustainable usage of water. Biotechnology offers one of the means of rapidly improving the drought tolerance of crops and opening new growing environments to meet the challenges of climate change. Furthermore, recent advances in greener technologies has created a dynamic FEW Nexus landscape. The balance of water requirements and greenhouse gases produced by animals is an

example of FEW Nexus dynamics that are impacted by population growth and food preferences.

AGFD003G 3552105 1:00 PM Agricultural Conservation
Planning Framework (ACPF): A planning approach for agricultural watersheds based on precision conservation Mark Tomer mark.tomer@usda.gov Nutrient and sediment losses from agricultural watersheds impacts aquatic ecosystems and presents risks to environmental and public health. Improving agricultural water quality requires careful planning and producer engagement to encourage voluntary installation of new conservation practices that are effective, and appropriate to each landscape. USDA scientists have developed the Agricultural Conservation Planning Framework (ACPF) to provide watershed databases and software tools that can be used to present realistic options for placement of conservation practices that can improve water quality outcomes. High resolution data on land cover, soil survey, and topography are analyzed to identify a suite of conservation practice options to reduce impacts of runoff and subsurface tile drainage on water quality. Results are not prescriptive, but rather are meant to provide options to help identify conservation preferences for each farm. ACPF watershed databases are available online for more than 11,500 small watersheds covering virtually all the Corn Belt. The ACPF includes tools that identify options to control runoff and water erosion, mitigate nutrient losses from tile drainage, store water on the landscape, and enables site-specific riparian analysis and streamside buffer design. Along with watershed databases and the ACPF GIS toolbox, a detailed user manual, and tutorial videos are also available (see www.acpf4watersheds.org). Social research has shown use of ACPF can help engage farmers to become more engaged in watershed improvement projects. The ACPF has been used in watershed planning by conservation districts, state agencies, environmental consulting firms, and several agricultural and environmental organizations.

AGFD003G 3561101 1:00 PM New methods for quantifying
behavioral responses to environmental and policy change Meagan Mauter mauter@stanford.edu Amanda Quay amandaq@stanford.edu Enhancing the sustainability of agricultural systems requires insight into how these complex techno-environmental-behavioral systems are likely to respond to changes in production technologies, anthropogenic environmental shocks, and public policies. Yet integrated models of food-energy-water systems tend to draw primarily on economic models, citing a need for increased biophysical and environmental process details as well as better human behavior feedback loops. We propose a suite of field-resolution models for estimating the effects of environmental and policy changes on cropping behavior. This work estimates a Ricardian model for measuring the impacts of climate (i.e., temperature and precipitation) anthropogenic (i.e., soil salinization and groundwater depletion) change on agriculture cropping practices using panel data in the California Central Valley in 2014 and 2015 ($N = 640,028$). This panel regression, at the scale of soil salinity data, empirically demonstrates that salt-robust crops replace more salt-sensitive crops as soil salinity increases. We corroborate the panel data econometrics by further estimating a multinomial logit regression at the field-scale, using the same dataset but reducing model complexity from 18 to six crops ($N = 101,418$). Compared to previous Ricardian analyses which focus mainly on long-term climate trends in temperature and precipitation, our approach captures adaptation to short-term anthropogenic change. We apply the fitted multinomial logit model to varying soil salinities and predict crop shares across the study area; we then pair these crop share yields with a biophysical model of crop salinity tolerance to estimate revenue changes and compare these results to the status quo scenario where growers maintain fixed crop shares regardless of soil salinity. The

scenario analysis illustrates the grower behavior's influence on economic impact assessments of soil salinization, with implications for future salinity management policies.

AGFD003G 3550162 2:00 PM **Managing water quality of surface runoff in agricultural field** Arlene Adviento-Borbe arlene.advientoborbe@ars.usda.gov Nutrient and sediment losses in surface runoff can be high that may cause water pollution and can represent a significant portion of total farm costs in irrigated cropped field. A field study with cotton (*Gossypium hirsutum*, L.) was conducted in production farms to quantify soluble nutrients and sediments losses from surface runoff associated with crop management practices: Conventional system, irrigated (CTIR), Conservation system, irrigated (FTIR), Conventional, rainfed (CTRA), and Conservation, rainfed (FTRA). Lint yields and concentrations of $\text{NH}_4\text{-N}$, $\text{NO}_3\text{-N}$, $\text{NO}_2\text{-N}$, dissolved P, soil sediments, other water quality metrics in irrigation runoff water were measured in all management systems. Mean lint yields ranged from 792 to 1,774 kg ha⁻¹ and were not significantly affected by irrigation or conservation practice ($P = 0.179 - 0.371$). The intensity and chemical form of nutrient losses were primarily controlled by volume of water runoff and agronomic practice. Across all systems, average concentrations of N in the runoff were $\approx 4.6 \text{ mg L}^{-1}$ and dissolved P were $\approx 0.58 \text{ mg P L}^{-1}$ and were affected by amounts of runoff water. Average nutrient concentrations in surface runoff were significantly higher in Conservation systems than in Conventional system. Water pH, specific electrical conductivity, alkalinity and hardness were within the levels that characterize irrigation water and less likely to impair pollution in waterways. Soil sediment concentrations (SSC) and total suspended solids (TSS) ranged from 27 to 1,831 mg sediments L⁻¹ and 1.4 to 1,555 mg L⁻¹, respectively. Sediment losses were reduced by 43 to 59% in Conservation system compared to Conventional systems. On average, the levels of soluble nutrients measured during field outflow were relatively small and within the range of values observed in agricultural fields. Results of this study show continuous measurements of runoff water quality are needed to better assess multiple benefits of implementing conservation management practices in the region.

AGFD003G 3536163 2:00 PM **Biochar surface oxygenation** through ozonization and unlocking of phosphorus in soil mineral phases for environmental and agroecosystems sustainability James Lee jwlee@odu.edu A novel biochar surface-oxygenation ozonization chemical process system concept has recently been created (2020 PCT International Patent Application Publication No. WO2020005760 A1). This process system could have at least four beneficial functions that may be transformative in helping to solve the environmental and sustainability grand challenges: a) Dramatically (by a factor of nearly 10 times) improving biochar cation exchange capacity (2019 Sustainable Chem. Eng. 7(19):16410-16418) which is the key property central to better retain soil water and nutrients for better water filtration, cleaner water environment and agroecosystems sustainability; b) Creating "humic acid-like" oxygenated biochar molecular fragments that can be water soluble with the potential capability to serve as a new innovative way to employ biochar materials through irrigation engineering systems to benefit the agroecosystems; c) Detoxifying aromatic toxins, which may have practical implications to inactivate any potential toxic component in biochars and other industries such as waste water treatments for sustainable water purification and resource recovery systems; d) Enabling to unlock phosphorus from insoluble phosphate materials (ACS Sustainable Chem. Eng. 8(18):7068-7077) in soil mineral phases. We have recently demonstrated that the surface-oxygenation biochar

products can unlock/solubilize phosphorus from insoluble phosphate mineral phases, a novel opportunity to overcome another major challenge of sustainability for food-energy-water systems. Note, phosphorus availability has also recently been identified as another major issue for long-term agricultural and environmental sustainability. Therefore, this function in unlocking P for plant uptake may be a revolutionary approach to enhancing the long-term sustainability and to also store carbon in the soil to help mitigate climate change. This presentation will discuss these four functions for environmental and agroecosystems sustainability.

AGFD003G 3559604 3:05 PM **Bringing sustainability to the bench** Rachael Relph rachael@mygreenlab.org In recent years, the global green labs movement has greatly accelerated with thousands of scientists looking at how they can minimize the environmental footprint of their research. Laboratories are approaching this challenge from a variety of angles and finding creative ways to bring sustainability to the bench. In this presentation we will look at practical examples of how different laboratories have been able to make small, simple changes that have a big impact on reducing energy, water, and waste in the lab.

WEDNESDAY AFTERNOON AND EVENING 4/14/21

start 5:00 PM end 7:50 PM

Modern Food Chemistry

AGFD002D 3547538 5:05 PM **Zeolitic imidazolate framework-8**

applied in functional food for curcumin intestinal delivery Situ Wenbei 842363390@qq.com For the purpose of ensuring the bioavailability of bioactive ingredients, a nano-delivery system was developed using metal organic framework. Two kinds of zeolitic imidazolate framework-8 loading with curcumin (CCM@ZIF-8) was synthesized by high-temperature one-pot method and room-temperature two-steps method respectively. The characteristic of CCM@ZIF-8 particle was also demonstrated by the analysis of morphology and crystalline structure. From the results of FTIR and BET, CCM@ZIF-8 by high-temperature one-pot method (CCM@ZIF-8-HT) had encapsulated CCM molecular into the framework structure of ZIF-8, and those by room-temperature two-steps method (CCM@ZIF-8-RT) had a few curcumins embedded into the surface of ZIF-8. This difference lead CCM@ZIF-8-HT with higher curcumin encapsulation efficiency than CCM@ZIF-8-RT. An in vitro release study showed that $96.57 \pm 0.79\%$ curcumin released from CCM@ZIF-8-HT during simulated gastric fluid transportation because ZIF-8 had no resistance to low pH environment. Compared to this, CCM@ZIF-8-RT could retained a large part of curcumin and transported to simulated small intestine and colon, which related to the curcumin embedded into ZIF-8 and reduced the erosion from acidic medium. Furthermore, with room-temperature two-steps method, a ZIF-8 nanoparticle loading with BSA was synthesized. Similarly, this nanoparticle also exhibited controlled releasing profile for protein delivery. This study will make a development of MOF as carrier material in functional food.

AGFD002D 3548547 5:00 PM **In-situ form graphitic**

$\text{C}_{3\text{-N}_4}$ -PDOL composite interlayer toward stable lithium metal anodes Zilong Zhuang zlzhuang1995@qq.com Lithium metal anode has the highest energy density among all anode materials while dendrite growth hinders the direct use of lithium metal anode in batteries. Herein, ultrathin graphitic $\text{C}_{3\text{-N}_4}$ -poly(1,3-dioxolane) (CN-PDOL) composite interlayer is in-situ polymerized upon lithium metal anode. Flexible PDOL could separate Li anode and electrolyte, suppress the continuous breaking/generating of SEI layer and consumption of electrolyte, while $\text{g-C}_{3\text{-N}_4}$ nanosheets could reduce the crystallinity of PDOL, increase ion-conductivity and uniform Li-ion flux. The synergistic effect of CN and PDOL could

enable stable Li plating/stripping process over 850 h at a high current density of 3 mA cm⁻² with a low overpotential of about 70 mV. This work demonstrates a promising strategy of functional buffer layer design for lithium metal anodes.

AGFD002D 3548745 5:00 PM **Metabolic fates of intraruminal rutin in dairy cows** Yue Guo guoxx390@umn.edu Rutin is a natural flavonol glycoside with diverse health-promoting properties through the bioactivities of quercetin, its aglycone. While widely distributed in the vegetables and fruits of human diet, rutin is either absent or inadequate in common animal feed ingredients. Rutin has been supplemented to dairy cows for performance enhancement, but its metabolic fate in vivo has not been determined. In this study, 100 mg/kg rutin was administered to 4 Holstein cows intraruminally, and the ruminal fluid, plasma, and urine samples collected before and after the rutin dosing were examined by both targeted and untargeted liquid chromatography-mass spectrometry-based metabolomic analysis. Targeted analysis of rumen fluid samples showed that rutin and quercetin were rapidly degraded in the rumen within 1 and 2 h of the dosing, respectively. Untargeted metabolomic analysis further identified 3,4-dihydroxyphenylacetic acid (DOPAC) and 4-methylcatechol as the microbial metabolites of quercetin in the rumen, peaking at 2 h and 4 h, respectively, after rutin dosing. Interestingly, quercetin and DOPAC as well as their conjugates were hardly detectable in plasma samples. Instead, 4-methylcatechol sulfate was identified as the major metabolite of quercetin in plasma and urine. The high abundance of 4-methylcatechol sulfate in the 6-h plasma samples and its absence in the pre-3h urine samples indicated the high bioavailability and slow absorption of 4-methylcatechol. Metabolomic analysis further revealed that rutin administration decreased the levels of p-cresol sulfate and hippuric acid, two phenolic microbial metabolites, in plasma and urine, suggesting potential competitive inhibition between quercetin degradation and microbial metabolism of aromatic amino acids in the digestive tract of dairy cows. Overall, these observations define the in vivo metabolic route of rutin and quercetin and further indicate that 4-methylcatechol, a bioactive metabolite, might contribute to the reported bioactivities of rutin and quercetin in dairy cows.

AGFD002D 3552541 6:05 PM **Physiological and molecular response of wheat (Triticum aestivum) exposed to perfluorooctanoic acid (PFOA)** Polycarp Ofoegbu polycarpsmart8@gmail.com PFOA is a prominent member of a class of straight chain fluorinated organic chemical compounds collectively called per and polyfluorinated alkyl substances (PFAS). Due to its peculiar properties (thermal stability, oils and water repellency, water solubility), PFOA is widely employed in firefighting, packaging, non-stick cookware, mattresses and others. However, it constitutes significant environmental and health concerns due to its disruptive nature in biological matrices. Wheat is widely consumed as a staple food owing to its high nutritional value (i.e., rich source of dietary fiber and protein). Physiological, ionome, and metabolome responses of wheat grown in soil treated with 0, 25, and 50 mg/kg PFOA were evaluated. Data revealed that PFOA impacted grain production in wheat. Ionomics revealed that PFOA modified elemental contents of major nutrients (e.g., magnesium, potassium, phosphorus, and iron). In addition, metabolomics showed alterations in several biochemical pathways such as citrate cycle, starch and sucrose metabolism, and unsaturated fatty acids biosynthesis.

