Division of Agricultural and Food Chemistry Spring 2016

CORNUCOPIA

including AGFD abstracts for the

251st American Chemical Society National Meeting

March 13 - 17, 2016

in

SAN DIEGO

BOSOON PARK, Program Chair

Attend AGFD oral technical sessions at the US Grant Hotel and view posters at the San Diego Convention Center

Join the AGFD Chair's Reception Tuesday, March 15, 6:00-8:00 pm at the San Diego Wine and Culinary Center 200 Harbor Drive

CONTENTS

page	
2	Message from the Chair
3	Future AGFD programs
5	Puzzle page
6	Membership application - join the team !
7	Roster of officers and committee leadership
8	Award news
9	Scenes from Boston
10	Executive committee meeting minutes
12	Business meeting minutes
12	AGFD technical program w/abstracts
back cover	Schedule of AGFD technical/business/planning meetings and merrymaking

Check this out → Caribbean Cooking Competition w/Master Chef Demo, Student team presentations & snacks - Tuesday 3/15 2:00 - 4:30PM at the San Diego Wine and Culinary Center 200 Harbor Drive See ACS Conference Registration (Ticketed Events) for Tickets ($10) Contact Gavin Sacks (gls9@cornell.edu) for more info

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

MESSAGE FROM THE CHAIR

It is my great pleasure and honor to serve the Division of Agricultural and Food Chemistry (AGFD) as the 2016 Chair. The 2015 AGFD program for the Fall ACS Meeting in Boston was well organized and attended.

The Division continues promoting outreach activities to serve our members who don't attend national meetings. We have begun international student chapters in Italy, Germany, Thailand, China, and several universities in the US. These student chapters are organizing their own symposium for the the 2016 Fall ACS meeting with an official name "AGFD Affiliate ACS Student Chapters". These activities are aimed at students and young professionals in our international student chapters and our student award programs.

There are several prestigious Division awards to recognize our members: Award for the Advancement of Application of Agricultural and Food Chemistry, AGFD Fellow Award, Roy Teranishi Graduate Fellowship in Food Chemistry, Young Scientist Symposium, Withycombe-Charalambous Graduate Student Symposium, Undergraduate Student Symposium, Award for Distinguished Service to the Division of Agricultural and Food Chemistry.

The Award for the Advancement of Application of Agricultural and Food Chemistry in Boston was won by Andy Taylor of Mars, Inc., who was honored at an AGFD Division Award Symposium on Tuesday. Wally Yokoyama won the AGFD Distinguished Service Award. Mike Appell, David McClements, Alyson Mitchell, and Kazuo Miyashita were the 2015 AGFD Fellow Awardees. Mike Appell won an ACS Fellow Award as well. The winner of the Young Scientist Award was Lili He, University of Massachusetts-Amherst. Thomas Selby of DuPont, who gave a talk at a symposium in his honor Wednesday morning and a ceremony in Kansas City on October, won the Kenneth Spencer Award.

Selecting leading scientists from around the world, the AGFD program in Boston included 17 symposia, 34 sessions, 335 papers, comprised of 216 oral presentations and 119 posters, which was the the largest program ever and the topics of symposia covered the broad areas of Phytonutrients to Nanoparticles in Food, Agricultural, & Environmental Settings cosponsored with COLL. Overall the meeting in Boston was another demonstration of AGFD leadership with numerous technical and networking opportunities. The Division also organized 4 symposia at the PACIFICHEM - Dec. 15-20, 2015, Honolulu.

During this spring meeting, the Division will host a Caribbean Cooking Competition with Student Team Posters on Tuesday, March 15 at the San Diego Wine and Culinary Center, 200 Harbor Drive at 4:30 PM followed by AGFD Chair's Reception from 6:00-8:00 PM. Join us for these events to meet people from across industry, academia, and government with a diversity of interests in AGFD research.

I would like to thank the numerous volunteers who have given me so much support. I especially would like to thank the past chair, Kathryn Deibler and vice-chair, Navindra Seeram for their invaluable leadership and assistance. I also want to thank Michael Appell, Mike Morello, Michael Tunick, Alyson Mitchell, Steve Toth, Neil Da Costa, Michael Qian, Lauren Jackson and many others, for their volunteered contribution in making the division successful. I'd like to give special thanks to Charles Brine who has been organizing student awards competition and Division Reception and Banquet many years. Thank you all for your support to the division.

Bosoon Park bosoon.park@ars.usda.gov

CORNUCOPIA EDITORIAL STAFF & CONTACT INFORMATION

Editor-in-Chief	C. Frey cfreyenterprises@gmail.com
General Manager	P. White
Staff	C. Kent, L. Lane, J. Olsen

Deadline for submission of content for Fall Cornucopia: Jun 15.

FUTURE PROGRAMS

PHILADELPHIA - August 21 – 25, 2016

Advances in Taste Research for Sodium & Sugar Reduction - Jane Leland Kraft Foods jleland@kraftheinzcompany.com Louise Slade Food Polymer Science Consultancy sladel@optonline.net Thomas Hofmann Technical University of Munich, Germany thomas.hofmann@wzw.tum.de

Flavor Stability: Chemical Changes in Flavor Molecules, Flavor-Food Matrix Interactions, Flavor Encapsulation - Michael Qian Oregon State University michael.qian@oregonstate.edu Bob McGorrin Oregon State University robert.mcgorrin@oregonstate.edu

Chemistry Behind Health Effects of Whole Grains - Shengmin Sang North Carolina State University ssang@ncat.edu Rikard Landberg Swedish University of Agricultural Sciences rikard.landberg@slu.se

Natural & Bio-based Antimicrobials for Food Applications - Xuetong Fan USDA, ARS xuetong.fan@ars.usda.gov Helen Ngo USDA ARS Helen.Ngo@ars.usda.gov Changqing Wu University of Delaware, changwu@udel.edu

Sample Preparation for Nutraceutical & Functional Food Analysis - Dave L. Luthria USDA d.luthria@ars.usda.gov

Young Scientist Award Symposium - Charles Brine Princeton ChitoCare LLC brinec11@verizon.net

AGFD Division Award Symposium - Bosoon Park USDA, ARS, USNPRC bosoon.park@ars.usda.gov

International Student Symposium - Philipp Schmidberger, Technical University of Munich,Germany philipp.schmidberger@lrz.tum.de Roberta Tardugno, University of Modena and Reggio Emilia, Italy roberta.tardugno@unimore.it

Microencapsulation of Pigments and Bioactives for Food Applications - Coralia Osorio, Universidad Nacional de Colombia, cosorior@unal.edu.co Agnes Rimando, USDA, ARS Agnes.rimando@ars.usda.gov

Chemistry of Mediterranean Foods (Co-sponsor: IAC) - Ellene Tratras Contis, Eastern Michigan University, econtis@emich.edu; Agnes Rimando, USDA, ARS agnes.rimando@ars.usda.gov

Sterling Hendricks Memorial Lectureship (co-sponsored with AGRO) - Michael H. Tunick USDA-ARS Eastern Regional Research Center michael.tunick@ars.usda.gov Kim Kaplan USDA-ARS kim.kaplan@ars.usda.gov

Challenges in Flavor Chemistry Associated with Developing Healthy Foods & Beverages - Kawaljit Tandon, Constellation Brands, Inc. Kawaljit.tandon@cbrands.com; Ryan Elias, Penn State University Ryan.elias@gmail.com

High-Resolution Mass Spectroscopy Techniques for Identification and Quantification of Phytochemical Metabolites - Luke Howard, University of Arkansas, lukeh@uark.edu; Youngmok Kim, Synergy Flavors, ykim@synergytaste.com; Steve Talcott, Texas A&M University, stalcott@tamu.edu; Mathias Sucan, Pfizer, mathias.sucan@pfizer.com

Nano-Biotechnology in Foods and Nutraceuticals - Fereidoon Shahidi, Memorial University of Newfoundland, fshahidi@mun.ca

Nutritional Oils and Omega-3s - Fereidoon Shahidi, Memorial University of Newfoundland, fshahidi@mun.ca

General Papers and General Posters - Navindra Seeram nseeram@uri.edu

Recent Advances in Functional Biopolymers - Yoshihiro Ito, RIKEN, Japan LinShu Liu, Linshu.liu@ars.usda.gov

continues on next page

continued from previous page

Synthetic and natural colors in foods - Youngmok Kim (ykim@synergytaste.com) and Kevin Goodner (kgoodner@synergytaste.com)

ACS National Meeting Theme: Chemistry of the People, by the People and for the People

SAN FRANCISCO - April 2-6, 2017

Biotransformation in the Body - Alyson Mitchell U. of California Davis aemitchell@ucdavis.edu - *needs support*

Chemistry of Nonvolatile Compounds in Beverages - Mathias Sucan Pfizer mathias.sucan@gmail.com

Emerging Trends in Nano-bioactives for the Prevention of Chronic Diseases - Bhimu Patil Texas A&M University b-patil@tamu.edu G. K. Jayaprakasha Texas A&M University gjayaprakasha@ag.tamu.edu

Chemistry of Phenolics from Fruits and Vegetables - G. K. Jayaprakasha Texas A&M University gjayaprakasha@ag.tamu.edu Bhimu Patil Texas A&M University b-patil@tamu.edu

Nano-Biotechnology in Foods and Nutraceuticals - Fereidoon Shahidi, Memorial University of Newfoundland, fshahidi@mun.ca

Chemistry of Korean Foods and Beverages - Choon Ho Do, National Fisheries R&D Institute, choondo@sunchon.ac.kr Agnes Rimando, USDA, ARS, agnes.rimando@ars.usda.gov

Graduate Student Symposium - Charles Brine Princeton ChitoCare LLC brinec11@verizon.net

Undergraduate Symposium - Charles Brine Princeton ChitoCare LLC brinec11@verizon.net

The Bliss Point: Food Satiety and Food Mood Effects - blissful organizer needed

Metabolomics: Diet and Effect - organizer needed

General Papers and General Posters - Navindra Seeram

ACS National Meeting Theme: Advanced Materials, Technologies, Systems and Processes

WASHINGTON DC - August 20-24, 2017

Food Safety & Labeling - Deepthi K Weerasinghe; dP3Consulting; dkweerasinghe@att.net Lauren Jackson, FDA, lauren.jackson@fda.hhs.gov