AGFD002D 3549948 6:00 PM **Food-borne nanoparticles from undaria pinnatifida as an efficient nanocarrier for zinc delivery** Shuai Hou houshuai009@126.com Zinc is an essential micronutrient in human body with diverse functions, however, due to the effect of dietary inhibitors of zinc absorption such as phytate, the bioavailability of zinc salts is too low. Nanoparticles were

extensively applied as bioactive compounds carrier to improve their absorption and bioavailability. Here we showed that food-borne nanoparticles from undaria pinnatifida (UPFNs) as an efficient nanocarrier for zinc delivery. Water-soluble UPFNs were first prepared by hydrothermal synthesis and green purification methods and then chelated with zinc. The chelating optimization results showed that the most optimal pH was 10 and mass ratio of UPFNs to zinc was 1:3. Compared with the well dispersed sphere of UPFNs, the formed UPFNs-Zn complex presented the aggregation morphology. In addition, Zinc ions mainly interacted with active functional groups such as carboxyl and amino groups on the surface of UPFNs. Thermodynamic analysis revealed that UPFNs were spontaneously interacted with Zinc by electrostatic interaction with a negative Gibbs free energy change. Meanwhile, compared with commercial zinc sulfate, UPFNs-Zn showed higher stability both in phytic acid solution and the process of gastrointestinal digestion. Finally, no obvious cytotoxicity was found in UPFNs-Zn. These results revealed that UPFNs might be served as an efficient, stable, and safe nanocarrier for zinc delivery

AGFD002D 3553969 6:00 PM **Urea pseudopeptidic organogelators for the encapsulation and delivery of (R)-limonene** Belen Altava altava@uji.es Adriana Valls avalls@uji.es The encapsulation of essential oils for flavors and fragrances is of great interest. They are volatile compounds synthesized by plants and having strong odor. Different natural flavor-oils have been described to have antimicrobial, antioxidant, antifungal, anticancer, antiviral, insecticidal and anti-inflammatory properties. Their encapsulation is a good strategy to avoid fast volatilization and degradation during storage, with their controlled release allowing a longer activity for the same amount of active substance. In this regard (R)-Limonene is present in a variety of products for food and cosmetic industries and for household purposes, being amongst the first natural pesticide ingredients used for environmentally-friendly pest control. Therefore, the encapsulation of this flavor-oil is of great interest for different applications. Gel formulations are of clear interest in this regard. We present here the use of low molecular weight compound containing alkylurea fragments of different mimetic pseudopeptidic structures as excellent organogelators. Both the topology and the symmetry of the corresponding urea compounds play a role in defining their organogelator behavior and this can also be tuned by the presence of additional supramolecular guests as is the case of suberic acid. They also achieve the gelation of relevant active substances like terpenic natural oils and complex mixtures of flavors and fragrances, providing a simple and mass efficient supramolecular systems for the quantitative encapsulation of the active substance under consideration and the consequent controlled release.

AGFD002D 3553260 7:10:00 PM **Presence and Interaction with Dopamine of Carbon Dots from Salmon (Salmo salar L.) during Roasting Process** Yukun Song 593186461@qq.com The safety of fluorescent carbon dots (CDs) in food has drawn great attention in recent years. In this paper, the presence and formation mechanism of CDs from roasted salmon and their interaction with dopamine (DA) were investigated. The size and morphology of the fluorescent CDs highly depend on the roasting time, which also affect the functional groups on their surface. The fluorescence properties of the CDs were affected by the roasting time, and displayed excitation-dependent emission behavior. The formation of CDs is believed to go through a process of morphology evolution, including formation of polymer-like CDs, carbon core and carbon core growth. The overlap and close-distance interaction was confirmed by the Förster resonance energy transfer (FRET) effect between CDs and DA. In addition, the fluorescent CDs had a potential biological impact to active substance with small molecule. This work represents the first report of foodborne fluorescent CDs and interaction with DA of CDs from

salmon during roasting process provide new knowledge about CDs in food which expands their biological impact.

AGFD002D 3553340 7:00 PM **Characterization of moisture migration, microstructure and quality of sea cucumber during microwave vacuum drying and rehydration process** shasha cheng chengshasha880321@126.com Moisture migration, microstructure and quality of sea cucumber during microwave vacuum drying (MVD) and rehydration process were characterized in this study. Three water components were identified in sea cucumber using low-field nuclear magnetic resonance (LF-NMR) relaxation, and the three peaks of water components shifted to short relaxation time during MVD process. The peak area of major water component immobilized water decreased significantly due to water evaporation induced by MVD. Magnetic resonance imaging (MRI) found that the water in the internal layer of sea cucumber body wall was firstly removed due to the internal heating of microwave, and then the water in the outer layer. Higher microwave power could accelerate the moisture migration during drying process, and shorten the drying time. Porous microstructure was observed by Cryo scanning electronic microscope images in sea cucumber dried with microwave power of 200 and 250 W, which might be responsible for high values of rehydration ratio and water holding capacity. High microwave power caused the increase of amino acids content, the change of saponins content was not significant. In addition, excellent prediction models of moisture ratio have been developed by partial least squares regression analysis based on transverse relaxation data, which proved the feasibility of LF-NMR to monitor water changes of sea cucumber during MVD.

WEDNESDAY EVENING 4/14/21 start 5:00 PM end 8:00 PM Nanotech that Drives Sustainability

AGFD003H 3559075 5:00 PM **Bio-inspired nano-fibrous structures for advanced functions** You-Lo Hsieh ylhsieh@ucdavis.edu Biosynthesized high length-to-width aspect ratio molecules and fibers are structural and functional materials in life and biology. Most biopolymers including polysaccharides and proteins are, however, challenging to engineer into fibrous structures due to limited solubility or dispersibility in solvents and difficulty in molecular reorganization in the solid state. This paper presents diverse approaches to create novel materials from the abundant polysaccharides, proteins, and phenolics among the under-utilized agricultural and forest by-products. Robust solubility and electrospinning of cellulose, chitin, and chitosan derivatives have been exploited to create high specific surface fibers with unique morphologies (multi-component hybrids, sheath-core, hierarchical porosity, etc.) and chemistries (stimuli-responsive, enzyme/ligand binding, antimicrobial). Globular proteins have been facilely processed into amphoteric and amphiphilic colloids and semi-crystalline microfibers to enable formation of high-internal-phase and double emulsions, templates for control release of hydrophobic and hydrophilic compounds as well as amphoteric and amphiphilic coatings and films. Nanocelluloses with designed surface chemistries have been derived from crop residues to self-assemble into nanofibers, hydrogels, and aerogels or to be engineered into unique hierarchical hybrids, sheath-core, porous structures for applications in catalysis, separation, bioremediation, antimicrobial, chemical/drug-delivery, sensing, etc. Biological nanomaterial innovations from agricultural and energy crop residues can offer versatile solutions and opportunities to meet future demand in advanced materials while reduce demand on fossil fuel resources while also minimize negative environmental impact from our food and bioenergy systems.

AGFD003H 3554467 5:00 PM **Sustainable nanomaterials as biosensors for food security and environmental applications** Omowunmi Sadik sadik@njit.edu Sustainable nanotechnology is the research and development of nanomaterials with economic and

societal benefits while minimizing adverse environmental impacts. In the last decades, we have developed robust methods for creating sustainable materials compatible with biological systems. An example is the discovery of a new class of nanostructured, π -conjugated, poly(amic acid) $\frac{3}{4}$ or BioTerc PAA. The uniqueness of BioTerc PAA lies in its excellent chromatic, electronic, biodegradable, and mechanical properties. PAA properties can be tuned via electronic coupling between the sequestered nanoparticles and their neighboring moieties, and where relevant, they can be interfaced with the biological systems. This presentation will focus on how the delocalized π -electron system in the BioTerc PAA has been exploited for green nanosynthesis, as well as sensors for food security, metal detoxification, and bio-batteries. BioTerc PAA materials provide superior properties that can meet the requirements of society's expectations for a safer environment and a sustainable future

AGFD003H 3558510 5:00 PM **Towards rational design of efficient and targeted foliar-applied agrochemicals** Greg Lowry glowry@andrew.cmu.edu Agrochemical application practices are inefficient and require more sustainable approaches. Foliar application of engineered nano-carriers could provide highly efficient and controlled delivery of agrochemicals into plants, but the physical chemical properties controlling leaf uptake and translocation in plants are unknown. Here, we systematically evaluated the effect of nano-carrier size, charge, and hydrophobicity on their uptake, phloem loading, and distribution in tomato (*Solanum lycopersicum*) plants. Poly(acrylic acid)-block-poly(2-(methylsulfinyl)ethyl acrylate) (PAA-*b*-PMSEA) and poly(acrylic acid)-block-poly((2-(methylsulfinyl)ethyl acrylate)-*co*-(2-(methylthio)ethyl acrylate)) (PAA-*b*-P(MSEA-*co*-MTEA)) star polymers were synthesized using controlled polymerization methods to provide carriers with different sizes (6-35 nm), negative charge content (17-83% PAA) and hydrophobicity (varying MSEA/MTEA ratio). All of the foliar applied star polymers displayed similar rapid and high rates of phloem loading (~30 wt%). However, the property differences affected their distribution to other plant compartments including younger leaves, older leaves, stems and roots. The smallest ~6 nm star polymers translocate most to younger leaves, while the largest ~35 nm star polymer moved preferentially to roots, likely due to different transport pathways in the leaf mesophyll tissue for the different sized materials. Charge content also affected the distribution of star polymers in the plants. The lower charge content star polymer moved more into the non-vascular tissues (younger leaf, older leaf and root), while the higher charge content star polymers mainly stayed in stem. This is likely due to charge dependent interactions with cell walls. Hydrophobicity did not affect star polymer translocation after entering the mesophyll but did affect their interaction with the leaf surface and the ability to penetrate the epidermis. These results can promote rational design polymer nano-carriers for more efficient and targeted agent delivery in plants, and more sustainable agricultural practices

AGFD003H 3551943 6:00 PM **Biodegradable zein and lignin nanoparticles as methoxyfenozide delivery systems in soybean plants** Cristina Sabliov csabliov@lsu.edu Biodegradable polymeric nanoparticles have the potential to significantly impact the agrochemical industry. It is imperative to study their behavior in plant systems to determine their effectiveness as sustainable agrochemical delivery systems. In this study we explore translocation of methoxyfenozide (MFZ) delivered by zein and lignin nanoparticles (ZNPs and LNPs) in soybean plants exposed to the particles through the roots under hydroponic conditions. ZNPs were synthesized by nanoprecipitation from zein with SDS as a surfactant, and LNPs were synthesized by emulsion evaporation from lignin-graft-poly(lactic-*co*-glycolic) acid. Both types of particles were loaded with MFZ, a non-

systemic pesticide (6.2 % (w/w) in ZNPs, and 2.7 % (w/w) in LNPs). Dynamic light scattering confirmed that LNPs measured 106 nm in diameter, with a narrow size distribution and a zeta potential of -42 mV. ZNPs measured 126.4 nm and had a zeta potential of 44.75 mV. Soybeans were grown hydroponically and were treated with 0.02, 0.2 or 2 mg/ml of LNPs or ZNPs at 28 days after germination. Plants were harvested after 6, 12, and 24 hours of continuous particle exposure to the root. Root, stem and leaves were collected and concentration of methoxyfenozide was quantified. Results indicated that both ZNPs and LNPs were effective at translocating MFZ from the hydroponic solution to the roots, and from the roots to the leaves of the plants relative to the control, free MFZ. LNPs were more effective than ZNPs at transporting MFZ from the hydroponic solution to the roots of the plants. For example, MFZ concentrations in the roots of plants treated with high concentration of LNPs were 184, 377, and 519 µg/g at 6, 12, and 24 hrs, relative to the much smaller 33, 46, and 143 µg/g delivered by the ZNPs even though the amount of MFZs available in the Hoagland solution spiked with ZNPs was higher than for LNPs at the same NP concentration, due to the higher loading of MFZ in the ZNPs. ZNPs translocated 16.2, 10.2 and 2.8 % of the available MFZ in the roots to the leaves (equivalent to 1.94, 3.68, and 5.08 µg) at low, medium, and high concentrations respectively. The LNPs translocation percentages were smaller 2.9, 3.4, 0.3 %, but led to similar amounts (0.23, 1.13, and 5 µg) in the leaves. In conclusion, ZNPs and LNPs were found suitable as sustainable delivery systems for MFZ and can be further developed to efficiently deliver other types of agrochemicals to plants.

AGFD003H 3554868 6:00 PM **Size and shape-dependent** antimicrobial activities of silver and gold nanoparticles: a model study as potential fungicides Francis Osonga francis.j.osonga@njit.edu Ali Akgul aliakgul@ufl.edu Idris Yazgan iyazgan1@binghamton.edu Ayfer Akgul aa1625@msstate.edu Gaddi Eshun gbe4@njit.edu Laura Sakhae lsakhae1@binghamton.edu Omowunmi Sadik sadik@njit.edu Plant-based pathogenic microbes hinder the yield and quality of food production. Plant diseases have caused an increase in food costs due to crop destruction. There is a need to develop novel methods that can target and mitigate pathogenic microbes. This study focuses on investigating the effects of Luteolin tetraphosphate derived silver nanoparticles (LTP-AgNPs) and gold nanoparticles (LTP-AuNPs) as a therapeutic agent on the growth and expression of plant-based bacteria and fungi. In this study, the silver and gold nanoparticles were synthesized at room temperature using Luteolin tetraphosphate (LTP) as the reducing and capping agents. The synthesis of LTP-AgNPs and LTP-AuNP was characterized by Transmission Electron Microscopy (TEM) and size distribution. The TEM images of both LTP-AgNPs and LTP-AuNPs showed different sizes and shapes (spherical, quasi-spherical, and cuboidal). The antimicrobial test was conducted using fungi: *Aspergillus nidulans*, *Trichaptum biforme*, *Penicillium italicum*, *Fusarium oxysporum*, and *Colletotrichum gloeosporioides*, while the class of bacteria employed include *Pseudomonas aeruginosa*, *Aeromonas hydrophila*, *Escherichia coli*, and *Citrobacter freundii* as Gram (-) bacteria, and *Listeria monocytogenes* and *Staphylococcus epidermidis* as gram (+) bacterium. The antifungal study demonstrated the selective size and shape-dependent capabilities in which smaller sized spherical (9 nm) and quasi-spherical (21 nm) AgNPs exhibited 100% inhibition of the tested fungi and bacteria. The LTP-AgNPs exhibited a higher antimicrobial activity than LTP-AuNPs. We have demonstrated that smaller sized AgNPs showed excellent inhibition of *A. nidulans* growth compared to the larger size nanoparticles. These results suggest that LTP-AuNP and LTP-AgNPs could be used to address the detection and remediation of pathogenic fungi, respectively.

AGFD003H 3562070 7:05 PM **Treating Grapevine Viral** Diseases with RNAi Avi Schroeder avis@technion.ac.il Grapevine leafroll disease (GLD) is a globally spreading viral infection that causes major economic loss by reducing crop yield, plant longevity and hampering berry quality, with no effective treatment. Grapevine leafroll associated virus 3 (GLRaV-3) is the most severe and prevalent GLD strain. We evaluated the ability of RNA interference (RNAi), a non-GMO gene-silencing pathway, to treat GLRaV-3 in infected vines. We synthesized lipid-particles as a carrier for double-stranded RNA (dsRNA, 250-bp-long) to target two conserved sequences in GLRaV-3's viral genome. The RNAi lipid particles, 220 nm in diameter, displayed a fibrillar structure with high-contrast locally ordered domains, correlating to the aminated lipid wrapping spirally around the dsRNA. The formulation effectively protected RNA from degradation by ribonucleases. Furthermore, particles trafficked distantly from the application site, after being applied to the grapevine leaves. In three field experiments conducted on Cabernet Sauvignon vines, foliar administration of RNAi particles knocked down GLRaV-3 titer and initiated recovery of the vine and berries. This study demonstrates RNAi as a promising platform for treating viral diseases in agriculture.

THURSDAY MORNING 4/15/21 start 9:00 AM end noon **Food Safety and Security**

AGFD003I 3558260 9:00 AM **Sustainability: Advances and** applications of chemicals prediction tools in food safety and security Y. Jane Tseng yjtseng@csie.ntu.edu.tw In silico or computational tools have been widely used in the fields of drug discovery, development, and chemicals used in environmental protection to assess chemical's physical properties as well as their physiological effects in humans. It would be of great benefit that those tools can be applied to food safety and security to better reduce the risk of toxins and potentially harmful components in food for the general public. This talk will focus on computational tools towards food safety and food security as well as regulatory considerations

AGFD003I 3550371 9:00 AM **Reducing exposure to mycotoxins** using computational toxicology and nanostructured materials to improve food safety and security Michael Appell michael.appell@gmail.com Food safety and security are important to ensure a safe, nutritious, and sustainable food supply. Foodborne illnesses are serious public health problems that often occur due to pathogen contamination of commodities and lack of adequate detection and monitoring efforts. Contamination of grains and fruits by mycotoxin producing fungi poses health risks to humans and animals. Computational assessments of toxins and antifungal agents with genetic functional approximation methods have developed predictive models to improve toxin detection and aid the development of better antifungals and materials to remove toxins. In an iterative process, rationally designed nanostructured synthetic materials have been developed that enable more robust and rapid methods to reduce exposures to ochratoxin A in wines, patulin in apple juice, and citrinin and fusaric acid in corn. The approaches presented contribute to broader efforts to realize sustainable food security and safety.

AGFD003I 3533800 9:00 AM **Making natural sustainable: New** routes to natural products of commercial interest Derek McPhee mcphee@amyris.com Driven by eco-conscious consumerism, there is currently increased interest in the use of natural products. Consumers (and the companies marketing their products to them) often use colloquially and indistinctly terms like "green", "eco-friendly" or "sustainable" to refer to these natural products, but whereas sustainability represents a higher standard that encompasses green products and eco-friendly practices, many green products are decidedly unsustainable. In this work we will present some examples

of how white biotechnology can provide truly sustainable natural products of commercial interest and discuss some of the sustainability challenges being addressed in each case (land use, biodiversity preservation, energy consumption, etc).

AGFD003I 3557027 10:00 AM **Use of carboxymethyl cashew gum** grafted with immobilized antibody for potential biosensor applications Roselayne Furtado roselayne.furtado@embrapa.br Atanu Biswas atanu.biswas@usda.gov In this work, cashew gum (CG) was derivatized and used as a platform for antibody (Ab) immobilization, which was then incorporated into a biosensor for bacteria detection. The CG was first isolated and characterized, followed by conversion to carboxymethyl cashew gum (CMCG). The CMCG film was a viable support for antibody immobilization; it was electrodeposited on a gold surface using the cyclic voltammetry technique, applying a potential sweep from -1.0 V to 1.3 V with a scan rate of 50 mV s⁻¹ and 10 scans. The COOH groups on the surface of the film were critical in promoting protein A (PrA) bonding. The immobilization of the Ab was mediated by PrA for recognition of the antigen. Voltammetry was used to study and monitor the Ab immobilization. Finally, the analytical response of the CMCG-PrA-Ab system was evaluated with the chronoamperometry technique and was found to detect *Salmonella Typhimurium* bacteria rapidly and efficiently. This result is significant because it opens up a range of possibilities for the use of CG derivatives to immobilize biomolecules that can function as bioreceptors in the development of biosensors and bio-devices.

AGFD003I 3552315 10:00 AM **Role of innovative processing technology of aquatic product in blue granary** Dayong Zhou zdzyfl@163.com Aquatic product is an important source of high quality food, and is regarded as "blue granary". According to the statistics of Food and Agriculture Organization of the United Nations, the world total output of aquatic products reached 179 million tons in 2018, and the global per capita aquatic product consumption has set a new record of 20.5 kg per year. Aquatic product plays an important role in ensuring the supply of high-quality protein, improving the health level of human and expanding the strategic space of food security. Therefore, the development of innovative processing technology of aquatic product is important as which provides support for comprehensive processing and development of high value products. The present presentation is aimed to introduce the latest progresses in the fundamental and applied research of aquatic products in China. Researchers have clarified the characteristics of shellfish under fatigue state, determined the dominant mechanism of sea cucumber autolysis, illustrated the mechanism of quality change of fresh aquatic products during storage and transportation. Researchers also revealed the effects of processing microenvironment on the structure changes of important components of aquatic products and its correlative mechanism on flavor quality. They revealed the changes of nutrient components, endogenous enzymes, microbial distribution, precursors and decomposition products of safety hazard factors during the processing of aquatic products. The changes of nutritional quality of some important aquatic products in the process of cold chain and normal temperature circulation were revealed and the influencing mechanism of different storage and transportation conditions on the quality of aquatic products was clarified.

AGFD003I 3534118 11:05 AM **Balancing microbial and chemical safety for hydroponically grown vegetables** Thanh Nguyen thn@illinois.edu Hydroponic production of vegetables is becoming more common, especially in regions with unfavorable climate for year-round crop production. However, if viruses are present in the feed water, then there is a chance that infectious viruses will be internalized into the tissues of hydroponically-grown vegetables. When this happens, surface sanitization of postharvest vegetables

may not be effective because the sanitizer cannot disinfect the internalized viruses. We conducted two sets of experiments to evaluate the cytotoxicity of hydroponic water after chlorination and ozonation and efficacy of virus inactivation by peracetic acid (PAA), an organic sanitizer with low toxicity risk. The overall results indicate that hydroponic water's cytotoxicity may increase when higher concentration and shorter exposure time were used to inactivate recalcitrant pathogens. To counteract the potential increase in cytotoxicity, a lower disinfectant dose and longer contact time may be adopted for both ozonation and chlorination. We also determined if peracetic acid (PAA) effectiveness is affected by the location of viruses (virus-contaminating produce surfaces or inside the tissues) in crops. The PAA disinfection efficacy was higher when the RV was on the arugula surface instead of the arugula interior. However, PAA disinfection efficacy of TV was not dependent on the virus location in arugula. For both internalized TV and RV, the disinfection efficacy was less than 2-log₁₀ using all PAA concentrations and exposure times examined here. Thus, both the type and location of viruses in fresh vegetables may influence postharvest vegetables' virus disinfection. Therefore, the optimization of sanitation for postharvest fresh vegetables is needed to reduce foodborne viral infection risks.

THURSDAY MORNING 4/15/21 start 9:00 AM end 11:45 PM Recent Topics in Food Chemistry

AGFD002E 3556611 9:00 AM **Fate of Brassicaceae seed meal derived biopesticides in soil** John Randall jrandall@uidaho.edu The emergence of pesticide-resistant species has increased significantly during the last 50 years, which has necessitated an increase in the use of synthetic pesticides and the development of novel pesticides. The environmental and health effects of many of these pesticides are not well understood, and any adverse effects may only be exacerbated with increased use. Botanical pesticidal compounds may offer a safe alternative to synthetic pesticides. Brassica species produce a wide range of glucosinolates, which break down to toxic isothiocyanates (ITCs) that can be used in pest control. ITCs have shown pesticidal activity against a wide range of pests, including insects, nematodes, and noxious weeds. Derived from mustard seed meal, a low-cost feedstock, these pesticides are an economically viable alternative to synthetic pesticides for farmers and land managers. However, for these pesticides to be widely adopted for grower use, there needs to be more knowledge about their transport, degradation, and reactivity in agricultural soil. Here we present a fate study of mustard meal extract biopesticides from *Sinapis alba* and *Brassica juncea* using soil lysimeters with dimensions 30 x 20 x 6-inches equipped with vertical water sampling ports and a modular drip line for irrigation. A moisture regime representative of agricultural soil was used for the experimental setup. The concentration of the glucosinolates sinalbin and sinigrin from *Sinapis alba* and *Brassica juncea*, respectively, as well as their hydrolysis products, and the activity of endogenous enzyme myrosinase were quantified in soil and leachate using high-performance liquid chromatography/mass spectrometry and ion chromatography. The data obtained from this study can be used to develop application recommendations that will maximize the efficacy of the pesticides and limit the cost to farmers and land managers

AGFD002E 3556767 9:00 AM **Powerful dendritic antioxidants** free of pro-oxidant effects Choon Lee leelcy@cmich.edu Free radicals are generated during the normal metabolism. Inflammation, infection, lifestyle, and environmental factors also contribute to increasing free radical formation in the body. Overly produced free radicals cause oxidative damage to cells, causing oxidative stress, which can lead to pathogenesis of various human ailments. Antioxidants neutralize harmful free radicals and prevent cells from oxidative cellular damage. There is mounting evidence showing the benefits of natural antioxidants like flavonoids, vitamins C and E in

the prevention of various human diseases. However, many of these popular antioxidants in the presence of transition metal ions, such as iron and copper, generate large amounts of harmful free radicals, resulting in cellular damage (pro-oxidant effect). This contradicting antioxidant and pro-oxidant behavior of these antioxidants is a significant concern in the use of antioxidants as preventative therapeutics. To overcome this antioxidant dilemma, we utilized a nanotechnology approach; we designed and synthesized antioxidants in dendritic architectures to separate the antioxidant property from pro-oxidant effects. These dendritic antioxidants displayed far superior free radical scavenging activities than the naturally occurring antioxidants. Most importantly, they did not show pro-oxidant effects in the presence of physiological amounts of transition metals. In this presentation, we will report synthesis and characterization of macromolecular dendritic antioxidants as well as their protective effects on human low-density lipoproteins and DNA.

AGFD002E 3557911 9:00 AM **Interactions of carbon dots with plant cell walls** Su-Ji Jeon jsuji@ucr.edu Cell walls are a unifying feature of plants and a key barrier limiting nanoparticle uptake into plant cells. Herein, we systematically investigated the influence of nanoparticle surface charge on the interactions with chemically heterogeneous plant cell walls. We assessed the interactions of fluorescent carbon dots (CDs) with positive, neutral, and negative zeta potentials with model plant cell wall surfaces composed of cellulose or pectin. Our results based on confocal fluorescence microscopy imaging, XPS, FTIR, and QCM-D indicate that the interaction between plant cell walls and nanoparticles is dominated by electrostatic interactions. The positively charged CDs have the strongest affinity to plant cell walls, which is dominated by the electrostatic interaction between the surface amine groups of CDs and the carboxyl groups of pectin, while CDs with negative or neutral zeta potential exhibit negligible interactions with plant cell walls. We validated our analysis based on interactions of CDs with model plant cell wall surfaces in isolated native cell walls of land plants (*Arabidopsis*) and green algae (*Coleochaete*). This study provides insight into nanoparticle surface charge design for optimizing delivery into crop plants and contributes to improve our understanding of nanoparticle interactions with plant biosurfaces in the environment.

AGFD002E 3558831 10:00 AM **The key impact odorant from the fungus, *Daldinia childiae*** Andrew Moore amoor140@vols.utk.edu A study was conducted to identify the odorant responsible for a pleasant woody cologne-like aroma produced from the fermentation broth of the fungus *Daldinia childiae* (J.D. Rogers & Y.M. Ju). Odorants that impart woody aroma attributes to flavors and fragrances hold significant value to both the food and cosmetic industry. Solvent-assisted flavor evaporation (SAFE) and aroma extract dilution analysis (AEDA) applied to 30-day old fungal fermentations led to the identification of guai-11-en-10-ol, also known as pogostol, as the key impact odorant. Guai-11-en-10-ol has been previously identified in the plant *Pogostemon cablin*, the source of “patchouli oil,” which is widely used in the flavor and fragrance industry. The odorant was isolated from *D. childiae* by means of solid-phase extraction (SPE) and normal phase column chromatography. The compound was then deuterated and subsequently used as an internal standard. Stable isotope dilution assays (SIDA) were then used to quantitate guai-11-en-10-ol in 30-day old fermentations. Additionally, the odor threshold of the odorant was determined. A high odor activity value (OAV) was determined for guai-11-en-10-ol (OAV; 102689). This study lays the groundwork for future investigations aimed at the utilization of *D. childiae* as a source of guai-11-en-10-ol for flavor and fragrance applications.

AGFD002E 3558830 10:00 AM **On the role of substrate recognition in modulating strigolactone receptor selectivity in witchweed** Diwakar Shukla diwakar@illinois.edu Witchweed, or *Striga hermonthica*, is a parasitic weed that destroys billions of dollars worth of crops globally every year. Its germination is stimulated by strigolactones exuded by its host plants. Despite high sequence, structure, and ligand binding site conservation across different plant species, one strigolactone receptor in witchweed (ShHTL7) uniquely exhibits a picomolar EC50 for downstream signaling. Previous biochemical and structural analyses have hypothesized that this unique ligand sensitivity can be attributed to a large binding pocket volume in ShHTL7 resulting in enhanced ability to bind substrates. Additional structural details of the substrate binding process can help explain its role in modulating the ligand selectivity. Using long-timescale molecular dynamics simulations, we demonstrate that mutations at the entrance of the binding pocket facilitate a more direct ligand binding pathway to ShHTL7, whereas hydrophobicity at the binding pocket entrance results in a stable “anchored” state. We also demonstrate that several residues on the D-loop of AtD14 stabilize catalytically inactive conformations. Finally, we show that strigolactone selectivity is not modulated by binding pocket volume. Our results indicate that while ligand binding is not the sole modulator of strigolactone receptor selectivity, it is a significant contributing factor. These results can be used to inform the design of selective antagonists for strigolactone receptors in witchweed.