Young Scientist Award Symposium - Charles Brine Princeton ChitoCare LLC brinec11@verizon.net

AGFD Division Award Symposium - Navindra Seeram, nseeram@uri.edu

Sterling Hendricks Memorial Lectureship (co-sponsored with AGRO) - Michael H. Tunick USDA-ARS Eastern Regional Research Center michael.tunick@ars.usda.gov Kim Kaplan USDA-ARS kim.kaplan@ars.usda.gov

Impact of Glycative and Carbonyl Stress on Diabetic and Aging Related Diseases - Shengmin Sang, NC State University, ssang@ncat.edu Chitang Ho, Rutgers University, ho@aesop.rutgers.edu Lishuang Lv, Nanjing Normal University, lishuanglv@126.com

ACS National Meeting Theme: Chemistry's Impact on the Global Economy

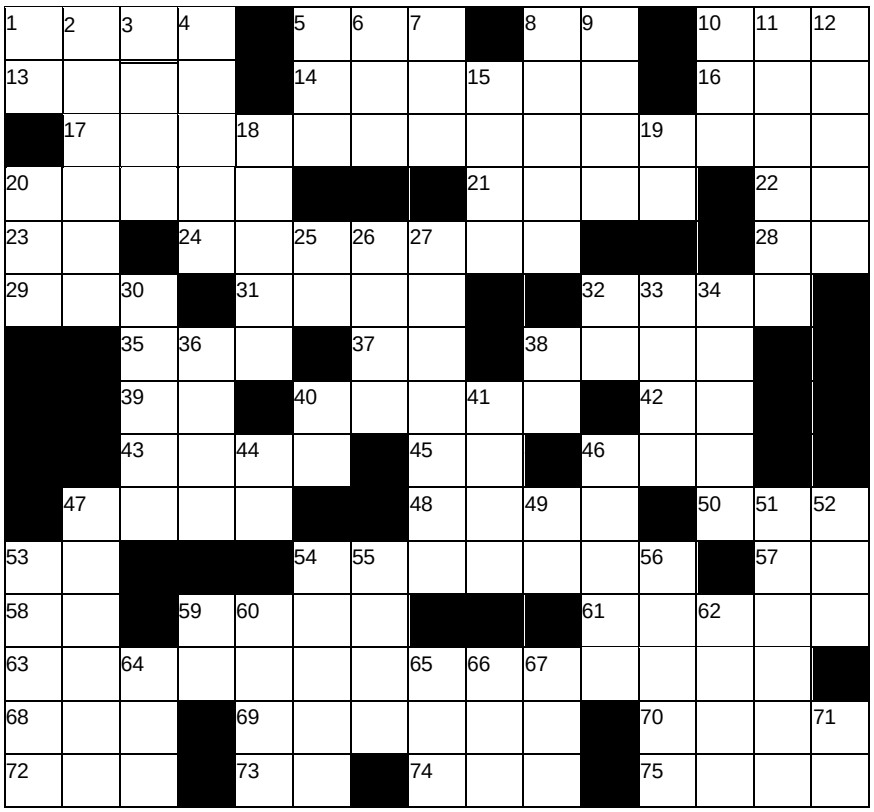
BEYOND 2017

Advances in Flavor Analysis - Michael Qian, Oregon State University, michael.qian@oregonstate.edu

INTERNATIONAL FLAVOR AND FRAGRANCE CONFERENCE (replaces Greece flavor meeting) -

Michael Qian Oregon State University Fereidoon Shahidi Memorial University of Newfoundland fshahidi@mun.ca Stephen Toth; IFF, stephen.toth@iff.com Coralia Osoria Roa, Universidad Nacional de Colombia, cosorior@unal.edu.co

WEST COAST WORDPLAY



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

ACROSS

1 warning to tag sale buyer
5 shipping carrier option
8 element or 4 year degree
10 refreshing energy drink
13 retained or held
14 they go up and down but don't move
16 Kingston Trio hit about rider Charlie
17 San Diego beach resort
20 a burning problem
21 alliance born in 1949
22 -- No or -- Evil
23 a guy or an element
24 see 30 DOWN
28 many an RIT grad
29 ten and twenty dispenser
31 13 in binary
32 really catty remark
35 8X Norris Trophy winner
37 nap time
38 mineral w/Mohs scale=1
39 syllable of hesitation
40 harbor barrier structure
42 Paris runway: -- Bourget
43 close by
45 workplace for an RN
46 airspace safety overseer
47 '---- the Man' Musial
48 cloud by stirring up mud
50 Now --- and Improved!
53 photocell element
54 San Diego border (w/34 DOWN)
57 Are you talkin' to --?
58 film about a retired balloon salesman.
59 status of GI out too late
61 relaxed or reduced
63 historic San Diego neighborhood
68 India Pale ---
69 continue where left off
70 R. Descartes: 'Cogito ---- sum'
72 Q followers
73 modern female address
74 rowboat propeller
75 really smell nasty

DOWN

1 -- 47
2 unshared information
3 some stock market launches
4 barbershop sharpening tool
5 source of many NASA astronauts
6 school support org.
7 gloomy
8 thorn or sticker
9 aide to a Mgr. or Dir.
10 org. for Drs.
11 refreshing citrus beverage
12 player at Petco Field
15 home of the Gaels
18 broadcasting or floating
19 -- and behold!
20 gotcha!
25 XV + XXXVI
26 slow messy leak
27 the Fonz' address for Richie's dad.
30 site of the 200" Hale Telescope (w/24 ACROSS)
32 degree following 8 ACROSS
33 tuneful Fitzgerald
34 see 54 ACROSS
36 Perlman of *Cheers*
38 nasty Cobb
40 Sr's son
41 *StarTrek* counselor/empath
44 -- eye for -- eye
46 a plane or its passenger
47 parts covering a blossom
49 --, then, else
51 appear or enter
52 unify
53 sweet source of energy
54 apples & pears, for instance
55 Matterhorn and Mont Blanc Locale
56 prepare food for a crowd
59 an element of cookware
60 like a welcome greeting
62 really dry & withered
64 chemistry ---
65 status ---
66 actress --- Thurman
67 --- Lingus
71 Roger!

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
- 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

Join the 3000 members of the AGFD division. At ACS National Meetings you can meet and discuss division activities at the AGFD Information table located near the AGFD technical session rooms. Use the membership application form (below) or join on-line at www.acs.org (click on Technical Divisions and then select Join a Division) or by mail American Chemical Society; Member and Subscriber Services; PO Box 182426; Columbus, Ohio 43218-2426 or call ACS at (800)333-9511 in US. Payment by Visa/Master Card or American Express.

	APPLICATION FOR AGFD DIVISION MEMBERSHIP (7623P)
title	
name	
1st address line	
2nd address line	
city	
state	
Zip code	
country	
e-mail address	
phone	
check one	**MEMBERSHIP FEE**
[ ]	I am an ACS member and wish to join AGFD ($10.00)
[ ]	I am not an ACS member and wish to join AGFD ($15.00)
[ ]	I am a full time student and wish to join AGFD ($10.00)
Be cool **J O I N** **A G F D**	Return application, with payment (payable to American Chemical Society), to AGFD Membership Chair: Dr. Lucy Yu University of Maryland Department of Nutrition & Food Science, 3303 Marie Mount Hall College Park MD 20742

AGFD OFFICERS & COMMITTEE LEADERSHIP

Chair - Serves 1 year. Presides over Division meetings & appoints committees
Bosoon Park
US National Poultry Research Center
950 College Station Rd.
Athens GA 30605
706-546-3396, Bosoon.Park@ars.usda.gov

Chair-Elect - Serves 1 year. Substitutes for the chair as needed
Navindra Seeram
University of Rhode Island
7 Greenhouse Road Kingston, RI 02881
401-874-9367, nseeram@uri.edu

Vice-Chair - Serves 1 year. Assists Chair-elect. Develops future technical programs.
Brian Guthrie
Cargill Food System Design
2301 Crosby Road
Wayzata MN 53391
952-742-3983 brian_guthrie@cargill.com

Secretary - Responsible for Division correspondence and meeting minutes.
Michael Tunick
USDA-ARS
Eastern Regional Research Center
600 E. Mermaid La.
Wyndmoor PA 19038
215-233-6454
michael.tunick@ars.usda.gov

Treasurer - Responsible for Division finances.
Stephen Toth
International Flavors & Fragrances R&D
1515 Hwy. 36 Union Beach NJ 07735
732-335-2772
stephen.toth@iff.com

Cornucopia Editor - Edits newsletter.
Carl Frey
cfreyenterprises@gmail.com
203-918-6007

Councilors - Represent Division for 3 years on ACS council.
Michael Appell (thru '16)
michael.appel@ars.usda.gov
John Finley (thru '17) jfinle5@lsu.edu
Michael Morello (thru '17)
mike.morello@pepsico.com
Agnes Rimando (thru '18)
agnes.rimando@ars.usda.gov

Alternate Councilors - Substitute for Councilors that can not attend Council meetings. Serves 3 years.
Charles Brine (thru '18)
brinec11@verizon.net
Keith Cadwallader (thru '17)
cadwlldr@uiuc.edu
Alyson Mitchell (thru '16)
aemitchell@ucdavis.edu
Fereidoon Shahidi (thru '16)
fshahidi@mun.ca

At-Large Executive Committee Members - Assist in management of Division. Serves 3 years.
Terry Acree (thru '18) tea2@cornell.edu
Jane Leland (thru '17)
JaneLeland@ameritech.net
Robert McGorrin (thru '17)
robert.mcgorrin@oregonstate.edu
Mathias Sucan (thru '18)
mksucan@pfizer.com

Awards Committee - Solicits nominations, oversees awards process.
Chair Michael Morello (thru '17)
mike.morello@pepsico.com
Student Awards Chi-Tang Ho
ho@aesop.rutgers.edu
Fellow Awards Fereidoon Shahidi
fshahidi@mun.ca
Canvassing Stephen Toth
stephen.toth@iff.com; Artemio Tulio, Jr.
artemio.tulio@fda.hhs.gov

Finance - Monitors the Division's finances for 1 year. Filled by Immediate Past Chair
Kathryn Deibler kdd3@cornell.edu

Hospitality - Organizes receptions and banquets.
Charles Brine brinec11@verizon.net

Membership - Recruits and retains Division members.
Lucy Yu lyu5@umd.edu

Multidisciplinary Program Planning coordinates nat'l mtg programming
John Finley jfinle5@lsu.edu

Nominations - Develops officer slate Served by Immediate Past Chair.
Kathryn Deibler kdd3@cornell.edu

Public Relations - Publicizes Division.
Charles Brine - brinec11@verizon.net

Web Master - Maintains web site.
Michael Appell
michael.appell@ars.usda.gov

Sub-divisions Develop symposia.