AGFD002E 3552320 10:00 AM **Engineered bacteriophage-based-electrochemical biosensor via hierarchical conductive nanofibers for rapid bacterial detection in food/fresh produce** Ahmed El-Moghazy aelmoghazy@ucdavis.edu Foodborne illnesses resulting from bacterial pathogens pose a serious threat to human health worldwide. The ability to more rapidly and sensitively detect bacteria in food samples is critical to ensure food safety and minimize the risk of human exposure to potential hazards. This study demonstrates the development of a highly sensitive and a selective electrochemical biosensor platform using a unique combination of hierarchical PEDOT nanofibrous-modified-chip with genetically engineered bacteriophage T7 for the detection of *Escherichia coli* without the need for extensive culturing or nucleic acid extraction. This biosensor platform is based on engineered bacteriophage mediated specific lysis of target bacteria and electrochemical detection of alkaline phosphatase enzyme induced by the genetically modified phages infecting bacteria and its release upon lysis of the bacteria by T7 phages. The conductive nanofibrous membranes as a sensor matrix increased the electroactive surface area by 4 fold compared with the casted PEDOT membrane and non-conductive nanofibrous membranes, respectively. The integration of the phage, nanofiber, and electrochemical technologies demonstrated successful detection of 1 CFU g⁻¹ of *E. coli* BL21 in spinach leaves within 1 h after the enrichment. Moreover, the developed biosensor exhibited high specificity toward the *E. coli* in the presence of other common food bacterial contaminants and commensal bacteria.

AGFD002E 3545122 11:05 AM **Microfluidics-based synthesis of pH-responsive colon-targeted fucoxanthin nanoparticles** Wentao Su suwentao2020@yeah.net Fucoxanthin (Fx) has varieties of biological activities such as anti-tumor, anti-oxidation, anti-inflammatory, hypoglycemic, hypolipidemic and weight loss, which has become one of the hot spots in the exploration and development of marine drugs. However, its application is limited to its poor water solubility and strong environmental sensitivity. Microfluidic device has the ability of efficient fluid mixing and accurate fluid control. Compared with conventional methods, microfluidics-based approach for nanoparticle synthesis is more conducive to the production of Fx nanoparticles

(F_xNPs) with controllable structure and high water solubility. Recently, we have synthesized hybrid nanoparticles with fucoidin as core and shellac as shell by using microfluidic device (Fig.1). The mean particle size of synthesized F_xNPs was less than 200 nm and the zeta potential was about -25 mV. In addition, the FT-IR and ¹H-NMR confirmed well encapsulation of F_x into the shellac. Observed by SEM and TEM, it was found that F_xNPs were spherical with obvious core-shell structure. Furthermore, the releasing evaluation exhibited the release of nanoparticles in gastric and intestinal fluids was inhibited but promoted in colorectal. Moreover, F_xNPs didn't showed cytotoxicity to Caco-2 cells at the concentration up to 20 μg/mL. These results indicated that F_xNPs can be used as an effective colon-targeted delivery system to improve the bioavailability of lipophilic compounds.

AGFD002E 3557154 11:00 AM **Biodegradable chitosan-montmorillonite nanocomposite hydrogel for controlled fertilizer release and water retention** Zeou Dou zdou8@gatech.edu Overpopulation poses pressure on sustaining food production, demanding a significant increase in crop yield. However, traditional fertilizers are applied in the form of soluble salts of the nutrients, a significant portion of nutrients is lost during leaching and runoff causing economic loss and environmental threats. Enhanced efficiency fertilizers are rendered critical in mitigating adverse environmental effects and increasing the productivity and profitability of crop production. Here, we present a controlled fertilizer release strategy based on widely available and biodegradable chitosan. Hydrophilic chitosan polymer chains were mainly crosslinked through freeze-thaw physical crystallization association to form polymer network hydrogels. Physical crosslinking ensures the excellent biodegradability of the chitosan hydrogels. Interpenetrating long chains with short chains facilitated the swelling of the synthesized chitosan hydrogel with interconnected pores, which achieved a steady fertilizer release. Two-dimensional montmorillonite nanoclay flakes with a thickness around 1 nm were mixed with the polymer to form microporous structures for enhanced diffusion of fertilizer ions. Improved cumulative fertilizer release ratio was achieved with the sponge-like porous hydrogel/nanoclay composite. Over the course of around 20 days, up to 80% of loaded nutrient ions were released into the aqueous medium. The addition of nanoclays also fortified the crosslinking between the polymer chains to slow down the degradation of chitosan hydrogels in water sustaining the fertilizer release. In addition to the controlled release of fertilizers, the as-prepared hydrogels containing varying nanoclay content exhibited excellent water absorbency ranging from 25 to 140 g/g dry gel. If applied in the soil, these hydrogels could significantly improve the water retention capacity of the soil, promoting the growth of crops.

THURSDAY AFTERNOON 4/15/21 start 1:00 PM end 4:00 PM Nutritional Science in Food Chemistry

AGFD002F 3553436 1:00 PM **Integration of metabolomics and lipidomics reveals the effects of metallothionein on the arsenic-induced metabolic disorder in PC12 cells** Haitao Wang wanght6@foxmail.com Arsenic ions (As³⁺) have been recognized as a hazard that threatens the health of humans. However, previous studies regarding arsenic-induced cytotoxicity were mainly focused on the activation of specific intracellular receptors, the underlying mechanisms still need further investigation, especially at the metabolic level. Additionally, As³⁺ was easily binding to the sulfhydryl groups in protein, which may change the normal function of the protein and resulted in cytotoxicity. Metallothionein (MT) is rich in cysteine which may provide a favorable condition for the chelating of As³⁺. Therefore, the pretense of MT may attenuate arsenic-induced cytotoxicity. However, the influence of MT on As³⁺-

induced toxicity and the underlying mechanisms are poorly understood. Herein, the interaction between As³⁺ and MT was investigated by isothermal titration calorimetry. The results demonstrated the formation of As³⁺-MT complex. Cell viability analysis suggested MT alleviate As³⁺-induced cytotoxicity through reduced the production of reactive oxygen species (ROS) and maintain the mitochondrial membrane potential. Furthermore, the metabolic response of PC12 cells to As³⁺ was investigated by lipidomics and metabolomics. The results reveal that As³⁺ disrupt amino acid metabolism, energy metabolism, and phospholipids metabolism. The presence of MT alleviated As³⁺ induced metabolic disorder. Compared with As³⁺ treated group, the level of metabolites in MT-As³⁺ co-exposure groups altered significantly, which were similar to the ones in control groups. The results suggested MT alleviated As³⁺ induced cytotoxicity by scavenging ROS and chelating As³⁺. Our findings obtained in this study were helpful to fill the gap about As³⁺-induced toxicity, which might provide clues for studying other food composition on As³⁺ toxicity.

AGFD002F 3549149 1:00 PM **Protein-polysaccharide complex** coacervates improve the viability of encapsulated probiotics during Encapsulation of probiotics in protein-polysaccharide complex coacervates has been proven to be as an effective method for improving the viability of probiotics during human digestion. In recent years, plant protein gains popularity for number of reasons such as affordable price, sustainable protein sources. As such, the main purpose of this study was to investigate the impact of different protein sources (animal vs plant) and drying methods on physicochemical properties and the viability of encapsulated probiotics Lactobacillus rhamnosus GG (LGG) in simulated sequential gastrointestinal (GI) digestion. Casein sodium salt (CS) and pea protein isolate (PPI) were selected to represent the animal and plant protein source, respectively. Complex coacervates was formed between CS, or PPI to sugar beet pectin (SBP) at ratios (5:1 and 2:1) under pH 3, and subsequently probiotics contained liquid coacervates was dried by two drying methods, spray-dry and freeze-dry. According to the state diagram, ζ-potential and viscoelastic measurements, complex coacervates were successfully formed at tested conditions and the Fourier transform infrared (FTIR) results confirmed the formation of non-covalent bonds between proteins and SBP. In terms of impacts of drying processing on particle size of probiotics encapsulated powders, the spray-dried CS-SBP samples tended to form bigger particles than that of PPI, and as the SBP ratio increased, the particle size increased as well. With respect to the protective effects of the coacervates on the encapsulated LGG, the spray-dry process turned the coacervates into spherical particles with smooth and intact surface which seemed to favor the protection of LGG, compared to the extreme porous and weak structure formed through freeze-dry process. Moreover, the drastic loss of viable cells (~2 Log CFU/g) in CS-SBP samples in the first hour of intestinal digestion indicated that the protein source played an important role on the protective effects by means of complex coacervates.simulated sequential gastrointestinal digestion: Effect of protein source, protein to polysaccharide ratio and drying method Xiaoxi Qi xiaoxi.qi@ndus.edu

AGFD002F 3556198 1:00 PM **Gossypol decreased cell viability** and down-regulated the expression of a number of genes in human colon cancer cells Heping Cao heping.cao@ars.usda.gov Plant polyphenol gossypol has anticancer activities. This may increase cottonseed value by using gossypol as a health intervention agent. It is necessary to understand its molecular mechanisms before human consumption. The aim was to uncover the effects of gossypol on cell viability and gene expression in cancer cells. In this study, human

colon cancer cells (COLO 225) were treated with gossypol. MTT assay showed significant inhibitory effect under high concentration and longtime treatment. We analyzed the expression of 55 genes at the mRNA level in the cells; many of them are regulated by gossypol or ZFP36/TTP in cancer cells. BCL2 mRNA was the most stable among the 55 mRNAs analyzed in human colon cancer cells. GAPDH and RPL32 mRNAs were not good qPCR references for the colon cancer cells. Gossypol decreased the mRNA levels of DGAT, GLUT, TTP, IL families and a number of previously reported genes. In particular, gossypol suppressed the expression of genes coding for mRNAs of CLAUDIN1, ELK1, FAS, GAPDH, IL2, IL8 and ZFAND5 mRNAs, but enhanced the expression of the gene coding for GLUT3 mRNA. The results showed that gossypol inhibited cell survival with decreased expression of a number of genes in the colon cancer cells.

AGFD002F 3529882 2:00 PM **Effects of emulsifiers on an in vitro model of intestinal epithelial tight junctions and the transport of food allergens** Sefat E Khuda sefat.khuda@fda.hhs.gov
Understanding the effects of food emulsifiers on gut barrier functions and how these may influence the absorption of allergens will help provide an adequate risk characterization analysis. Methods: We challenged monolayers of human epithelial cells, an in vitro model of tight junctions, with polysorbate-80 or lecithin, or in combination with known allergens (egg proteins: ovalbumin, ovomucoid and ovotransferin; and an allergen of increasing concern, alpha-gal), at 0.01-0.5% concentrations. Results: We observed >90% cell viability and <15% cytotoxicity with individual emulsifiers and allergen treatments, except for emulsifiers at a concentration of 0.5%. Only 0.2% polysorbate-80 treatment reduced the monolayer integrity (~20%) demonstrated by increased lucifer yellow penetration. Dose-related differences in the expression of tight junction genes and occludin proteins were observed with both emulsifier treatments. The transport of tested allergens, excluding ovotransferin, nearly doubled in the presence of 0.2% polysorbate-80 compared to the emulsifier lecithin. Conclusion: By modulating paracellular permeability, certain emulsifiers may enhance absorption of allergens in a size-dependent manner

AGFD002F 3529907 2:00 PM **Quality and quantity of gluten in commercial wheat flours used in the bakery industry in Peru** Ivan Best ibest@usil.edu.pe
Wheat (*Triticum aestivum* L.) is part of the basic consumption of the Peruvian population, but its production is deficient. Wheat cultivation is used for the production of farinaceous products; however, it does not cover the internal demand that annually amounts to 2 million metric tons of wheat, being supplied mainly by imports (around 90% of the total). The objective of this study was to evaluate the quality and quantity of gluten in commercial wheat flours used in the Peruvian bakery industry. Physicochemical and rheological properties were evaluated in 14 commercial wheat flours from Peru. Moisture, ash, fat, and protein were determined according to AOAC methods 925.10, 923.03, 922.06, and 920.87, respectively. Wet gluten, dry gluten and gluten index, as well as the falling number, were evaluated according to the AACC 38-12 and AACC 56-81 methods, respectively. The correlation between the different variables was performed using the Pearson method ($p \leq 0.05$). According to our results, the moisture, ash, fat and protein content of wheat flours ranged from 13.00 and 14.42%, 0.39 to 1.38%, 0.56 to 1.55% and 8.51 to 12.72%, respectively. Regarding the quality of the gluten protein, the levels of wet gluten, dry gluten and gluten index varied between 22.59 to 37.60%, 7.20 to 12.29% and 86 to 99%, respectively; while the falling number ranged from 295 and 483 s. Wet gluten was significantly correlated with the content of protein and dry gluten ($r = 0.857$ and $r = 0.970$, respectively; $p \leq 0.01$), as well as with the falling number ($r = -0.381$, $p \leq 0.05$). Gluten index was significantly

correlated with the moisture and falling number ($r = 0.527$ and $r = 0.739$, respectively, $p \leq 0.01$, Table 1). Our results suggest that the quality of gluten in commercial wheat flours is associated with the moisture content and falling number, while the amount of gluten is associated with the protein content of commercial wheat flours.

AGFD002F 3532500 3:10:00 PM **Comparison of rice bran oil composition between parental and hybrid lines** McKinley Fox mckinley.fox@lyon.edu
Rice, the staple food of half of the human population over thousands of years, is mainly composed of starch. A much smaller percentage of lipids is present in a rice grain that contributes to the processing and nutritional value of rice. An important by-product of rice milling is rice bran, outer layer of rice grain, which contains high percentages of edible lipids. Rice bran oil has been a popular choice of cooking oil in several Asian countries for decades. The interest in rice bran oil is fast growing in the Western countries due to high levels of hearty unsaturated fats and Vitamin E present, and other benefits such as improving antioxidant and anti-inflammatory effects and reducing blood sugar and LDL cholesterol in the human body. Nevertheless, the production of rice bran oil is costly due to the special techniques involved in preserving oil composition during extraction and storage. Consequently rice bran mainly limits to animal feeds. It is reported that further knowledge of unsaturated fatty acid content in the rice lines will assist in improving the quality of rice bran processing, allowing robust extraction of rice bran for oil production. Several studies have been conducted in analyzing the composition of rice bran oil. However, the majority is restricted to Asian origin and the studies focused on beneficial genotypes are scarce. In this presentation, we will discuss how the bran lipid content and free unsaturated fatty acid composition vary between selected parental and hybrid rice lines. In our study, we utilized an efficacious organic extraction to collect rice bran oil from number of genetic variants including parental and hybrid lines, and developed an user-friendly reverse-phase high performance liquid chromatography (HPLC) to investigate the composition of three of the most abundant, healthy, unsaturated fatty acids that freely exist in rice bran oil: oleic, linoleic, linolenic

AGFD002F 3548411 3:00 PM **Triacylglycerols compositions, soluble and bound phenolics of red sorghums, and their radical scavenging and anti-inflammatory activities** Yanfang Li Zoe_Li@sjtu.edu.cn
Six commercial red sorghum varieties (Tong Za 117, 141, 142 and 143, Chi Za 109 and 101) were investigated for their triacylglycerol (TAG) profiles, soluble and bound phenolics, and radical scavenging and anti-inflammatory activities. A total of 21 TAGs were identified in red sorghum oils for the first time. Total phenolic (TPC) and flavonoid contents (TFC) in the soluble or bound phenolic fractions differed among red sorghums. Significant correlation among TPC, TFC and DPPH radical scavenging activities was observed in both fractions. Except for caffeic acid, most of phenolic acids in red sorghums are in the bound form. Soluble 3-deoxyanthocyanidins contents (2.12–57.14 $\mu\text{g/g}$) were significantly higher than those of bound forms (0.01–0.18 $\mu\text{g/g}$) regardless of sorghum varieties and types of 3-deoxyanthocyanidins. Moreover, the stronger anti-inflammatory capacity of soluble phenolic fraction in Tong Za 117 correlated with its higher TPC, TFC and radical scavenging activity than those of its bound counterpart.

THURSDAY AFTERNOON 4/15/21 start 1:00 PM end 4:00 PM Sustainable Food Systems for Health

AGFD003J 3550246 1:00 PM **Advanced food science approaches to tackle global food challenges: COVID, global warming, population growth, and health** David McClements mcclements@foodsci.umass.edu
This presentation highlights some of the approaches that modern science is using to tackle global food-related challenges, including COVID, global warming, population

growth, and diet-related chronic diseases. Technological innovations such as food architecture, robotics, machine learning, artificial intelligence, advanced diagnostics, nanotechnology, biotechnology, gene editing, vertical farming, alternative proteins, and soft matter physics are all being utilized for this purpose. Many of these technologies are being applied across the food chain, from farmers to distributors to manufacturers to consumers, so as to improve the quality, nutrition, safety, and sustainability of the global food supply. In the case of coronavirus, automation of food production and distribution chains can reduce disease transmission by enabling social distancing and reducing face-to-face contact. Moreover, certain combinations of nutraceuticals are being promoted for their ability to strengthen the immune system, thereby improving resistance to the virus. In the case of global warming and population growth, the transition to a more plant-based diet would reduce greenhouse gas emissions, land use, water use, pollution, and biodiversity loss, thereby providing more food without causing as much damage to the environment. Moreover, genetic engineering and nanotechnology may be able to increase yields, raise resilience, and reduce losses of agricultural crops.

AGFD003J 3559580 1:00 PM **Next-generation technologies to program microbial communities for health and sustainability** Harris Wang hw2429@columbia.edu Soil and animal-associated microbiomes play crucial roles in the trophic networks of the biosphere and have an important impact on biosustainability in the context of climate change. In the rhizosphere, microbes fix nitrogen, degrade complex organic substrates, and protect roots from pathogens. In humans, microbes colonize the gastrointestinal tract to modulate host metabolism, immunity, and homeostasis. Better tools to study and alter these microbial communities are essential for unlocking their vast potential to improve human health and the environment. This talk will describe emerging technologies to engineer microbial communities in different settings. Specifically, I will discuss platforms for in situ programming of the gut microbiome using CRISPR technologies and the genetic modification of soil-associated bacteria to build engineered living materials. These enabling capabilities provide a foundation to accelerate the development of next generation solutions to tackle the most pressing challenges we face in the next decades.

AGFD003J 3552946 1:00 PM **Advances in self-assemble peptide nanomaterials for 3D ex vivo models: functional food compounds for cancer prevention and mitigation** Xiuzhi Susan Sun xss@ksu.edu In vitro cell culture models on monolayer surface (2D) have been widely adapted for chemopreventive food compound identification. However, the low correlation between 2D models and in vivo animal studies has always been a concern; this gap is mainly caused by the lack of a three-dimensional (3D) extracellular microenvironment. In 2D models, cell behaviors and functionalities are altered and consequently result in varied responses to external conditions (i.e., antioxidants) and hence lead to low predictability. Novel peptide hydrogel 3D scaffolding technologies for cell culture have been recently reported to physiologically mimic the 3D microenvironment and can serve as an ex vivo model for cell activities, which hopefully will improve the prediction rate. Thus, this seminar will focus on the advances in self-assemble peptide nanomaterials, particularly hydrogels, as novel 3D cell culture tools with potential for ex vivo 3D models for cancer-related research with regard to toxicity and efficacy of functional food compounds.

AGFD003J 3556635 2:00 PM **Preparation of pea protein aggregates and their gelling property study** Wenhao Cai wcail@ualberta.ca Pea protein has attracted attentions as an alternative for soy protein, but its weaker gelling properties has limited its applications in food formulations. In this study, the pea

protein aggregates were prepared and their gelling properties were studied. The mechanical property measurement indicated that the gel strength can be modulated by modifying the pea protein aggregate properties to achieve compressive strength up to more than 10 kPa, which comparable to soy protein based gels. In addition, the strong gels were achieved at relatively low concentration of protein (< 10% thus are advantageous for practical applications. Nowadays, novel products are designed based on the growing preference of consumers for natural and healthy foods, and pea protein aggregates-derived ingredients show excellent potential to be well adopted by consumers. The utilization of pea protein gels to produce food products of different textures could potentially contribute to the growth of the food and agricultural industry.

AGFD003J 3558433 2:00 PM **Diabetes as an environmental risk factor: Biological significance of metabolic inhibitors and their curcumin adducts** Bishambar Dayal dayalb77@gmail.com A very recent report described treatment of pancreatic cancer patient-derived xenograft panel with metabolic inhibitors such as metformin and phenformin demonstrating much better efficacy of a biguanide phenformin than metformin <http://clincancerres.aacrjournals.org/> April 25, 2018. Studies by Brownlee et al. (Science 1986) elucidated that glycosylation products in diabetes patients are toxic mediators of macro- and microvascular complications and a monoguanide, 2-aminoguanidine prevented diabetes-induced arterial wall protein cross-linking. Protein cross-links are also formed spontaneously not only in diabetes individuals but also are formed in aging populations. Our recent studies elucidated the anti glycosylation effect of flavonoids present in Okra Seed Extracts (OSE) (ACS Book Chapter 2012, ACS 255). Specifically, the okra seed water extract had very much enhanced antiglycosylation/inhibitory activity. Furthermore, inhibition and anti-glycosylation activity of methylglyoxal-induced modification of human serum albumin and lysozyme by stereo-chemically well-defined OSE was also illustrated by SDS-PAGE, fluorescence spectroscopy and changes in protein concentrations via Nano-drop spectrophotometry. Studies on the microwave-induced organic synthesis and LC-MS/MS characterization of curcumin adducts of metformin and phenformin and 2-aminoguanidine were also described (2016-2018). Since curcumin is slightly soluble in water by masking the diketone moiety of curcumin with the nucleophilic metabolic inhibitors its solubility was enhanced. Since phenformin suffers from lactic acidosis side effects is not being used clinically for the treatment of diabetes type-2 patients, the curcumin adducts had enhanced antiglycosylation activity. We believe these compounds may have potential not only for treatment of diabetes but also for pancreatic ductal adenocarcinoma cancer (PDAC).

AGFD003J 3557019 3:05 PM **Value-added utilization of agricultural and food processing by-products** Liangli Yu lyu5@umd.edu By-products or wastes from agricultural and food processing, such as tomato and berry seeds, are environmental hazardous. These by-products may contain significant levels of health components and nutrients for human health, or can be further processed into valuable functional ingredients for food applications. This presentation will discuss the chemical components and nutraceutical properties of the selected edible seeds and seed flours, the by-products from seed oil processing. The nutraceutical properties may include free radical scavenging, anti-proliferative, anti-inflammatory, and gut microbiota modulating activities. The presentation also will discuss how additional processing may produce potential value-added utilization of tomato skins and soybean coats. The results of these studies serve as a scientific basis for value-added use of the agricultural and food processing by-products while reducing environment hazards.

THURSDAY AFTERNOON & EVENING 4/15/21

start 1:00 PM end 7:50 PM

Chemistry of Fruits and Vegetables

AGFD002G 3531563 5:05 PM **Quantifying insecticide**

application efficacy and degradation within a citrus greening disease infected grove Rachelle Rehberg RRehberg@colostate.edu Citrus greening disease (Huanglongbing, HLB) has damaged the citrus industry worldwide. With over 90% of Florida's oranges infected, growers are desperate to improve management strategies and slow the spread of this detrimental disease. Insecticide application efficacy in the field was investigated with liquid chromatography tandem mass spectrometry to determine if insecticide applications to citrus were effective at killing the responsible pest, Asian citrus psyllids (ACP). Sample discs attached to leaves were sprayed with imidacloprid, malathion, dimethoate, and afidopyropen at a field site in Florida. Application method, canopy height and depth, cardinal side of tree, and leaf side were considered to assess spatial distribution of insecticides throughout citrus trees. Leaf samples were collected at various times after insecticide application to assess degradation. ACP were inspected in trees before and after insecticide applications to quantify psyllid reductions and application efficacy. Our findings show that while concentrations were high enough to kill ACP, the spatial distribution of insecticides throughout individual trees was highly variable and live ACP were detected after application. Inadequate distribution to different areas of the tree canopy, including top side of leaves receiving significantly more insecticide than undersides, was observed for all application methods tested. Preliminary results show insecticides degrading below the LOD within 3 days after application. Inspections of ACP populations before-and after-insecticide applications resulted in efficacies of 85-100% (malathion), 48-80% (imidacloprid), 60-84% (dimethoate), and 33-77% (afidopyropen) with a majority resulting in population increases (ranging 145-600%) when inspected 9 days after application. The variability in insecticide spatial distribution due to application method and rapid degradation of insecticide active ingredients allows remaining ACP to continue spreading citrus greening disease to unprotected trees. Further research is needed to improve insecticide application methods for citrus trees and implement effective pest management strategies and fully target ACP to eliminate HLB.

AGFD002G 3538835 5:00 PM **Ultrasound-aided extraction of** soybean okara byproduct: analysis of their physicochemical and conformational changes Carmen Lammi carmen.lammi@unimi.it Soybean okara is a by-product generated during tofu or soymilk production processes. It contains about 50% dietary fiber, 25% protein, 10% lipid, and other nutrients. Due to its high protein content and low production costs, okara is a good raw material for protein extraction. Hence, the ultrasound protein extraction was carried out at 20, 60, and 80 °C and a greatly enhanced of their yields was achieved. The ultrasound treatments at different temperatures modified in a significant way the protein secondary and tertiary structure. The atomic force microscope (AFM) analysis demonstrated a significant morphological transition from well-defined single round structures to highly aggregated ones after the ultrasonication at the highest temperature, suggesting that these aggregates possess more hydrophilic surfaces and more hydrophobic cores than the untreated sample. This feature was confirmed by measuring their water contact angles and wettability. Hence, the improvements of protein solubility and water binding capacity appears to depend on the temperature in a similar way in the ultrasound extraction. On the contrary, no protein viscosity change was observed. The improvement of peptides generation and the different amino acid exposition within the protein after the ultrasound process led to an increase of the antioxidant properties of the samples and to a reduction of their phytic acid content. The integrated strategy applied in this study, allows to foster the okara protein obtained after ultrasound extraction as valuable

materials for new application and provides, therefore, a more sustainable way to solve the environmental criticism related to the huge quantities of okara produced annually.

AGFD002G 3533949 5:00 PM **Changes in the volatile**

composition of blueberry during storage: Emphasis on molecular regulation of fruit aroma deterioration Fang Yuan fyuan@mail.hzau.edu.cn Aroma is important to determine fruit quality and its market value. However, aroma change and off-flavor development are often problems during postharvest handling and storage. In this study, the effects of different storage condition from harvest to market on blueberry volatile composition and sensory quality were evaluated by SPME-GC-QTOF-MS and sensory panel. The biosynthesis mechanisms of important aroma compounds in blueberry were evaluated by transcriptome analysis. The results showed that esters were dominant in rabbiteye blueberries, especially for ethyl acetate. No distinct pattern of volatile profile was found for the highbush and half-highbush blueberry cultivars. The grassy descriptor was positively correlated with linalool and hexanal. The minty descriptor was positively correlated with eucalyptol. Volatile compounds generally showed a downward trend during cold storage. However, the subsequent shelf life was the most remarkable period of volatile change, and was represented by the strong fluctuation of ethyl acetate and the rapid decrease of terpenoids, resulted in a quick deterioration in sensory acceptability. Our study reveals that during postharvest storage, blueberry volatile composition changed by regulating several secondary metabolic pathways, in particular, by stimulating the expression of pyruvate decarboxylase (PDC) genes, resulting in a high production of ethyl acetate. Postharvest storage also modulated some terpene synthase (TPS) genes associated with linalool production. The concentration of C6 aldehydes and alcohols decreased during the postharvest storage accompanied by lower lipoxygenase (LOX) gene expression. These findings illustrate the molecular and biochemical mechanisms that occur in blueberry during the postharvest storage period, especially with regard to volatile composition changes.