Flavor
Chair- Kawaljit Tandon
kawaljit.tandon@cbrands.com
Chair-Elect Ryan Elias elias@psu.edu
Vice-Chair Julie Anne Grover,
JulieAnne.Grover@Kraftfoods.com

Functional Foods & Natural Products
Chair- Steve Talcott
stalcott@tamu.edu
Chair-Elect Mathias Sucan
mathias.sucan@pfizer.com
Vice Chair Kwang-Geun Lee,
kwglee@dongguk.edu
Secretary Hyang-Sook Chun
hschun@cau.ac.kr

Biotechnology
Chair Joey N. Talbert
jotalber@iastate.edu
Chair Elect Rashmi Tiwari
rashmi.tiwari@pepsico.com
Vice Chair Nitin Nitin
nnitin@ucdavis.edu

Nutrition
Chair Anne Kurilich
anne.kurilich@mccain.com
Chair-Elect Indika Edirisinghe
iedirisi@iit.edu
Vice Chair Luke Howard
lukeh@uark.edu

Food Safety
Chair Lucy Yu, lyu5@umd.edu
Chair-Elect Bosoon Park,
bosoon.park@ars.usda.gov
Vice Chair Alyson Mitchell,
aemitchell@ucdavis.edu
Secretary Michael Granvogl
michael.granvogl@tum.de

AWARD NEWS

ACS Fellows

Congratulations to Division of Agricultural and Food Chemistry members who were selected as 2015 ACS Fellows: Michael Appell, U.S. Department of Agriculture, Agricultural Research Service (AGFD Nominee); Rodney Morris Bennet, Critical Path Services, LLC; Bonnie Charpentier, Cytokinetics, Inc; John J. Johnston, U.S. Department of Agriculture, Food Safety and Inspection Service

Ernest Guenther Award in the Chemistry of Natural Products

Congratulations to Division of Agricultural and Food Chemistry member Eric Block, SUNY at Albany, for receiving the Ernest Guenther Award in the Chemistry of Natural Products – sponsored by Givaudan Flavors. His award and address will be presented before the Division of Organic Chemistry.

2015 AGFD Distinguished Service

Dr. Wally Yokoyama, USD-ARS, WRRC will receive the 2015 AGFD Distinguished Service Award for continuing service to the Division.

AGFD Fellows

Drs. Mike Appell, David J. McClements, Alyson Mitchell, and Kazuo Miyashita are the 2015 AGFD Fellow Awardees for continuing service to the Division.

2015 Award for Advancement of Application of Agricultural & Food Chemistry

The 2015 Award for Advancement of Application of Agricultural & Food Chemistry was presented to Dr. Andrew Taylor Ph.D., FIFST at the Fall 2015 ACS National Meeting in Boston.

2015 Graduate Student Research Award

Lindsay Springer, Cornell University won the 2015 Graduate Student Research competition.

2015 Teranishi Fellowship

Cansu Ekin Gamus, University of Massachusetts won the 2015 Teranishi Fellowship.

2015 Undergraduate Student Research Awards

The 2015 Undergraduate Student Research Awards winners, determined by a competitive symposium at the Denver ACS Meeting in March are: 1st Place: Sebastiaan Groothuis, Hanze University of Applied Science (Groningen, The Netherlands), and, 2nd Place: Santiago Bukovsky-Reyes, University of Colorado at Colorado Springs.

AGFD Young Scientist Award

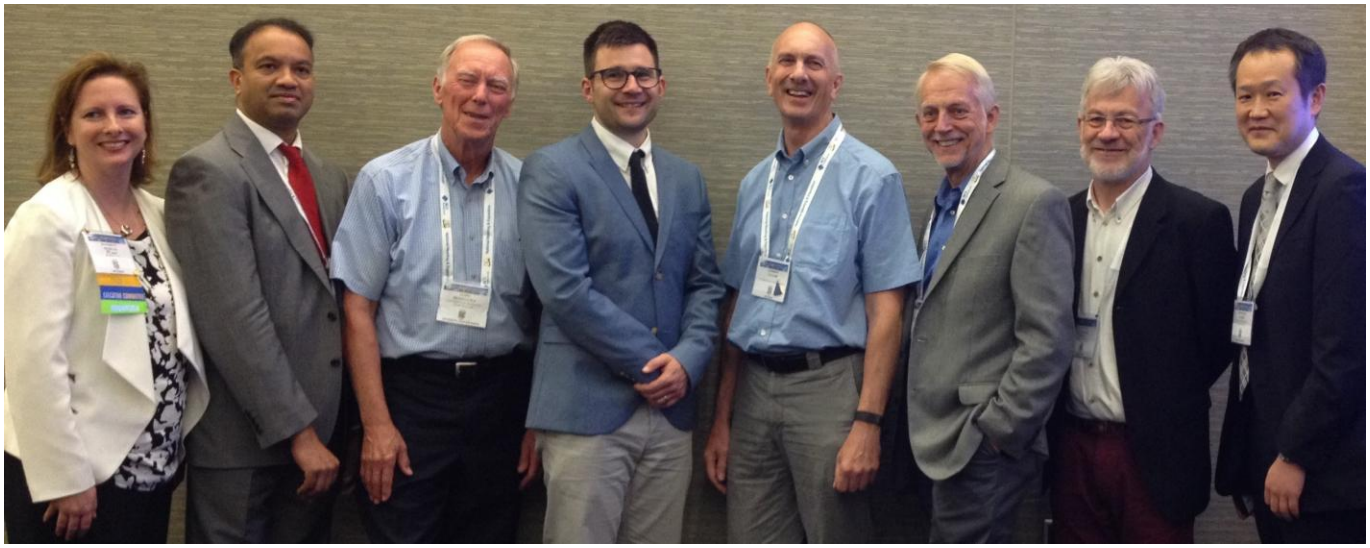
Assistant Professor Lili He from the University of Massachusetts-Amberst, Department of Food Science won the AGFD Young Scientist competition.

IPG grant

AGFD won an IPG Grant to support the "Caribbean Cuisine Chemistry and Flavors" student outreach program being held during the Spring national meeting in San Diego. http://www.hws.edu/news/caribbeancuisine.aspx

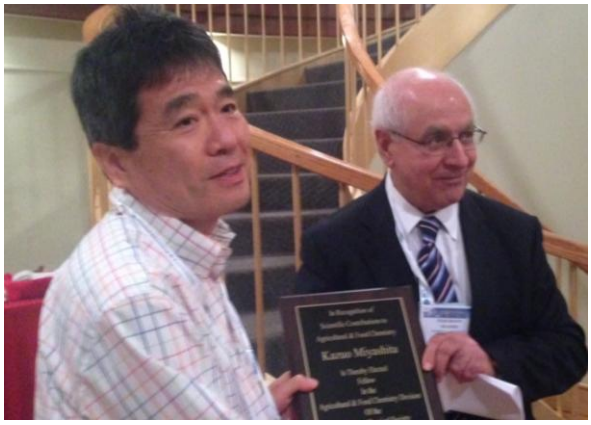
AGFD congratulates all these awardees and looks forward to their continued successes and contributions.

SCENES FROM BOSTON



above - Participants in the 2015 AGFD Division Award Symposium honoring Dr. Andrew Taylor. (from left) Kathryn Deibler (symposium organizer), Neil Da Costa, Gary Reineccius, Lewis Jones, Andrew Taylor, Gary Beauchamp, Jean-Luc Le Quere, Masayuki Yabuki. Don Mottram also participated but is camera shy.

below – clockwise from upper left - Lili He (Young Scientist Award Winner) & Charlie Brine, Kazuo Miyashita & Fereidoon Shahidi, Mike Appell, Alyson Mitchell, Neil Da Costa, Kathryn Deibler & Wally Yokoyama



Executive Committee Meeting Minutes

Sunday, August 26, 2015 Massachusetts Convention Center, Boston, MA

Takes place at each ACS National Meeting

Attendees: Terry Acree, Michael Appell, Charles Brine, Anthony Clark, Neil Da Costa, Kathryn Deibler, Indika Edirisinghe, John Finley, Kevin Goodner, Lauren Jackson, Jahan Marcu, Alyson Mitchell, Robert McGorrin (on phone), Michael Morello, Bosoon Park, Ezra Pryor, Michael Qian, Agnes Rimando, Gavin Sacks, Fereidoon Shahidi, Mathias Sucan, Stephen Toth, Michael Tunick, Lucy Yu

AGFD Chair Kathryn Deibler called the meeting to order at 5:02 p.m. She noted that Robert McGorrin was listening to the meeting by conference call.

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

Stephen Toth distributed the **Treasurer's Report**. AGFD received $11,840 in dues and a $29,620 allotment from ACS. The revenues this year have been $69,200 and expenses $37,700. Investments gained $31,500. The total in the treasury is $694,350. The Denver meeting cost $26,360, though $30,000 was allocated. The Boston budget was $50,000.

Bosoon Park distributed the **Program Report.** AGFD has 17 symposia, 34 sessions, and 335 papers, including 119 posters and 32 Sci-Mix posters. Seventeen presentations were withdrawn and there were 20 registrations sponsored by the division. Kathryn Deibler said that the MAPS abstract system wanted the list of symposia for the March 2016 San Diego meeting by June 29 so it could be published in C&EN in August. John Finley pointed out that co-sponsorship of a symposium, even if nominal, gives us credit for attendance. Having symposia within the meeting theme also helps. Steve Toth proposed a $37,000 budget for San Diego, and the motion passed. The theme will be Computers in Chemistry and 14 symposium proposals have been submitted with three pending. A Caribbean Cuisine program by Gavin Sacks will take place in San Diego, instead of having a Colonial Cuisine program in Boston. Ten symposia have been proposed for Philadelphia in August 2016 and five for San Francisco in April 2017, with two pending for each. The theme for Washington, DC in August 2017 will be Chemistry's Impact on the Global Economy and theme for New Orleans in March 2018 will be Food, Energy, and Water. Michael Qian reviewed the four symposia that AGFD will have at Pacifichem in December. He also said that he, Fereidoon Shahidi, and Steve Toth will help organize the IFF Flavor Conference in Colombia in 2017. Steve Toth and Fereidoon Shahidi will help organize the final Greek Flavor Conference in 2016.