AGFD002G 3549976 6:05 PM **Chinese yam polysaccharide**

plays an immunomodulatory role based on its metabolites of intestinal flora Yajuan Bai xbaizxyq@sina.com Chinese yam (*Dioscorea Opposita* Thunb.) is an important functional food as well as a source for natural medicine due to its several pharmacological activities. Polysaccharide is one of the important bioactive substances of Chinese yam. The biological activity of natural polysaccharide is closely related to how it is digested, absorbed and utilized in the host. We invested the gastrointestinal digestion and fecal fermentation behavior of polysaccharide from Chinese yam (CYP). The molecule weight of CYP remained unchanged in vitro gastric and intestinal digestion. Following 24 h of fecal fermentation, 49.0% of the total carbohydrate in the CYP was consumed. The total short chain fatty acids (SCFAs) productions, acetic, propionate, butyrate acid, and lactate acid significantly increased compared to the blank group. Simultaneously, CYP modulated the composition and abundance of beneficial microbiota, especially *Lactobacillus* spp. and *Bifidobacterium* spp. Compared with non-fermented CYP, CYP fermentation stimulated TNF- α and IL-10 secretion of macrophage RAW 264.7. The results suggest that CYP could potentially be a functional food to improve gut health.

AGFD002G 3551679 6:00 PM **Nutrients characteristics of the**

leaf, stem and root of *Eclipta prostrata* (L) Abiodun Sodamade sodamade1@gmail.com *Eclipta prostrata* (L) is one of the plant samples used locally in the south western part of Nigeria in preparation of herbs for treatment of some ailments, diseases and hormonal disorder. The sample was purchased, and authenticated with a view to evaluate its nutritional composition by determining the

proximate composition, mineral content, and amino acid profile using standard analytical method. The proximate analysis revealed; the moisture content for the root to be the highest followed by the stem, while the leaf has the least value. The ash content and protein values respectively were (7.54±0.00)g/100g, 12.48±0.03g/100g for the root and the highest followed by the stem (7.54±0.23)g/100g; (11.36±0.47)g/100g and the leaf had the least values; (5.55±0.00)g/100g, 4.38±0.61) g/100g respectively. More crude fat and crude fibre were found in the root followed by the stem. The leaf had the highest value of nitrogen free extractive; (70.15±0.71)g/100g while the root had the least (56.51±0.26)g/100g. The dietary mineral revealed highest concentration of Na, K, Ca, Mg, Zn and Fe in the root than other parts. Other minerals that were detected in the three parts of the plants samples in trace amount are: Cu, Mn, P, and Cd. Lead was not detected in the samples but the stem showed trace amount of selenium of concentration, 0.05±0.16mg/100g. The amino acid profile revealed significant proportion of both essential and non-essential amino acid. The amino acid values were higher in the stem than the leaf and the root of the plant samples. The consumption and pharmaceutical use of the whole part of the plant is therefore encouraged. The plants could serve as raw material to produce essential supplements needed by man

AGFD002G 3550729 6:00 PM **Spatial distribution and metabolism of forchlorfenuron in oriental melon under greenhouse cultivation** Qi Wang 497750075@qq.com Forchlorfenuron is a widely used plant growth regulator. It was noticed that forchlorfenuron affected fruit quality and its metabolite poses a potential risk for human health. However, its spatial distribution and metabolism in agricultural food has been fully unrevealed. Therefore, we performed matrix-assisted laser desorption/ionization (MALDI-IMS) and high-performance liquid chromatography tandem mass spectrometry (HPLC-MS/MS), analysis to investigate their spatial distribution and metabolism in oriental melons under greenhouse cultivation. Forchlorfenuron parent was degraded rapidly in melon at the recommended application concentration (20mg/L) and gradually migrated from exocarp to endocarp. In 0-2 d, the concentrations of forchlorfenuron parent were higher(254.24-1122.03 µg/kg), which were mainly activity in exocarp and mesocarp of melon; In the 3-4 d, the forchlorfenuron were decreased rapidly and evenly distributed in entire oriental melon body. The metabolite 4-hydroxyphenyl-forchlorfenuron was first identified in oriental melon, which exhibited the highest level of residues of 5.12 µg/kg on the 4 days after application. The dissipation rate of 4-hydroxyphenyl-forchlorfenuron was greater than the metabolic rate of forchlorfenuron and mainly activity in mesocarp of melon. The results obtained in this study offer important insights into the potential migration and effects of forchlorfenuron in oriental melons.

AGFD002G 3552583 7:10:00 PM **Elucidation of the pawpaw (*Asimina triloba*) aroma: North America's largest native fruit** LiLi Zyzak lili.zyzak@eku.edu The pawpaw fruit is the largest native fruit to North America. This fruit grows in the eastern half of the United States and many different cultivars exist today. However, most people have never tried this delicious, tropical like fruit. The descriptors used to characterize this fruit are banana, pineapple, custard, and mango-like. Its flesh is yellow and it ripens very quickly, which leads to a very short shelf-life. That is one reason why it is not commonly known and presents a problem for retail logistics. However, for those who have tasted the fruit, it is very pleasant and has found application in deserts such as ice cream, pies, and pastries. Indeed, many innovative chefs will provide desert applications of pawpaw fruit at their restaurants in the fall. Even though this fruit has been known and enjoyed for centuries, an exhaustive look into the compounds responsible for its tropical flavor and aroma has not been published in research journals. Traditional headspace GC-MS

methods have identified esters as the major volatile compounds in pawpaw. However, these esters alone do not account for the complex creamy, fruity, dairy, and vanilla character. It is our goal to provide a deeper understanding of the pawpaw aroma through the use of gas chromatography - olfactometry (GC-O) and gas chromatography - mass spectrometry (GC-MS) on extracts obtained through the use of solvent extraction and solid phase microextraction (SPME). Through the use of GC-O and GC-MS, we have identified several intense aroma active compounds which have never been reported to be present in pawpaw fruits. These compounds, some present at low levels, are contributing significantly to the aroma of pawpaw. In addition, their aroma character is responsible for some of the dairy and sweet, vanillin character of the pawpaw fruit. Some of the new compounds identified include: 2,3-butanedione, gamma-octalactone, vanillin, butyric acid, eugenol, and gamma-decalactone. These new discoveries now provide additional insights into the pawpaw flavor. Additional quantitation and reconstitution steps are underway to validate the importance of this research into aroma of pawpaw fruit elucidation.

AGFD002G 3558600 7:00 P **Persistence and metabolism of the diamide insecticide cyantraniliprole in tomato plants** Khang Huynh huynhkha@msu.edu Plant uptake and metabolism of pesticides are complex and dynamic processes, which contribute to the overall toxicity of the pesticides. We investigated the metabolic fate of cyantraniliprole, a new diamide class of pesticide, during various growth stages of tomato. Cyantraniliprole was the major residue in leaves, flowers, and fruits, with the relative metabolite-to-parent ratios maintained at <10% up to 28 days after treatment (DAT). Mature leaves contained consistently higher concentrations of cyantraniliprole than young leaves throughout the study. Flowers contained the highest cyantraniliprole concentrations up to 21 DAT, which then gradually decreased. Immature green fruits had the highest cyantraniliprole concentrations (5.2 ± 0.7 ng/g; 42 DAT), which decreased toward red ripening stages (1.2 ± 0.1 ng/g; 84 DAT). Metabolism of cyantraniliprole primarily occurred in the foliage, where 21 metabolites were tentatively identified. Flowers and fruits contained four and 14 of these metabolites, respectively. Major transformation pathways were characterized by ring closure, followed by N-demethylation, and glycosylation. Additionally, plant metabolism of cyantraniliprole was also associated with several minor phase-I, phase-II, and breakdown metabolites. The occurrence of these metabolites in plants varied as a function of tissue types and their developmental stages. Our study highlights a tissue-specific biotransformation and accumulation of metabolites of cyantraniliprole in tomato.

FRIDAY MORNING 4/16/21 start 9:00 AM end 11:50 AM
Chemistry of Fermented Hispanic Foods - Beverages
 AGFD004A 3552534 9:05 AM **Mediterranean fermented beverages: potential source of melatonin and other bioactive compounds** Maria Martin-Cabrejas maria.martin@uam.es Melatonin is a powerful antioxidant molecule that exists in all living organisms and also found in plant foods and proposed as a new bioactive component. In recent years, the incorporation of melatonin-rich plant foods in our diet could improve human health through to its prevention of chronic diseases related to the aging and oxidative stress such as cardiovascular diseases, obesity, and type-2 diabetes. Melatonin contents vary widely in foods and, most of food-processing technologies reduce its levels; however, the fermentation process increase this neurohormone. The most popular beverages (wine and beer) in the Mediterranean diet exhibit high levels of melatonin. These increases were mainly due to melatonin synthesis during the alcoholic fermentation by yeasts. These microorganisms are the ability to use tryptophan and their metabolites as nitrogen source but also produce tryptamine, molecule require in the

biosynthetic pathway of melatonin. Nevertheless, wine and beer making techniques might be important for melatonin production. Steps such as maceration times and fermentation period may probably improve the extraction and solubility of this indoleamine. Factors as pH, presence of phytochemical components such reducing sugars, organic acids or polyphenols are key aspects in the formation of melatonin. Of interest here, notable differences have also found in red, white, and rose wines, possibly due to grape melatonin levels, red grapes show higher levels of melatonin than white grapes, and by other hand, in red wines grape skins are included, and higher temperatures required. Studies indicate that the more alcohol contains these beverages the higher the melatonin levels as consequence of its physicochemical properties. The melatonin molecule may form isomers, and, in recent years, they have been paid attention because of its enhanced biological activities and bioavailability. These isomers were identified not only in wine and beer but also in other fermented beverages as orange juice obtained by controlled alcoholic fermentation. In summary, moderate consumption of these fermented beverages present in the Mediterranean diet may influence on the total antioxidant capacity of blood plasma levels in humans, given them protection from overall oxidative stress, and therefore, could improve the health benefits.

AGFD004A 3558841 9:00 AM **Fermentation of honey water** from agave in the production of pulque Gloria Davila Ortiz gdavilao@yahoo.com Pulque is a non-distilled alcoholic beverage native to Mexico and pre-Hispanic origin. Likewise, its extraction and fermentation process has not undergone major modifications since pre-Hispanic times. As for its elaboration, it is carried out by a Tlachiquero who knows in depth the biology and care of the maguey. Additionally, the entire process for obtaining it occurs with the fermentation of the mead which is a substrate extracted from the maguey that is mainly consumed in the central states of Mexico. Mead is the slightly cloudy, thick, sweet, and yellow agave sap that is obtained between 8 and 10 years of age. Regarding fermentation, this will depend on the quality of the mead, maturity of the seed, season, region where it is produced, as well as other factors. On the other hand, as it is a fermented drink, it will have the presence of probiotic microorganisms (*Lactobacillus*) that will have a positive effect on health, helping in the prevention and treatment of intestinal diseases. In the same way, it presents an interesting nutritional content where it is necessary to highlight the presence in high concentrations of amino acids such as tryptophan and sulfur amino acids. So, it is particularly important to evaluate new low-cost sources of protein and functional nutrients from native products that help combat the special needs of people with inflammatory bowel diseases.

AGFD004A 3554177 9:00 AM **Mexican traditional** fermentations from corn (*Zea mays*): An overview Javier Arrizon jparrizon@ciatej.mx Maize (*Zea mays L.*) constitute the most important crop for the Mexican diet, it was the basic grain for the ancient pre-hispanic cultures settled in Mexico. These cultures developed the nixtamalization process, which involves the steps of cooking of corn grains with lime (Calcium oxide), followed by a milling process to obtain the maize dough used for the elaboration of tortillas and other Mexican traditional dishes. The corn grains or the maize dough have been used by different local ethnic groups to elaborate a variety of traditional fermented beverages, by applying different elaboration processes and by mixing different ingredients, and they have been consumed in Mexico since ancient times. "Tejuino", "tesguino", "pozol", "tejate" and "atole agrio" are the principal fermented beverages produced from corn in Mexico. This review is focussed in the diversity of the processes involved in the elaboration of these traditional beverages, as well as their chemical composition and their microbial diversity, which determine their functional properties for the health of consumers

AGFD004A 3558604 10:00 AM **Production of a fermented** beverage from vanilla coproducts Gloria Davila Ortiz gdavilao@yahoo.com Mexico is a diversity rich country in culture, food. It has been related since pre-Hispanic times by the fermented beverages production such as tepache and pulque, where its consumption has been related to the health care. The Mexican Vanilla (*Vanilla planifolia* , Jackson) is considered one of the most important worldwide flavorings. Once it has harvested, it must undergo a traditional curing process to develop its characteristic aroma and flavor (more than one hundred compounds). Once it has cured, vanilla bean produces a large amount of aromatic, phenolic, organic acids, fatty acids and essential oil compounds, which together give it a high antioxidant capacity. The commercialized gourmet beans are in specific sectors, while the smaller pods are used to produce an alcoholic extract corresponding to 2-3% of the vanilla production. The present work aims to evaluate the use of small cured vanilla beans, subjecting them to a fermentation process using microorganisms to obtain a drink with low alcohol content (digestive drink) rich in phenolic and aromatic compounds with antioxidant capacity. According to the preliminary results of the proximal chemical analysis, the cured beans contain a high amount of carbohydrates (79.26%) of which approximately 60% corresponds to fiber, which is partially hydrolyzed during the curing process by the endophyte flora. In such way these storage sugars and those from the hydrolysis of structural polysaccharides remain available to be fermented and obtain a beverage with flavor, aroma, quality and biological properties

AGFD004A 3554861 11:00 AM **Fermented zarzaparrilla-based** beverage as potential source of bioactive compounds Audry Peredo-Lovillo aperedo88@outlook.com The zarzaparrilla is a plant belonging to the genus *Smilax*, and like all the same genus has climbing or trailing stems. With about 300 species growing around the world, some of them have been used in traditional medicine as anti-hypertensive and anti-rheumatism agents as well as a diuretic and for cutaneous affections. Besides, they have recently also been explored for cytoprotective, antifungal, antioxidant, and hypoglycaemic purposes. Such biological activities have been attributed to the presence of bioactive compounds (steroidal saponins, phytosterols, triterpenoids, flavonoids, and phenolic acids) mainly found in roots and rhizomes. In Mexico, particularly in the center of the state of Veracruz, the roots of *Smilax aristolochiifolia* and *Smilax morenensis* (native species from Mexico), also known as "blanca" and "roja", respectively; are commonly used as raw material to elaborate a traditional beverage call it "zarzaparrilla". The elaboration process is based on a Spanish traditional recipe. Briefly, the dried roots are mixed with an aqueous infusion prepared from star anise, ginger, and brown sugar, although other ingredients are also added to improve the taste. The beverage is ready for consumption after 8 days of spontaneous fermentation. Despite zarzaparrilla have mostly used as a simple light-refreshing beverage, it has also been used as a folk medicine to treat gastrointestinal affections, skin reactions, arthritis, and syphilis, probably because contains a wealth of plant chemicals thought to have a beneficial effect, but which have not yet been fully identified. Therefore, the aim of this chapter is to provide an overview of zarzaparrilla as a potential source of bioactive compounds.

AGFD004A 3558679 11:00 AM **Fermentation of vanilla beans** enzymatic hydrolysates after aromatic compounds extraction Gloria Davila Ortiz gdavilao@yahoo.com Food fermented production is growing in interest because through biotechnological processes the integral use of agro-industrial waste can be used to generate products with added-value. In this sense, vanilla (*Vanilla planifolia* Jackson) is considered the best flavoring agent used in food, flavor, fragrance,

and cosmetic industries. For its production, vanilla beans are subjected to a traditional curing process in which color, aroma, and flavor characteristics are developed, in which more than one hundred volatile compounds of various types of chemical groups. However, only 2 to 3% of vanilla bean, is used as an alcoholic extract, and the material residual is considered as waste. The objective of this work is to use the vanilla bean waste to be subjected to enzymatic hydrolysis and finally to be fermented, generating added-value products. Sequential enzymatic hydrolysis fractions of the vanilla waste were characterized by Fourier Transform Infrared Spectroscopy (FTIR) and Mass Spectrometry (SM), getting spectra associated with the presence of carbohydrates (monosaccharides, disaccharides and trisaccharides) from the degradation of compounds belonging to the cell wall, the FTIR spectra show functional groups associated with pectin, cellulose, hemicellulose and lignin. All these carbohydrates can be fermented by microorganisms and yeasts and in this way obtain a nutritious and healthy beverage.

FRIDAY AFTERNOON 4/16/21 start 1:00 PM end 3:35 PM

Chemistry of Fermented Hispanic Foods – Other Foods

AGFD004B 3544840 1:00 PM **Aging of Hispanic cheese**

Michael Tunick mht39@drexel.edu Hispanic cheeses such as Oaxaca and Queso Fresco are meant to be consumed within a few days, but other varieties such as Queso Chihuahua and Cotija are allowed to ripen over a period of weeks before being offered for sale. The lactose and citrate in the cheese is fermented by lactic acid bacteria (LAB), producing a host of compounds responsible for the characteristic flavors of the product. The action of the bacteria as well as the coagulant also break down casein, resulting in textural changes. Microbiological studies isolated 16 LAB species from artisanal and semi-industrial Cotija, and 17 LAB species were found in Queso Chihuahua made from raw milk; 12 of these were also found in the pasteurized version. A number of enzymatic pathways that produce aroma and flavor compounds were detected in Cotija. Proteolysis during aging resulted in reductions in hardness, cohesiveness, and springiness. The fermentation occurring in aged Hispanic cheese varieties causes the development of the desired flavor and texture.

AGFD004B 3554848 1:00 PM **Tepache: A pre-Hispanic**

fermented beverage as a potential source of probiotic microorganisms Haydee Romero roluna88@hotmail.com In Mexico, there is a great variety of traditional fermented beverages of pre-Hispanic origin, which are prepared from vegetables and fruits. Its consumption has been associated with improved human health, such as Tepache, which is prepared from pineapple peels and by adding tibicos, and that although it has been used for curative purposes, just a few studies allow defining that their benefits are owed; however, it is thought that the benefits could be associated with the presence of microorganisms (probiotics), which carry out the fermentation and which remain viable in the beverage when ingested. So, the aim of this study was to evaluate in vitro the probiotic potential of microorganisms isolated from Tepache and tibicos. In this investigation, 44 microorganisms (17 lactic acid bacteria (LAB) and 27 yeast) from Tepache and tibicos (9 and 35, respectively) were isolated. A preselection was made for LAB based on the structure of the cell wall (Gram-positive) and absence of catalase, while yeasts were preselected by the growth parameters at 37 °C. A survival test at pH 2 and bile salts allowed the selection of a total of 12 microorganisms, of which 1 was molecularly identified as *Lactobacillus paracasei* (CT12B), 8 as *Saccharomyces cerevisiae* (CT02L, CT32L, CT1L, GT3L, CT41L†, GT31L†, GT41L†, and GT42L†), 2 as *Saccharomyces paradoxus* (Tep1L and Tep4L), and 1 as *Saccharomycodes ludwigii* (Tep5L), these last two are for the first time reported in Tepache. All of them were able to survive under conditions that simulate the gastrointestinal tract, to adhere to mucin

in high percentages and they did not present hemolysis. Furthermore, the 11 yeasts showed an important capacity to inhibit the DPPH radical, they did not degrade mucin, they were able to resist osmotic stress, they remained active from 10 to 37 °C, and they were inhibited with nystatin. For its part, *Lactobacillus paracasei* (CT12B) was sensitive to 3 clinically important antibiotics, resistant to nisin, and presented the ability to produce compounds that can inhibit harmful bacteria and filamentous fungi. According to the results, isolates can be considered microorganisms with probiotic potential. In addition to pointing to tibicos and Tepache as a source of microorganisms with probiotic characteristics, which could generate benefits for the health of the host, including the prevention of diseases related to reactive oxygen species and infections generated by pathogenic bacteria.

AGFD004B 3552188 1:00 PM **Gastrointestinal resistance and diversity of microbiota in agave sap concentrate: an artisanal**

Mexican food Aurea Karina Ramirez Jimenez aramirezj@tec.mx Agave sap (AS) is an artisanal Mexican food produced by the evaporation of AS, also known as “aguamiel”. After collection, the AS rapidly undergoes fermentation to produce “pulque”. To avoid this step, AS is concentrated by a thermal treatment for a period of 5-6 hours. In this study, we determined the bacterial diversity of agave sap concentrate (ASC), as well as its metabolite profile and bacterial resistance to in vitro gastrointestinal digestion and fermentation. Thirteen samples from 3 different regions of Mexico were enriched with two culture media (NZ amine or R2A). A 16S rRNA sequencing was performed with the Illumina Miseq system. Selected ASC samples were digested and fermented under in vitro conditions and then analyzed by HPLC/ESI-MS/TOF to identify metabolites; the production of short chain fatty acids (SCFA) was quantified with GC-FID. Thermoresistant bacteria were recovered from ASC with NZ amine, the medium that allowed to obtain the highest bacterial diversity, which was highly dependent on the production region. Firmicutes predominate among other phyla, as well as the genus *Bacillus*. The strains *Gordonia* sp and *Arthrobacter globiformis* were isolated from ASC and showed to influence the metabolite profile. Acetic (1695 to 2731 ppm) and propionic (30 to 1043 ppm) acids were important metabolites produced after fermentation by the ASC microbiota. This study showed that despite the adverse conditions that predominate in the ASC and throughout the in vitro gastrointestinal digestion, it is possible to find a significant diversity of microorganisms with potential to produce SCFA.

AGFD004B 3557446 2:00 PM **Effects of isolated and symbiotic-**

associated kefir in gut and bone health Mariana Grancieri marianagrancieri@gmail.com Kefir is a fermentable food, with functional characteristics, since it is a rich source of natural probiotics that confer benefits to the host's intestinal health, mainly by preventing the growth of pathogenic microorganisms. Our studies demonstrate benefits resulting from the consumption of kefir in rats and humans, both in isolation and in a symbiotic way. In a study with adult rats (n = 30) that during 42 days received only kefir (1mL/day of the fermented kefir drink with 1000000000 CFU/mL) or kefir symbiotically associated with yacon flour, a rich source of the prebiotic fructooligosaccharides (FOS), improving the integrity of the intestinal mucosa, decreasing intestinal permeability, intestinal pH, and increasing levels of sIgA. The symbiotic was efficient in calcium balance and kefir proved to be effective in preventing bone resorption, reducing the levels of collagen type I (NTx) and C-telopeptide collagen type I (Ctx). Thus, kefir both isolated and inserted in a symbiotic has shown beneficial effects on intestinal and bone health, highlighting the promising use of this fermented food for the formation and maintenance of human intestinal and bone homeostasis. In order to observe these effects, in another study, kefir was inserted into a milk preparation and offered to constipated adult

women (n = 12). It was observed that these women had a significant increase in the Bristol scale and a reduction in the score of the Agachan scale, according to the Roma III criteria, confirming the effects of kefir on intestinal functionality. Furthermore, in addition to the benefits to the organism, the products developed with kefir are palatable, since in the sensory analysis, carried out with 59 adult participants, it was possible to observe an average of 7 points on the 9-point hedonic scale. In this way, kefir is a palatable fermentable probiotic that can be inserted in preparations and with promising effects on bone and, especially intestinal health.

AGFD004B 3557673 2:00 PM **Fermented black beans released peptides and phenolic compounds biological potential** Luis Mojica lmojica@ciatej.mx Solid state fermentation could improve the release of bioactive compounds from the food matrix. Bioactive compounds from foods could be used as adjuvants to prevent non communicable diseases such as type 2 diabetes. The objective of this work was to evaluate the effect of solid state fermentation on the release of phenolic compounds and bioactive peptides from black beans and their biological potential. *Bacillus subtilis* was utilized as an inoculum for the solid-state fermentation of black beans. Fermentation was performed during 48 and 96 h at 30°C and 90% relative humidity. Phenolic compounds and bioactive peptides were characterized. Antioxidant potential and α amylase and α glucosidase inhibition assays were performed using *in silico* and *in vitro* assays. Twenty eight peptide sequences and 12 phenolic compounds were identified on black bean samples. From *in silico* assays, sequenced peptides showed theoretical binding energies up to negative 8.3 kcal/mol and phenolic compounds up to negative 8.8 kcal/mol for analyzed enzymes. Protein hydrolysates after 96 h of fermentation showed the potential to block α amylase with IC₅₀ 0.57 mg protein/mL and 5.55 mg protein/mL for α glucosidase. Phenolic compounds after 48 h of fermentation blocked α glucosidase IC₅₀ 0.353 mg GAE/mL. Protein hydrolysates from solid state fermentation show higher antioxidant capacity compared with cooked beans to block ABTS radical. The antioxidant potential was maintained in phenolic compounds after fermentation for 48 h. Solid state fermentation improves bioactive compounds released and could generate functional ingredients rich in bioactive compounds with antidiabetes potential.

AGFD004B 3550076 2:00 PM **Chemical characterization of fermented whole blackcurrants and their value-added benefits** Regina Cortez rcortez826@gmail.com E Demejia edemejia@illinois.edu The objective was to characterize fermented whole blackcurrants (BC) and their effect on the activities of α -amylase, α -glucosidase, dipeptidyl peptidase, as markers of diabetes. In addition, the antioxidant capacity was measured using 2,2-diphenyl-1-picrylhydrazyl (DPPH), after water-based ultrasound assisted extraction, treatment with pectinase and fermentation. Enzymatic treatment doses and heating times (52 °C) were evaluated for their effect on the concentration of anthocyanins (TA) and it was determined that a dose of 400 mL/ton held for 150 min at 52 °C yielded the highest concentration. Positive correlations were noted

among the total time (min) of heating (52 °C) and total tannins (TT) and total polyphenols (TP) ($r = 0.725$ and $r = 0.731$, respectively at $\alpha = 0.05$). Heating during pectinase treatments increased the concentrations of both TT and TP, with a contribution of heating of the BC mash and the pectinase. Positive correlations were also noted for the fermentation temperatures (23 °C and 15 °C) for TA, TT, and TP ($r = 0.608$, $r = 0.569$, and $r = 0.546$, respectively at $\alpha = 0.05$). Dealcoholized wine-mix- 15 °C had the lowest (more potent) IC₅₀ for α -glucosidase. Fermentation increased TA approximately 5 times. LC-ESI-MS analysis confirmed the presence of four major TA (D3G, D3R, C3G, and C3R). Fermentation byproducts (BC pomace) proved to be a potent antioxidant when compared to 600 μ M gallic acid (100% inhibition), it achieved a DPPH free radical scavenging capacity of 83% (at 2 mg/ml). These results provide strong evidence that BC byproducts have great potential for reutilization by the food and beverage industries. In conclusion, to our knowledge, this is the first report quantifying the value-added benefits in BC fermented products using a water-based ultrasound extraction. BC fruits have potential to offer solutions for current issues facing the food industry such as consumer demand for more healthful colored processed foods.

AGFD004B 3550499 3:00 PM **Evaluation of bioactive properties of blackcurrants after lactic acid fermentation** Rebecca Kowalski rkowals2@illinois.edu E Demejia edemejia@illinois.edu Blackcurrants are powerful berries with many bioactive compounds. Previous research has shown other berries to have increased bioactive properties after lactic acid fermentation. The objective of this research was to look at the feasibility of fermenting blackcurrants with lactic acid bacteria and potential enhancement of antioxidant capacity and phenolic bioactive compounds. Different bacteria strains of *L. plantarum* Heal 19, *L. paracasei* 8700:2, and *L. rhamnosus* 271 were analyzed for tannase and glycosidase activity, and UHPLC and biochemical assays were conducted to analyze the change in phenolics and antioxidant capacity of blackcurrant juice after fermentation with these lactobacillus bacteria. Results suggest that *L. rhamnosus* 271 has 1.95x more tannase activity than *L. plantarum* Heal 19 and 8.88x more tannase activity than *L. paracasei* 8700:2. In addition, *L. rhamnosus* 271 contained the most glycosidase activity (1.3x more than the other two bacteria types). *L. plantarum* Heal 19 fermented the fastest and the juice started to get lighter in color after 8 h. The pH of the juice went from 6.00 to 4.35 after 44 h and the fermented juice became lighter than the untreated juice. The juice before fermentation had a total polyphenol concentration of 164.23 ± 1.41 mg eq GA/100 mL juice and a total antioxidant capacity of 30.13 ± 0.35 mmol eq Trolox/mL juice. It is expected that the faster the fermentation, the less likely the bacteria will affect polyphenols, and the bacteria with the most tannase and glycosidase activities will be the best candidate to enhance bioactive compounds. Producing a healthy fermented product with enhanced bioactive properties would allow the consumer to acquire the benefits of blackcurrants.