A **Subdivision** report was sent by Youngmok Kim, Functional Foods & Natural Products Chair. They organized two symposia in Boston and will have one or two in Philadelphia. Indika Edirisinghe reported that the Nutrition Subdivision held a symposium in Boston and would like to co-sponsor one with CARB. Food Safety Chair Lauren Jackson reported that they also held a symposium in Boston and plan one for San Diego. No reports were received from the Flavor and Biotechnology Subdivisions.

Ezra Pryor and Jahan Marcu reported on **Cannabis Chemistry** and possibly becoming a subdivision of AGFD. They are going to have a symposium in San Diego and are looking for 178 signatures from ACS members for taking the next step to becoming a division. Terry Acree pointed out that all subdivisions are involved in organizing symposia and publishing papers. He would like to have scientists come together and form a subdivision instead of forming it first and then attracting scientists. Ezra Pryor said that the group is attracting corporate sponsors and that they have a poster with SCHB in Sci-Mix.

Lauren Jackson reported that our **Strategic Planning** session will be next year, possibly just before or after the San Diego meeting, with 12 people. Mike Morello said that ACS feels that the sessions are more effective outside of the national meeting. He moved that we set aside $12,000 for this session, and the motion was passed.

continues on next page

continued from previous page

Mike Appell, John Finley, Mike Morello, and Agnes Rimando gave the **Councilor's Report.** Agnes Rimando said that ACS is actively going international. There are now ACS international offices in India and China. The International Activities Committee (IAC) is moving on International Chapters, with 11 approved and five to be presented to Council on Wednesday. IAC and DAC created a task force to look at international activities/engagements of ACS Technical Divisions. As IAC contact for the task force, Agnes wrote a white paper on international activities, which was approved at the IAC Executive Committee meeting on Saturday. The white paper will be passed on to DAC. International Student Chapters, which was stated as a pilot program in 2013 by SOCED, has been approved as a permanent ACS program this year. The pilot program started with six International Student Chapters, including two that AGFD chartered in Munich and Italy. There are now 15 international student chapters from 13 countries. Agnes Rimando circulated a copy listing these chapters. Kathryn recognized Charles Brine and Michael Tunick for being ChemLuminary Award finalists for this effort.

Mike Appell reported that the petition to allow preferential voting and a procedure for removing members will be voted upon at this meeting. ACS dues will increase $15 a year for the next five years. Mike Morello reported that IPG grants will require a poster to be presented, probably at the Divisional Activities Committee reception and Sci-Mix. Brazil, China, and India are being pushed for outreach. He is on a task force for employment and is rotating off the DAC. Rodney Bennett, another AGFD member, will be the new DAC Chair.

In **Awards**, Mike Morello said that the Kavli Award needs divisions to nominate people. Kathryn Deibler said that our Young Scientist winner will be nominated. She reported on the Awards Committee meeting held earlier in the day, saying that criteria should be clearly defined and that diversity should be increased in the nominations, which should reflect the geography and demographics of the division. Mike Morello will take over as Awards Chair. The Award for the Advancement of Application of Agricultural and Food Chemistry was won by Andy Taylor of Mars, Inc., who will be honored at a symposium on Tuesday. The AGFD Distinguished Service Award was won by Wally Yokoyama. Charles Brine reported that the Young Scientist Award will be announced at the banquet on Tuesday. (The winner was Lili He, University of Massachusetts-Amherst). Mike Appell reported that the Kenneth Spencer Award was won by Thomas Selby of DuPont, who will have a symposium in his honor Wednesday morning and a ceremony in Kansas City on October. Mike Appell won an ACS Fellow Award. Winners of awards announced at the Spring Meeting were reviewed.

Editor Carl Frey sent a report saying the current issue of the **Cornucopia** was the largest ever.

Mike Tunick and Charlie Brine reported that our **International Student Chapters** are expanding and are planning a symposium for Philadelphia. Their official name is "AGFD Affiliate ACS Student Chapters."

In **Hospitality/Public Relations,** Charlie Brine organized the banquet for this meeting at the Villa Victoria Center for the Arts and is working on a place for the reception in San Diego.

Membership Chair Lucy Yu said that AGFD had 2733 members, a loss of 100 since 2014. Membership retention will be covered at the Strategic Planning Conference. Agnes Rimando pointed out that new members get a free year of ACS membership if they publish five papers in ACS journals, and Mike Morello said that new members from Brazil, China, and India get three free years in a limited program. He moved to give free AGFD membership for these people if they choose to join AGFD, and the motion was passed.

Mike Qian gave the **Nominations** report. The slate of officers consists of Bosoon Park, Chair, Navindra Seeram, Chair-Elect, and Brian Guthrie, Vice-Chair, with Michael Tunick as Secretary and Stephen Toth as Treasurer. Mathias Sucan and Terry Acree will again be Executive Committee Members At-Large. The slate was approved.

The **Journal** report was written by new Editor-In-Chief Thomas Hofmann and read by Kathryn Deibler. There were 6207 submissions in 2014 and 1483 papers were accepted. Almost 85,000 citations were

continues on next page

continued from previous page

made of JAFC papers. The time from submission to acceptance is averaging 83 days. The scope has changed somewhat and a new Associate Editor was added in March. John Finley added that Thomas is doing a great job and that James Seiber is owed a debt of gratitude for the job he did.

Mike Appell gave a report about the **Communications Committee.** The four main ways we communicate with members are by e-mail blast, Facebook, web site, and Cornucopia. We have 170 web site members, and the site is updated within a few days after he receives ne information. ACS webinars are now being done in Spanish, and C&EN is being translated into that language. Alyson Mitchell said that announcements should be sent to her for e-mail blasts.

Mike Tunick reported that the revised **Bylaws** were approved by the membership with no dissenting votes and that they will be voted on at the Business Meeting Tuesday.

There was no **Old Business** or **New Business**.

The meeting adjourned at 7:13 p.m. *Submitted by Michael Tunick, AGFD Secretary*

Annual AGFD Business Meeting Minutes

Tuesday, August 18, 2015 Massachusetts Convention Center, Boston

Takes place at each Fall National Meeting and is open to all AGFD members

Attendees: Terry Acree, Mike Appell, Keith Cadwallader, Neil Da Costa, Kathryn Deibler, Robert McGorrin, Alyson Mitchell, Mike Morello, Navindra Seeram, Fereidoon Shahidi, Mathias Sucan

--- AGFD Chair called the meeting to order at 12:00 p.m.

--- A motion to approve the new **bylaws** was made and the bylaws were approved.

--- A motion to accept the slate of **officers** was made and the slate was approved.

--- Kathryn Deibler summarized the **Executive Committee** meeting.

In **New Business**, the group discussed having a provision that any official activity of the Division (e.g. awards banquet) cannot be moved without notifying the executive committee, and especially the program organizing committee, as soon as possible. Notification of changes needs to be published on the AGFD website at least one week prior to the meeting.

Meeting adjourned 12:10 PM *Submitted by Alyson Mitchell*

Schedule of AGFD Technical Sessions

SUNDAY MORNING March 13

Bioactives & Neurodegenerative Diseases Section A US Grant Hotel Celestial Ballroom

H. Ma, N. P. Seeram, Organizers, Presiding

8:00 Introductory Remarks.

8:15 1. Role of polyphenols in promotion of healthy brain aging and Alzheimer's disease preventative initiatives. G.M. Pasinetti

8:45 2. Curcumin bioavailability and potential for prevention of neurodegenerative disease. G.M. Cole, S.A. Frautschy

9:15 3. Neuroprotective effects of the extra-virgin olive oil component oleocanthal in Alzheimer's disease. A. Kaddoumi

9:45 Intermission.

10:00 4. Maple syrup extract inhibits the beta-amyloid and tau oligomerization of Alzheimer's disease. D.F. Weaver, C. Hawco, Y. Wang, M. Taylor

10:30 5. Withanamides in aswagandha botanical to treat and prevent Alzheimer's disease. M.G. Nair

11:00 6. Blueberry fruit supplementation in human cognitive aging. R. Krikorian

Flavor Chemistry of Alcoholic Beverages Section B US Grant Hotel Grant Hall
M. Granvogl, K. Tandon, Organizers, Presiding
8:00 Introductory Remarks.
8:05 7. Unraveling the key aroma compounds of different types of beer: Are differences in aroma profiles caused by quantitative or qualitative differences in key odorants? P.H. Schieberle
8:35 8. Hop, the spirit of the beer. M.C. Qian
9:05 9. Odor-active compounds in novel special flavor hop cultivars and their impact on beer aroma. M. Steinhaus, S. Neiens
9:35 Intermission.
10:00 10. Options to mitigate sunstruck-flavor formation in beer. S. Stingl, P.H. Schieberle
10:30 11. Characterizing aroma components of rum. C. Ickes, K.R. Cadwallader
11:00 12. Cachaça flavour. A.R. Alcarde, J. Piggott
11:30 Concluding Remarks.

Undergraduate Symposium Section C US Grant Hotel Crystal Ballroom
C. J. Brine, Organizer, Presiding
8:00 Introductory Remarks.
8:05 13. Bioproduction and anti-inflammatory activity of delta-tocotrienol enriched extracts from hairy roots of annatto. J. Creameans, K. Vellanki, M. Dolan, F. Medina-Bolivar
8:35 14. Quinone intermediate mediates the cytotoxicity effects of tert-butylhydroquinone (TBHQ). E. Sukamtoh
9:05 15. Selectivity of separation of natural antioxidants in gradient reversed-phase liquid chromatography. M. Palmieri, P. Cesla, F. Pellati
9:35 Intermission.
9:50 16. Effect of elemental sulfur and yeast strain on hydrogen sulfide production in wine post-bottling. E. Friedberg, G.L. Sacks
10:20 17. Structure-property study of the selective Raman spectroscopy detection of fusaric acid and analogs. E. Martinez Rosado, M. Appell, L.E. Orellana
10:50 18. Determination of the effect of dissolved oxygen on the rate of oxidation presented by trans-2-nonenal in beer. D. Kazal, W.H. Steel
11:20 Concluding Remarks.