PRESENTER / DATE / TIME INDEX
sorted by presenter's last name

LAST	FIRST	DATE	TIME
Abdi	Reihaneh	4/5	6:00 AM
Acharya	Pratibha	4/8	9:45 AM
Ackerman	Luke	4/6	9:45 AM
Adhikari	Jayashan	4/8	3:15 PM

Adviento-Borbe	ARLENE	4/14	2:15 PM
Akgul	Ali	4/14	6:40 PM
Akgul	Ayfer	4/14	6:40 PM
Al-Taher	Fadwa	4/5	6:00 AM
Alfonso-Prieto	Mercedes	4/14	9:25 AM
Almeida	Vitor	4/13	3:05 PM

Altava	Belen	4/14	6:50 PM
Appell	Michael	4/15	9:25 AM
Arrizon	Javier	4/16	9:55 AM
Asenjo	Stephen Bryan	4/14	1:55 PM
Azoubel	P	4/8	5:45 PM
Bai	Jinhe	4/6	5:45 PM
Bai	Yajuan	4/15	6:05 PM
Barringer	Sheryl	4/5	1:20 PM
Beauchamp	Jonathan	4/5	3:25 PM
Bertolo	Mirella	4/6	1:05 PM
Best	Ivan	4/15	2:45 PM
Bhandari	Sneh	4/13	3:10 PM
Bhunja	Arun	4/7	5:25 PM
Biradar	Kishan	4/8	6:05 PM
Biswas	Atanu	4/15	10:15 AM
Boonprab	Kangsadan	4/5	6:00 AM
Brinas	Raymond	4/6	9:05 AM
Brown	Eric	4/13	11:30 AM
Cai	Wenhao	4/15	2:15 PM
Candian	Joara	4/7	9:25 AM
Cao	Heping	4/15	1:50 PM
CHEGN	LU	4/13	10:05 AM
Chen	Hongda	4/12	9:25 AM
Chen	Wan-Ting	4/13	1:50 PM
Cheng	H.N.	4/13	2:40 PM
Cheng	Shasha	4/14	7:30 PM
Cheung	Chin	4/12	1:50 PM
Chiang	Nancy	4/14	2:50 PM
Chicilo	Farley	4/13	10:50 AM
Cochran	Eric	4/13	9:25 AM
Collias	Dimitris	4/13	5:00 PM
Compton	David	4/13	10:40 AM
Cooperstone	Jessica	4/8	9:25 AM
Cortez	Regina	4/16	2:55 PM
Crosby	Kevin	4/7	9:05 AM
Davila Ortiz	Gloria	4/16	9:30 AM
Davila Ortiz	Gloria	4/16	10:35 AM
Davila Ortiz	Gloria	4/16	11:25 AM
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Demejia	E	4/16	2:55 PM
Demejia	E	4/16	3:15 PM
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Dhowlaghar	Nitin	4/7	2:35 PM
DJAUI	Souad	4/5	6:00 AM
Doshna	Noah	4/6	3:25 PM
Dou	Zeou	4/15	11:25 AM
Duan	Xuguo	4/5	6:00 AM

Eischeid	Anne	4/5	6:00 AM
El-Moghazy	Ahmed	4/15	10:45 AM
Eshun	Gaddi	4/14	6:40 PM
Fan	Xuetong	4/6	7:05 PM
Farmer	Jason	4/13	10:30 AM
Feng	Yaohua	4/7	6:55 PM
Finley	John	4/14	9:00 AM
Fox	McKinley	4/15	3:10 PM
Frollini	Elisabete	4/12	3:05 PM
Furtado	Roselayne	4/15	10:15 AM
Gallegos-Peretz	Tiffany	4/5	6:00 AM
Ganjyal	Girish	4/8	1:25 PM
Gao	Boyan	4/13	5:25 PM
Gaydhane	Mrunalini	4/6	1:45 PM
Giraldo	Juan Pablo	4/14	11:10 AM
Goddard	Julie	4/6	5:05 PM
Graham	James	4/6	10:45 AM
Grancieri	Mariana	4/16	2:00 PM
Guo	Mingming	4/6	2:05 PM
Guo	Yue	4/14	5:45 PM
Handa	Sachin	4/12	10:40 AM
Hart-Cooper	William	4/13	9:50 AM
Harvey	Benjamin	4/13	10:15 AM
Haverhals	Luke	4/13	1:25 PM
He	Zhanglan	4/5	6:00 AM
Hendon	Christopher	4/13	9:25 AM
Honda	Hiroshi	4/5	6:00 AM
Honda	Hiroshi	4/5	6:00 AM
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Hsieh	You-Lo	4/14	5:00 PM
Hu	Yaxi	4/13	2:14 PM
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Hwang	Hong-Sik	4/14	10:15 AM
Jeon	Su-Ji	4/15	9:40 AM
Jia	Ruixin	4/7	1:25 PM
Jifon	John	4/7	10:15 AM
Jin	Tony	4/6	11:25 AM
Jo	Hyeong Wook	4/5	6:00 AM
Jurado	Jaime	4/13	9:45 AM
Kang	Seung Yoon	4/5	6:00 AM
Kang	Seung Yoon	4/9	5:30 PM
Kaur	Lajpreet	4/8	2:35 PM
Khomenko	Iuliia	4/5	10:55 AM
Khuda	Sefat E	4/15	2:15 PM
Kim	Chyer	4/8	6:50 PM

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Klasson	Thomas	4/5	6:00 AM
Koiwa	Hisashi	4/7	2:05 PM
Kotamarthi	V. Rao	4/14	9:50 AM
Kowalski	Rebecca	4/16	3:15 PM
Krueger	Dana	4/13	2:47 PM
Kuhn	Eberhardt	4/13	1:28 PM
Kumar	Devendra	4/6	6:05 PM
Lagaron	Jose Maria	4/12	1:25 PM
Lahne	Jacob	4/7	7:15 PM
Lammi	Carmen	4/15	5:25 PM
Le Quere	Jean-Luc	4/5	10:40 AM
Lee	Changhoon	4/5	6:00 AM
Lee	Choon	4/15	9:20 AM
Lee	James	4/14	2:40 PM
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Li	Qing	4/13	11:05 AM
Li	Jun	4/13	2:15 PM
Li	Yanfang	4/15	3:35 PM
Li	Jia	4/12	5:05 PM
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Lindinger	Christian	4/5	9:20 AM
Lipshutz	Bruce	4/12	10:15 AM
Lister	Andee	4/14	3:15 PM
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Lo	Yu-Chen	4/5	6:00 AM
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Lowry	Greg	4/14	5:50 PM
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Lu	Mei	4/8	1:05 PM
Lu	Weiying	4/13	5:50 PM
Luo	Shiyuan	4/5	6:00 AM
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Majithia	Drishti	4/8	10:35 AM
Marco	Maria	4/7	5:45 PM
Martin-Cabrejas	Maria	4/16	9:05 AM
Mauter	Meagan	4/14	1:50 PM
McClements	David	4/15	1:00 PM
McPhee	Derek	4/15	9:50 AM
Menghi	Leonardo	4/5	11:10 AM
Metrani	Rita	4/7	1:45 PM
Miller	Rhonda	4/7	1:05 PM
Miller	Michael	4/12	6:25 PM
Miri	Massoud	4/14	9:25 AM

Mitchell	Alyson	4/8	10:05 AM
Mohanty	Amar	4/13	5:25 PM
Mojica	Luis	4/16	2:35 PM
Monagas	Maria	4/13	7:20 PM
Moore	Andrew	4/5	6:00 AM
Moore	Andrew	4/15	10:00 AM
Mosher	Michael	4/5	6:00 AM
Munafo	John	4/12	6:50 PM
Munoz	Carolina	4/5	9:50 AM
Murthy	Chidambara	4/7	10:35 AM
Mustafa	Fatima	4/14	9:50 AM
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Nguyen	Thanh	4/15	11:05 AM
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Oehrl	Lisa	4/7	6:35 PM
Ofoegbu	Polycarp	4/14	6:05 PM
Orts	William	4/13	1:00 PM
Osonga	Francis	4/14	6:40 PM
Padayachee	Diandree	4/5	9:35 AM
Paoletta	Celina	4/5	6:00 AM
Paoletta	Celina	4/9	5:30 PM
Park	Richard	4/7	2:55 PM
Pascall	Melvin	4/6	3:05 PM
Patel	Dinesh	4/5	6:00 AM
Patel	Dinesh	4/5	6:00 AM
Pedrotti	Michele	4/5	11:25 AM
Peng	Han	4/5	6:00 AM
Peredo-Lovillo	Audry	4/16	11:00 AM
Perez	Jose	4/8	7:10 PM
Phetxumphou	Katherine	4/8	2:55 PM
Pokhrel	Lok	4/5	6:00 AM
Pulatsu	Ezgi	4/5	6:00 AM
Qi	Xiaoxi	4/15	1:25 PM
Qian	YanPing	4/5	6:00 AM
Qian	Xiaoning	4/7	11:15 AM
Quay	Amanda	4/14	1:50 PM
Rai	Rewa	4/8	2:05 PM
Raliya	Ramesh	4/14	10:40 AM
Ramanathan	Ranjith	4/5	6:00 AM
Ramirez Jimenez	Aurea Karina	4/16	1:40 PM
Randall	John	4/15	9:00 AM
Rao	Jiajia	4/13	9:00 AM
Ratnawati	Susana Endah	4/5	2:55 PM
Ravindranath	Varsha	4/8	6:30 PM
Ravishankar	Sadhana	4/7	3:35 PM
Reddivari	Lavanya	4/8	10:55 AM
Rehberg	Rachelle	4/15	5:05 PM

Relph	Rachael	4/14	3:05 PM
Ren	Gui	4/5	6:00 AM
Richards	Todd	4/14	1:30 PM
Romero	Haydee	4/16	1:20 PM
Sabliov	Cristina	4/14	6:15 PM
Sadik	Omowunmi	4/14	5:25 PM
Sadik	Omowunmi	4/14	6:40 PM
Saha	Supradip	4/8	7:30 PM
Sakhaee	Laura	4/14	6:40 PM
Sapozhnikova	Yelena	4/6	9:25 AM
SARKAR	ROHAN	4/8	1:45 PM
Scherf	Katharina	4/12	7:15 PM
Scholz	Carmen	4/13	5:50 PM
Schroeder	Avi	4/14	7:05 PM
Schultheis	Jonathan	4/7	9:45 AM
Schwartz	Eric	4/13	3:33 PM
Seiber	James	4/14	1:00 PM
Serber	Zach	4/12	9:50 AM
Sharma	Heena	4/5	6:00 AM
Shen	Hongchen	4/6	1:25 PM
Shivanagoudra	Siddanagouda	4/8	11:15 AM
Shukla	Diwakar	4/15	10:25 AM
Silcock	Patrick	4/5	1:50 PM
Silva	Christopher	4/14	1:05 PM
Singh	Jashbir	4/7	10:55 AM
Sodamade	Abiodun	4/15	6:30 PM
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Song	Hyunjong	4/5	6:00 AM
Song	Yukun	4/14	7:10 PM
Spanel	Patrik	4/5	2:40 PM
Stanzione	Joseph	4/12	2:40 PM
Starowicz	Malgorzata	4/12	5:55 PM
Su	Wentao	4/15	11:05 AM
Su	Xueqian	4/13	11:10 AM
Sun	Xiuzhi Susan	4/15	1:50 PM
sun	jianghao	4/13	6:30 PM
Syed	Nisa	4/5	6:00 AM
Tan	Mingqian	4/13	9:05 AM
Taylor	Andrew	4/5	9:05 AM
Taylor	Andrew	4/5	1:05 PM
Tennyson	Andy	4/13	6:40 PM
Tian	Fei	4/12	5:30 PM
Timkovsky	Joseph	4/5	1:35 PM
Tomer	Mark	4/14	1:25 PM
Trinetta	Valentina	4/6	2:45 PM
Tse	Timothy	4/14	10:45 AM
Tseng	Y. Jane	4/15	9:00 AM

Tunick	Michael	4/16	1:00 PM
Tunick	Michael	4/13	7:05 PM
Ulberth	Franz	4/13	1:05 PM
Valls	Adriana	4/14	6:50 PM
Venkitanarayanan	KUMAR	4/7	5:05 PM
Vitha	Stanislav	4/7	3:15 PM
Vitrac	Olivier	4/6	10:05 AM
Waite-Cusic	Joy	4/7	6:05 PM
Waman	Ajit	4/8	5:25 PM
Wang	Yi	4/5	6:00 AM
Wang	Zhen	4/14	9:00 AM
Wang	Haitao	4/15	1:00 PM
Wang	Harris	4/15	1:25 PM
Wang	Qi	4/15	6:50 PM
Warner	John	4/12	9:50 AM
Washburn	Newell	4/12	2:15 PM
wenbei	situ	4/14	5:05 PM
Whaley	William	4/5	6:00 AM
Whaley	William	4/5	6:00 AM
White	Jason	4/14	10:15 AM
WOO	SO YOUNG	4/5	6:00 AM
WOO	SO YOUNG	4/9	5:30 PM
Wu	Ying	4/6	5:25 PM
Xiao	Chang-Lin	4/6	7:25 PM
Xu	Tongtong	4/13	1:51 PM
Yan	Ru	4/5	6:00 AM
Yang	Ruiwen	4/5	6:00 AM
Yazgan	Idris	4/14	6:40 PM
You	Hong	4/13	6:55 PM
Yu	Dajun	4/5	6:00 AM
Yu	Jianmei	4/5	6:00 AM
Yu	Jianmei	4/5	6:00 AM
Yu	Liangli	4/15	3:05 PM
Yu	Dajun	4/9	5:30 PM
Yuan	Fang	4/15	5:45 PM
Zhang	Jingyao	4/13	5:00 PM
Zhang	Xinyan	4/5	6:00 AM
Zhang	Yuxuan	4/5	6:00 AM
Zhang	Zhichao	4/14	2:25 PM
Zheng	Jia	4/5	6:00 AM
Zheng	Wenhao	4/13	5:25 PM
Zhou	Dayong	4/15	10:40 AM
Zhu	Danye	4/5	6:00 AM
Zhuang	Zilong	4/14	5:25 PM
Zyzak	LiLi	4/15	7:10 PM



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