Advances & Applications in Water Sensing Technologies for Drinking Water, Reuse, Agri-Tech & Research
Sponsored by ENVR, Cosponsored by AGFD

SUNDAY AFTERNOON March 13
Bioactives & Neurodegenerative Diseases Section A US Grant Hotel Celestial Ballroom
H. Ma, N. P. Seeram, Organizers, Presiding
1:00 Introductory Remarks.
1:05 19. Actions of bioactive phytochemicals in neuropathology. R. Hartman
1:35 20. Phenolic-enriched maple syrup extract shows neuroprotective effects in murine microglial cells and delays β-amyloid aggregation induced neurotoxicity and paralysis of Caenorhabditis elegans. H. Ma, W. Liu, P.P. Nahar, N. DaSilva, Z. Wei, P.P. Pharm, D.A. Vattem, N.P. Seeram
2:05 21. Back to the future: Using phenotypic screening to identify Alzheimer's disease (AD) drug candidates. P. Maher
2:35 Intermission.
2:50 22. Potential beneficial effects of a diet with walnuts in Alzheimer's disease. A. Chauhan, V. Chauhan
3:20 23. Bioactive compounds in dairy products and their relation to neurodegenerative disease. M.H. Tunick, D.L. Van Hekken, P.M. Tomasula
3:50 24. Assessment of the ability of dietary soy to impact age-related neurodegeneration. J. Deshane, S. Meleth, L. Wilson, S. Barnes, H. Kim
4:20 Concluding Remarks.

Flavor Chemistry of Alcoholic Beverages Section B US Grant Hotel Grant Hall
M. Granvogl, Organizer K. Tandon, Organizer, Presiding P. H. Schieberle, Presiding
1:00 Introductory Remarks.
1:05 25. Non-volatile profiling of cask aged spirits using UHPLC/QTOF-MS. T.S. Collins
1:35 26. Unraveling differences in key aroma compounds of a commercial American bourbon whiskey und a scotch single malt whisky by means of the sensomics concept. V. Mall, P.H. Schieberle
2:05 27. From the fruit to the spirit: Changes of key aroma compounds in pears and pear brandy. M. Granvogl, B. Willner, P.H. Schieberle

2:35 Intermission.
3:00 28. Identification of compounds that contribute to trigeminal burn of alcoholic spirits. S. Kokkinidou, D.G. Peterson
3:30 29. Grape pathogenesis related proteins (PRPs) – a factor responsible for low tannin extraction during winemaking. G.L. Sacks, L. Chen, L.F. Springer
4:00 Concluding Remarks.

Graduate Student Symposium Section C US Grant Hotel Crystal Ballroom
C. J. Brine, Organizer, Presiding
1:00 Introductory Remarks.
1:05 30. Anti-obesity and anti-hyperlipidemic effect of Gynostemma pentaphylla saponins and the possible mechanisms. J. Liu, H. Shi, X. Sun, L.L. Yu
1:35 31. Kafirin protein and its applications in nano-encapsulation, pickering emulsion and electrospinning fiber. J. Xiao, Q. Huang
2:05 32. Physicochemical modification of an immunostimulatory gluten peptide and the potential implications for Celiac disease. C. Van Buiten
2:35 Intermission.
2:50 33. Chemical modification of poultry feather keratin for biobased wood adhesive applications. N. Bandara, J. Wu
3:20 34. Advanced analytical techniques for the phytochemical investigation of essential oils. R. Tardugno, F. Pellati, S. Benvenuti
3:50 35. Colorimetric detection of Escherichia coli in drinking water based on bacteriophage infection. J. Chen, V.M. Rotello, S.R. Nugen
4:20 Concluding Remarks.

Advances & Applications in Water Sensing Technologies for Drinking Water, Reuse, Agri-Tech & Research
Sponsored by ENVR, Cosponsored by AGFD

MONDAY MORNING March 14
Bioactives & Neurodegenerative Diseases Section A US Grant Hotel Celestial Ballroom
H. Ma, N. P. Seeram, Organizers, Presiding
8:00 Introductory Remarks.
8:15 36. Dietary bioactives and neurocognitive function: The case for curcumin. A. Scholey, K. Cox
8:45 37. Identifying ache inhibitors as bioactives from Chinese herbal medicine. J. Xu
9:15 38. Evaluation of three tropical fruits on lifespan and experimentally induced neurodegeneration in Caenorhabditis elegans. K.C. Borges, J.C. Azevêdo, M.F. Bezerra, R. Crews, R.T. Correia, D.A. Vattem
9:45 Intermission.
10:00 39. Experimental and theoretical studies toward the development of new amyloid inhibitors against amyloid-β aggregation. J. Zheng
10:30 40. Neuroprotective effects of urolithins, pomegranate ellagitannin-gut microbial derived metabolites: In silico, in vitro, and in vivo studies. D.B. Niesen, T. Yuan, H. Ma, N. Shah, W. Liu, R. Crews, D. Vattem, N.P. Seeram
11:00 41. Metabolomics of urinary metabolites as well as in grape seed bioactives that may have a role in postmenopausal neurodegeneration. J. Cutts, L. Wilson, S. Barnes, H. Kim
11:30 Concluding Remarks.

Flavor Chemistry of Alcoholic Beverages Section B US Grant Hotel Grant Hall
K. Tandon, Organizer M. Granvogl, Organizer, Presiding M. Steinhaus, Presiding
8:00 Introductory Remarks.
8:05 42. Typicity of great Chardonnay wines, evidence for new potent markers. J. Gros, A. Marchal, V. Lavigne, V. Moine, P. Darriet
8:35 43. Unravelling fruitiness in Vitis vinifera cv. Carmenere red wines. E. Agosin, C. Pavez, M. Espinoza
9:05 44. Synergistic effects of copper and pH - wine making variables that significantly impact reductive aromas in wines. M.Z. Bekker, M.E. Smith, A. Mierczynska-Vasilev, P.A. Smith, E. Wilkes
9:35 Intermission.
10:00 45. Impact of vineyard exposure to smoke on wine composition and sensory properties. L. van der Hulst, C. Ford, R. Burton, R. Ristic, N. Lloyd, Y. Hayasaka, P. Boss, K. Wilkinson
10:30 46. Relating sensory attributes, notably 'tropical fruit' flavour, and volatile chemical composition in Chardonnay wines. D.L. Capone, A. Barker, P. Williamson, L. Francis
11:00 47. Role of selected microbial dehydrogenases in the synthesis of flavor compounds. S. Kermasha
11:30 Concluding Remarks.

Cannabis: Exploring the Chemistry, History & Future Section C US Grant Hotel Crystal Ballroom
Cosponsored by CHAS and SCHB R. W. Phifer, E. M. Pryor, Organizers J. Marcu, Organizer, Presiding
8:00 Introductory Remarks.
8:05 48. Building a subdivision at the ACS: Sowing the seeds of change. E.M. Pryor, J. Marcu, M.J. Wilcox
8:35 49. Potency trends in confiscated cannabis and analytical methods. M.A. Elsohly
9:05 50. Responsible cultivation policy: Preserving personal cultivation rights while regulating commercial cultivation as agriculture. K. Nevedal, J. Marcu
9:35 Intermission.
9:55 51. Improving quality control methods for cannabis using flash chromatography. J. Marcu, J.P. Kababick, M.J. Wilcox, M. Jacyno
10:25 52. Cannabis: Taxonomy and secondary metabolism. J. Fischedick
10:55 Panel Discussion.

MONDAY AFTERNOON March 14
Bioactives & Neurodegenerative Diseases Section A US Grant Hotel Celestial Ballroom
H. Ma, N. P. Seeram, Organizers, Presiding
1:00 Introductory Remarks.
1:05 53. Laboratory preparations of vinaxanthone and xanthofulvin, natural products enhancing CNS regeneration. D. Siegel
1:35 54. Salvia divinorum: A unique CNS active plant. T.E. Prisinzano
2:05 55. Discovery of anti-Alzheimer agents from Chinese herbal medicine. Q. Gu, J. Xu
2:35 Intermission.
2:50 56. Fungal metabolome as a rich resource for tau aggregation inhibitors. S.R. Paranjape, Y. Chiang, C.C. Wang, B.R. Oakley, T.C. Gamblin
3:20 57. Disaggregation of amyloid beta peptides by tabersonine and related compounds: Biophysical, bioanalytical, and cytotoxicity studies. T. Kai, L. Zhang, G.B. Yagnik, A. Jing, B. Zhao, F. Zhou
3:50 58. Efficient synthesis and neuroprotective activity of CN2097: A cyclic disulfide polyarginine peptidomimetic binding PDZ domain of PSD-95. R.K. Tiwari, S.R. Kotla, J. Marshall, D.J. Goebel, K. Parang
4:20 Concluding Remarks.

Advances in Food Peptide & Food Protein Research: Nutrition, Functionality & Food Safety
Section B US Grant Hotel Grant Hall Y. Zhang, Organizer, Presiding
1:00 Introductory Remarks.
1:05 59. Applied peptidomics and digestomics to guide protein nourishment in infants for optimal gut health. D. Dallas
1:30 60. Alpha-lactalbumin-catechin conjugates improve the chemical stability of the vitamin A precursor β-carotene in nanoemulsions. J. Yi, Y. Zhang, L. Zhao
1:55 61. Bioactive peptides generated from plant proteins in relation to molecular structures. L. Chen, Z. Tian
2:20 62. Ovomucin derived peptides as anti-adhesive agents against infectious diseases. X. Sun, M. Gänzle, J. Wu
2:45 63. New tree nut allergens. Y. Zhang, W. Du, B. Lee, Y. Fan, S. Lyn, K. Nadeau, T.H. McHugh
3:10 Intermission.
3:25 64. Studies on the mechanism of calcium ion on the allergenic activity of EF-hand domain food-induced allergen. S. Han, H. Che
3:50 65. Influence of free amino acids, oligopeptides and polypeptides on the formation of pyrazines in Maillard model systems. G. Leonardo Scalone, P. Lamichhane, T. Cucu, N. De Kimpe, B.E. De Meulenaer
4:15 66. Cold-adapted β-galactosidase from a psychrotrophic bacterium Rahnella sp. R3: Protein structure and enzymatic properties. Y. Fan, Y. Zhang, R. Yang
4:40 67. Structural modification of an immunodominant gluten peptide upon interaction with (-)-epigallocatechin-3-gallate. C. Van Buiten, C.N. Pacheco, E. Hatzakis, R. Elias
5:05 Concluding Remarks.

Cannabis: Exploring the Chemistry, History & Future Section C US Grant Hotel Crystal Ballroom
Cosponsored by CHAS and SCHB J. Marcu, R. W. Phifer, Organizers E. M. Pryor, Organizer, Presiding
1:00 Introductory Remarks.
1:05 68. Navigating the ever changing regulations and rules of the cannabis industry. C. Ludwig
1:35 69. Review of Bedrocan science: Patient-inspired and science-based. A. Hazekamp
2:05 70. Consumer safety and an accredited laboratory. S.A. Audino
2:35 Intermission.
2:55 71. Results from auditing medical cannabis operations in the United States. J. Marcu, S. Sherer, K. Nevedal

3:25 72. Understanding cannabis diversity in today's medical applications. J.C. Raber
3:55 73. Beyond cannabis and anandamide. R. Mechoulam
4:25 Panel Discussion.

MONDAY EVENING March 14 8:00 - 10:00pm
Sci-Mix/Agricultural & Food Chemistry Undergraduate Research Posters San Diego Convention Center Halls D/E
Sponsored by CHED, Cosponsored by AGFD and SOCED B. Park, Organizer
3, 8, 49, 59, 67, 71. See previous listings.
78, 96, 102, 110-111, 122, 136-137, 143, 158-159, 161, 166, 168, 186, 191. See subsequent listings.

TUESDAY MORNING March 15
Applied Nanotechnology for Food & Agriculture Section A US Grant Hotel Celestial Ballroom
M. Appell, S. R. Nugen, B. Park, Organizers, Presiding
8:00 Introductory Remarks.
8:05 74. Metal oxide nanoparticles for destructing dyes and bacteria. Y. Mao
8:35 75. Applications of nanoporous cyclodextrin polymers to prevent exposure to mycotoxins. M. Appell, M.A. Jackson, K. Evans
9:05 76. Enzyme nanotechnology: Moving towards next-generation biocatalytic materials for food applications. J.M. Goddard, J. Talbert
9:35 Intermission.
9:50 77. Comparative study of b- and g-cyclodextrin as ionophores in potentiometric sensors for naltrexone and some applications of ionophore in chemical sensors. G.A. Mostafa
10:20 78. Colorimetric detection of Escherichia coli based on the enzyme-induced metallization of gold nanorods. J. Chen, A. Jackson, V.M. Rotello, S.R. Nugen
10:50 79. Functionalization of biopolymer silver nanosubstrates for pathogen detection. J. Chen, B. Park
11:20 Concluding Remarks.

Public Health Perspectives of Mycotoxins in Food Section B US Grant Hotel Grant Hall
Cosponsored by AGRO and ANYL L. Jackson, D. Ryu, Organizers, Presiding
8:00 Introductory Remarks.
8:05 80. Short history of mycotoxin research. J. Pitt
8:55 81. Climate variability and mycotoxin exposure. J. David Miller
9:35 Intermission.
9:50 82. Worldwide occurrence of mycotoxins in foods. D. Ryu, H. Lee
10:20 83. Emerging mycotoxins: Beyond traditionally determined food contaminants. F. Berthiller, E. Varga, M. Sulyok, R. Krska
10:50 84. Aflatoxin and child growth: The critical first 1000 days of life in underdeveloped world regions. P.C. Turner
11:20 Concluding Remarks.

Chemical Modification of Natural Bio-based Material: Design & Application for Value Added Products
Section C US Grant Hotel Crystal Ballroom S. Chang, Organizer, Presiding
8:00 Introductory Remarks.
8:05 85. Effects of mechanical strain on average orientation and packing of polymeric constituents in onion epidermis cell walls. K. Kafle, Y. Park, S. Huang, D. Cosgrove, S.H. Kim
8:25 86. Swine odor removal with biochar. O. Hwang, S. Cho, D. Han, K. Ro
8:45 87. Thermally reprocessible polylactic acid grafted cellulose nanocrystal films through reactive extrusion process. P. Dhar, D. Tarafdar, A. Kumar, V. Katiyar
9:05 88. Chitosan-based multilayer nanocoatings that exhibit high gas barrier and flame retardant behavior. J.C. Grunlan
9:25 Intermission.
9:40 89. Investigation of solvent systems and potential applications of soy proteins. G. Sun, A. Aghanouri
10:00 90. Ammonia and hydrogen sulfide removal using biochar. K. Ro, I.M. Lima, G. Reddy
10:20 91. Effects of processing conditions on the structure of enzymatic modified soy protein isolate-based bioplastics. E. Zadeh
10:40 92. Mountain beetle pine infestation: Characterization of the polar components for Lodge pole pine (pinus contorta) acetone extractives. R.K. Moore
11:00 93. Innovative technologies for anti-flammable cotton fabrics. S. Chang, B.D. Condon
11:20 Concluding Remarks.

Cannabis: Exploring the Chemistry, History & Future Spons:SCHB, Cospons:AGFD, CHAS and ORGN

TUESDAY AFTERNOON March 15

Applied Nanotechnology for Food & Agriculture Section A US Grant Hotel Celestial Ballroom
M. Appell, S. R. Nugen, B. Park, Organizers, Presiding
1:00 Introductory Remarks.
1:05 94. Ultra-small-angle x-ray scattering study of zein self-assembly. S. Uzun, G. Padua
1:35 95. Isolation, characterization and anti-proliferative activities of Picroside compounds present in Picrohiza kurroa, (kutki) extract. B. Dayal, T. Roy, M.A. Lea, S. Patel, S. Ali, S. Li
2:05 96. Development and characterization of functionalized TiO2/polylactic acid nanocomposite films for food packaging applications. N. Baek, S. Duncan , Y. Kim, J. Marcy, S.F. Okeefe
2:35 Intermission.
2:50 97. Targeted delivery system based on chitosan and sulfated β-glucan for the colon. C. Yucel, J. Sotres, A. Rascon, J. Risbo, M. Cardenas
3:20 98. Dual-enzyme nanobiocatalyst for the cascade conversion of cellulose to fructose via a glucose pathway. C. Lai, D.R. Radu, G. Ozbay
3:50 Concluding Remarks.

Public Health Perspectives of Mycotoxins in Food Section B US Grant Hotel Grant Hall
Cosponsored by AGRO and ANYL L. Jackson, D. Ryu, Organizers, Presiding
1:00 Introductory Remarks.
1:05 99. Urinary biomarkers for human multi-mycotoxin exposure. M. Solfrizzo, L. Gambacorta, A. Logrieco
1:35 100. Risk of exposure to multiple mycotoxins from maize based complementary foods in Tanzania. A. Kamala, M. Kimanya, C. Lachat, L. Jacxsens, J. Ortiz, G. Haesaert, P. Kolsteren, B. Tiisekwa, B.E. De Meulenaer
2:05 101. Fumonisin exposure in women linked to inhibition of an enzyme that is a key event in farm and laboratory animal diseases. R.T. Riley, K. Voss, J.L. Showker, T. Mitchell, O. Torres, J. Matute, S.G. Gregory, A.E. Ashley-Koch, J.R. Maddox, J. Gelineau-van Waes
2:35 Intermission.
2:50 102. DNA Adduction by ochratoxin A: Insight for mechanism of action and aptasensor development for mycotoxin detection. R.A. Manderville
3:20 103. Mycotoxins at the blood-brain barrier: Metabolism, toxicity, barrier integrity and transfer to the brain. M. Behrens, S. Hüwel, H. Galla, H. Humpf
3:50 104. Renal gene expression changes in mice and rats exposed to dietary ochratoxin A. A. Nunnikhoven, I. Curran, A. Gannon, Z. Gillespie, L. Coady, C. Qiao, V. Liston, D. Lefebvre, N. Ross, R. Mehta, G. Bondy
4:20 Concluding Remarks.

Metabolomics in Agriculture & Food Chemistry: Current Status & Future Scope
Section C US Grant Hotel Crystal Ballroom S. Chakraborty, Organizer, Presiding
1:00 Introductory Remarks.
1:10 105. FlavonQ: An automated data processing tool for profiling flavone and flavonol glycosides with ultra-high-performance liquid chromatography−diode array detection−high resolution accurate mass−mass spectrometry. P. Chen, M. Zhang, J. Sun
1:55 106. Taking metabolomics beyond primary metabolism - challenges and opportunities for capturing plant chemical diversity. B.M. Lange, S.R. Johnson
2:40 Intermission.
2:55 107. Second-generation metabolomics in food research: Merging untargeted and targeted data acquisitions for food and exposome analysis. O. Fiehn
3:40 108. Breast milk or infant formula: Consequences for the microbiome and metabolome. C. Slupsky
4:25 109. Metabolomics for understanding the plant chemistry: Comparison of lipid extraction methods for lipid profiling in algae. N. Kaushik, T. Kind, O. Fiehn
4:50 Concluding Remarks.

General Posters Section C San Diego Convention Center Halls B/C
B. Park, Organizer
3:00 - 5:00
110. Comparison of volatile compounds in fermented rice broths. H. Lim, S. Lee, Y. Roh, J. Lee, B. Eum, J. Chang, Y. Kim
111. Crystal structure and catalytic mechanism proposal of cellobiose 2-epimerase from Caldicellulosiruptor saccharolyticus DSM 8903. Q. Shen, Y. Zhang, R. Yang, S. Pan

112. Inhibition of formation of advanced glycation end-products by an oligosaccharide-enriched fraction purified from cranberry (Vaccinium macrocarpon). J. Sun, H. Ma, W. Liu, J. Dain, D.C. Rowley, N.P. Seeram
113. Advanced glycation endproducts inhibitory compounds from amla (Phyllanthus emblica). K.N. Rose, C. Wan, H. Ma, W. Liu, N.P. Seeram
114. Antibacterial properties of common herbs and spices. B. Lipinski, D.F. Moriarty
115. Pea protein isolate as a natural nanocarrier for enhanced dispersibility and stability of curcumin. S. Chen
116. New approaches to the preparation and characterization of tormentic acid. E.J. Parish, H. Honda, T. Wei, J. Wu, H. Ho
117. Novel approaches to the chemical synthesis and biological activity of 24-ketolanosterol an inhibitor of HMG-CoA reductase. E.J. Parish, J. Yin, H. Honda, T. Wei, H. Yin
118. Facile synthesis and carbon-13 nuclear magnetic resonance spectral properties of cholest-4-en-3,6-dione. E.J. Parish, H. Honda, T. Wei, H. Shyu
119. Novel approaches to the chemical synthesis and spectral characterization of hydroxysterols. Y. Lo, H. Shyu, W. Huang, H. Honda, T. Wei
120. Chemical synthesis and characterization of lanosterol derivatives, inhibitor of cholesterol biosynthesis. E.J. Parish, W. Huang, H. Honda, T. Wei, H. Shyu
121. Novel preparation and characterization of kinsenoside. E.J. Parish, J. Wu, H. Ho, H. Honda, T. Wei
122. Elucidation of changes in non-volatile metabolites of amylolytic yeast, Saccharomycopsis fibuligera, according to the cultivation times. J. Jeong, N. Lee, Y. Kim
123. Microbial synthesis of myrcene by metabolically engineered Escherichia coli. E. Kim, J. Eom, Y. Um, Y. Kim, H. Woo
124. Structure activity related, mechanistic, and modeling studies of gallotannins containing a glucitol-core and a glucosidase. H. Ma, L. Wang, D.B. Niesen, W. Tan, Q. Gu, J. Xu, N.P. Seeram
125. Anti-glycative, reactive carbonyl scavenging and anti-amyloid fibrillation effects of ayurvedic medicinal plants. W. Liu, H. Ma, L. Zhang, C. Wan, J. Dain, N.P. Seeram
126. Vapor-Infusion of wine flavor volatiles in specialty dark chocolate and analysis via GC-MS. S. Richards, R. MacFarland, P.J. Iles, L.D. Giddings, M. Alvarez, R.V. Valcarce, R. Holcomb, N.R. Bastian
127. Pesticide mobility in soils: An initial characterization comparing productive vs non-productive soils. G.A. Querejeta, E.P. Beiguel, E.A. Hughes, J. Montserrat, A. Zalts
128. Evaluation of immunogenicity of hepatitis b vaccine referred to the clinic. E. Rezaei
129. Effect of pH and xanthan-locust bean mixtures on the physicochemical properties of whey protein-stabilized oil-in-water emulsions. C. Owens, H. Khouryieh, K. Williams
130. Comparison of a brewer's water analysis kit to standardized methods and implications for brewing. N.O. Flynn, D. Reasoner, J. Read, P.T. Baumgardner
131. Survey of amino acid composition in cider apples grown in Virginia by UPLC-PDA. S. Ma, G. Peck, A. Stewart
132. Physicochemical properties of amorphous granular starches prepared from corn, tapioca and non-waxy rice starches using high hydrostatic pressure. J. Choi, M. Song, B. Kim, M. Baik
133. Effects of processing and storage temperature on browning index, furosine, and HMF in aseptic cold break tomato paste during storage time. H. Yeom, J. Conte, R. Mohammed, S. DeMuri
134. Effects of storage and heating on serum viscosity of hot break tomato paste. H. Yeom, A. Janosko, M. Ramirez, S. DeMuri
135. Determination of ceftiofur and its metabolites in plasma using reverse-phase liquid chromatography. S. Cox, M. White, K. Gordon, J. Bailey
136. Reversed-phase high performance liquid chromatography (HPLC) studies of the sweet diterpene glycosides isolated from Stevia rebaudiana bertoni. V. Chaturvedula, S. Meneni
137. Analysis of volatile flavor components of steamed rice and identification of key odorants causing old rice smell. H. Takemitsu, Y. Sako, K. Shibakusa, S. Kitamura, H. Inui
138. Comparison between traditional-SERS and RCA-SERS assays for 35S promoter gene detection. B. Guven, I.H. Boyaci, U. Tamer, E. Acar-Soykut
139. Exposure estimate for semicarbazide from the use of azodicarbonamide in bread for the U.S. population. S. Bhagan, D.L. Doell, H. Lee, T. Croce, S.E. Carberry
140. Determination of total dietary fiber in extruded food products containing grape pomace. L. Hordge, J. Yu
141. Preparation of gelatin films incorporated with tea polyphenol nanoparticles for enhancing controlled-release antioxidant properties. F. Liu, W. Yokoyama, F. Zhong, Y. Li
142. Rapid front end cleanup of cannabis-infused edibles using automated flash column chromatography. M.J. Wilcox, J. Marcu, J.P. Kababick, M. Jacyno
143. Fatty acid profiles of marine fishes from Rhode Island coastal waters. M. Yurkevicius, J. Jacques, N.E. Breen, D.L. Taylor
144. Synthesis and fungicidal activity study of 2-(thiophen-2-yl)pyridine derivatives. Y. Xie, Y. Xu, Y.L. Chen, C.L. Liu

145. Design, synthesis, and biological activities of novel carboxylic ether derivatives containing oxime. Q. Wu, J. Yang, J. Zhang, G. Aiying, H. Ma, C.L. Liu
146. Herbicidal properties of substituted 3-(pyridin-2-yl)benzenesulfonamide derivatives. Y. Xie, H.W. Chi, G. Aiying, C.L. Liu, H. Ma
147. Synthesis and characterization of novel luminescent sodium carboxymethyl cellulose nanocomposites for potential safety inspection of food applications. M. Zhang, L. Qingyong, J. Ye, X. Jian
148. Characterization of pepsin-solubilized collagens and the hydrolysates from sea cucumber species. M. Saito
149. Red shortening: Characterization and utilization in formulating novel functional biscuits. H. Abou Gharbia, M.M. Youssef, M. Abd-El-Aal, N. Nabil
150. Presence of Protostrongylus stilesi in Rocky Mountain goats and the effects of infestation. C. Dunlap
151. Polyphenol-aluminum complex formation: Implications for aluminum tolerance in plants. A.E. Hagerman, L. Zhang
152. Natural soil benign bacterium with an insecticidal activity. S. Stark
153. Chemical and supramolecular structural modifications in lignin during acid catalyzed ionic liquid pretreatment: A case study of Arundo donax linn. T. You, L. Zhang, F. Xu
154. Seed-specific phosphate allocation with coordinated expression of genes involved in phosphate transport function during wheat grain development. V.K. Shukla, M. Kaur, S. Aggarwal, K. Bhati, S. Sharma, S. Mantri, A. Pandey
155. Detection of pesticides in edible oil using LC-MS analysis. S. Bhattacharya
156. Heated headspace solid phase microextraction of marijuana for chemical testing. A. Brown, J. Sweet, C.C. Yu
157. Nutritional value and total phenolics of tortillas obtained by extrusion cooking of red pigmented creole maize. A.K. Milan, C. Reyes-Moreno, J. Milan Carrillo
158. Evaluating Raman spectroscopic data by using principal component analysis to determine the freshness of fish samples. H. Temiz, H. Velioglu, I.H. Boyaci
159. Fatty acid composition as a tool for screening industrial applications of vegetable oils. B.R. Moser
160. Dolabella-3,7,18-triene:The main constituent of Nymphaea lotus essential oil. D.M. Navarro, M. Pottier, B.N. Albuquerque, A.C. Maia, F. Hallwass, A. Navarro-Vazques
161. Molecularly imprinted polymers with desorption electrospray ionization mass spectrometry for high throughput analysis of neonicotinoids pesticides in water and food. C.S. Bottaro, J. Gauthier, S. Egli
162. Chemical compositions of essential oils of Psidium guajava and Syzygium sp. and their in vitro antivirus activities. N. Mohamed, A.A. Abdalsalam, H. Osman, E.E. Kamarulzaman, H. Wahab
163. Detecting delta-9-tetrahydrocannabinol (Δ9-THC) and delta-8-tetrahydrocannabinol (Δ8-THC) by UV-HPL. K. Tseng, T. Ono, T. Hirose, K. Kimata
164. Nutritional variation and antioxidant properties of wild fruits revealed through a fluorescence-based method. S. Smith, F. Ulerio Nunez, M. Bida, T.E. Pagano
165. Using dietary preferences of wildlife to discover bioactive polyphenols in plants. D. Conner, H. Hoang, M. Fremgen, J.S. Forbey, C. Dadabay
166. Antimicrobial activity of extracts from seaweeds of northeast Brazil. P.C. Bezerra-Silva, B.N. Albuquerque, B.S. Santos, T.N. Reis, P.M. Paiva, M.V. Silva, D.M. Navarro
167. In situ analysis of interrelation between topochemistry and cellulose accessibility in poplar cell walls. X. Zhou, F. Xu, D. Ding
168. Bioassay-guided isolation of secondary metabolite inhibitors of Xylella fastidiosa produced by endophytic fungi. M. Papineau, L. D'Elia, P.E. Rolshausen, C. Roper, K.N. Maloney
169. Chemistry and mass spectral characterization of methylglyoxal adducts formed with metformin, aminoguanidine and okra seed extract: Relevance to diabetic complications. B. Dayal, R. Gohil, P. O'Connor, M.A. Lea
170. LC/MS metabolomic profiling of an amber ale fermented with four different yeast strains. C.A. Hughey, K.M. Foss, K. Fortmann
171. Antimicrobial spectrum and toxicology of a natural food grade additive obtained from avocado seed. A. Pacheco, R.C. Chávez, D.G. Rodriguez-Sanchez, R. Villarreal-Lara, M.I. Garcia-Cruz, C. Hernandez-Brenes

WEDNESDAY MORNING March 16
Natural & Modified Carbohydrate Polymers Effects on Obesity Related Metabolic Diseases
Section A US Grant Hotel Celestial Ballroom
M. Kale, Organizer M. Turowski, W. H. Yokoyama, Organizers, Presiding
8:00 Introductory Remarks.
8:05 172. Functional role of fiber in the diet: Prebiotics, metabolic benefits and beyond. C. Slupsky
8:30 173. Effects of indigestible polysaccharides on obesity related metabolic diseases and inflammation. Y. Egashira
8:55 174. Anti-obesity properties of mushroom polysaccharides: A review. M. Friedman

9:20 Intermission.
9:40 175. Polysaccharide structure and physiological effect: Glycemic and non-glycemic carbohydrates. M. Kale, B. Hamaker
10:05 176. Yeast β-glucan down-regulates blood glucose level in obesity/type 2 diabetes. X. Xu, Y. Cao, L. Zhang
10:30 177. Digestibility and health benefits of native and modified resistant starch. J. Jane, Y. Ai, M. Reed, H. Jiang, J. Hasjim, D. Birt
10:55 Concluding Remarks.

Public Health Perspectives of Mycotoxins in Food Section B US Grant Hotel Grant Hall
Cosponsored by AGRO and ANYL L. Jackson, D. Ryu, Organizers, Presiding
8:00 Introductory Remarks.
8:05 178. New strategy for the biocontrol of Fusarium verticillioides in corn based on endophytic bacterial-fungal interactions. C.W. Bacon, D.M. Hinton, T. Mitchell
8:35 179. Bioplastic formulation of beneficial microbes to control agricultural pests. H.K. Abbas
9:05 180. Reduction of fumonisin toxicity by extrusion and nixtamalization (alkaline cooking). K. Voss, D. Ryu, L. Jackson, R.T. Riley, J. Gelineau-van Waes
9:35 Intermission.
9:50 181. Mycotoxin deactivation strategies – past, presence and future. G. Schatzmayr
10:20 182. Molecular approaches for enhancing host resistance against Aspergillus flavus infection and aflatoxin contamination in corn and cottonseed. D. Bhatnagar, R. Brown, K. Rajasekaran, J. Cary, M. Gilbert
10:50 183. Tools to determine the identity, occurrence and toxicity of conjugated mycotoxins. V. Nagl, G. Adam, R. Schuhmacher, R. Krska, F. Berthiller
11:20 Concluding Remarks.

General Papers Section C US Grant Hotel Crystal Ballroom
B. Park, Organizer, Presiding
8:00 Introductory Remarks.
8:05 184. Making synthetic starch (amylose and amylopectin) from nonfood biomass. Y. Zhang
8:30 185. Effect of sulfite on the reactivity of exogenous acetaldehyde with wine flavonoids. M.K. Sheridan, R. Elias
8:55 186. Dietary flavonoid luteolin chemosensitizes ovarian cancer cells by inhibiting FAK-mediated epithelial-to-mesenchymal transition. V.P. Dia, P. Pangloli
9:20 187. Effect of cooking on saponins content in pigmented chickpea. A.K. Milan, J. Gutierrez-Uribe, S. Serna-Saldivar
9:45 Intermission.
10:05 188. Hydrophobically-modified nanoporous silica aerogel: Novel food-contact surface inhibiting adhesion of gram-negative and gram-positive bacteria. J. Oh, L. Cisneros-Zevallos, M. Akbulut
10:30 189. Bioavailability of cranberry flavonol glycosides and flavan-3-ols in healthy female adults. Y. Wang, T. Wilson, A.P. Singh, N. Vorsa
10:55 190. Inhibitory effect of Gynostemma pentaphylla saponin on adipogenesis of 3T3-L1 cells through modulating Wnt/β-catenin pathway and cell cycle in mitotic clonal expansion. J. Liu, P. Yang, H. Shi, X. Sun, L.L. Yu
11:20 191. Development of graphene based room temperature gas sensors for agricultural applications. H. Park
11:45 Concluding Remarks.

WEDNESDAY AFTERNOON March 16
Natural & Modified Carbohydrate Polymers Effects on Obesity Related Metabolic Diseases
Section A US Grant Hotel Celestial Ballroom
M. Turowski, Organizer M. Kale, W. H. Yokoyama, Organizers, Presiding
1:00 Introductory Remarks.
1:05 192. Bioactive pectic oligosaccharides and obesity. A.T. Hotchkiss
1:30 193. Prevention of metabolic diseases by HPMC, a non-fermentable fiber. M. Turowski, W.H. Yokoyama
1:55 194. Impact of processing on physicochemical properties and nutritional function of dietary fibers: Balancing consumer taste and tangible health effects. N. Bordenave
2:20 Intermission.
2:40 195. Characteristics of EGCG loaded modified starch during digestion. Y. Li, F. Wang, F. Zhong
3:05 196. Bioactive polysaccharides and gut microbiome. W.H. Yokoyama, M. Turowski
3:30 Concluding Remarks.

Public Health Perspectives of Mycotoxins in Food Section B US Grant Hotel Grant Hall
Cosponsored by AGRO and ANYL L. Jackson, D. Ryu, Organizers, Presiding
1:00 Introductory Remarks.
1:05 197. Immunochemical methods for rapid screening of (multi)mycotoxins. S. De Saeger, N. Beloglazova, I.Y. Goryacheva
1:35 198. Application of nanobodies, sensors and other immunochemical techniques for the analysis of mycotoxins and other small molecules. C.S. Bever, S.J. Gee, B.D. Hammock
2:05 199. Waveguide optical immunosensors for the simultaneous detection of melamine and aflatoxin M1 and kinetic analysis. H. Guo, X. Zhou, H. Shi
2:35 Intermission.
2:50 200. Development and evaluation of multi-mycotoxin analysis in foods by liquid chromatography-mass spectrometry (LC-MS/MS and LC-HRMS). K. Zhang, J.W. Wong, C. Liao, A.J. Krynitsky, M. Trucksess
3:20 201. FDA regulatory program for mycotoxins in food. H. Kim
3:50 202. Regulation of mycotoxins in Canada. E. Elliot, L. Pelletier, G. Bondy
4:20 Concluding Remarks.

General Papers Section C US Grant Hotel Crystal Ballroom
B. Park, Organizer B. D. Guthrie, Presiding
1:00 Introductory Remarks.
1:05 203. Withdrawn.
1:30 204. Synthesis of 1,2,4,5-tetraoxanes derived from naphtaleneacetic acid with potential herbicide activity. T.D. Silva, I. Antolinez, A. Silva, L. Barbosa, J. Boukouvalas
1:55 205. Effect of organic matter on phosphorus recovery in dairy waste. A. Silchuk, S.J. Parikh, K.M. Scow, S. Kim
2:20 206. Understanding flavor in California almonds. S. Charoenprasert, G. Huang, P. Wylie, A.E. Mitchell
2:45 Intermission.
3:05 207. Towards understanding induced resistance of ash (Fraxinus spp.) against emerald ash borer using proteomics and metabolomics. S. Chakraborty, S.O. Opiyo, A.L. Hill, D. Cipollini, D.A. Herms, P. Bonello
3:30 208. Formation of 3-MCPD fatty acid esters from monostearin and thermal decomposition of 3-MCPD mono-fatty acid ester. Y. Zhao, Y. Zhang, Z. Zhang, B. Gao, H. Shi, L.L. Yu
3:55 209. Tuning mechanical, barrier and thermal properties of poly(lactic acid) using polymorphic cellulose nanocrystals. P. Dhar, D. Tarafdar, A. Kumar, V. Katiyar
4:20 210. When in silico meets in vitro: Molecular basis of function of an anion-permeable efflux transporter from barley (Hordeum vulgare L.). A. Singh, Y. Nagarajan, M. Hrmova, Y.G. Yingling
4:45 Concluding Remarks.

AGFD Abstracts - 251st ACS Nat'l Meeting, San Diego

AGFD 1 Role of polyphenols in promotion of healthy brain aging and Alzheimer's disease preventative initiatives Giulio M. Pasinetti, giulio.pasinetti@mssm.edu. Neurology, Icahn School of Medicine at Mount Sinai, New York, NY Polyphenols are a large and diverse group of naturally occurring compounds widely distributed in many plant-derived foods and beverages. Polyphenols are receiving increasing attention for their roles in preventing the onset and progression of Alzheimer's disease (AD). In particular, preclinical evidence demonstrated the efficacy of certain polyphenols, acting individually or in combination, to modulate multiple diverse mechanisms relevant to AD, implicating the potential for novel development of polyphenols for multi-target engagement in AD. Despite the increasing efforts committed to clinical testing of polyphenols in AD, these are hindered by limited knowledge of polyphenol bioavailability, specific forms of brain-bioavailable bioactive polyphenols (including polyphenol metabolites) and their underlying mechanisms of actions. I will discuss the mechanistic implications of brain-bioavailable bioactive polyphenol metabolites in modulating key physiological processes that are relevant in early, preclinical AD. I will also summarize current efforts for the characterization of brain-bioavailable bioactive polyphenols and their potential drug-like properties for their successful clinical development into nutraceuticals. Moreover, promoting cognitive resilience and preventing cognitive deterioration in response to external stressors is one of the most difficult challenges in the promotion of healthy brain aging and the prevention of AD. Emerging evidence suggests that the promotion of resilience against psychological stress and other mood disorders by select microbiome derived polyphenol metabolites may be tightly associated with the onset and progression of AD. Based on this consideration, I will also discuss novel evidence on the role of the gastrointestinal microbiome, specifically the contributions of microbiota in modulating bioconversion and bioavailability of bioactive phenolic acids from the polyphenols. Collectively, I will critically discuss the current complex mosaic of evidence, which puts the investigation of brain-bioavailable bioactive polyphenols at the cross-roads between promotion of psychological resilience and prevention of AD cognitive deterioration, and eventually the translation of select brain-bioavailable bioactive polyphenols into therapeutic nutraceuticals.

AGFD 2 Curcumin bioavailability and potential for prevention of neurodegenerative disease Greg M. Cole, gregorycole@mednet.ucla.edu, Sally A. Frautschy. Depts of Neurology and Medicine, UCLA and GLA Veterans Affairs GRECC, Los Angeles, CA Alzheimer Disease (AD) and other neurodegenerative conditions involve protein aggregate accumulation and chronic

neuroinflammation that is implicated in both neurodegeneration and phagocytosis clearance of aggregates. This suggests immunomodulatory approaches that can limit pro-inflammatory mediators but sustain phagocytic clearance of amyloid, resolution of inflammation and "natural healing." Recent genetic data causally implicate innate immune genes like TREM2 and CD33 in AD pathogenesis while network analysis of gene expression in AD brains puts these genes in hubs central to altered gene expression in AD. Further unbiased bioinformatics analysis, implicates activation of oxidative damage and NFkB in disease pathogenesis. The curry spice curcumin is known to limit oxidative damage and NFkB activation with multiple targets and to promote resolution of inflammation and wound healing. Free curcumin meets Lipinski rules for rapid blood brain barrier penetration and effective dosing was obtained in rodent brains in a series of studies that demonstrated that curcumin can limit key soluble toxic Aβ and tau oligomers as well as AD plaque pathogenesis while promoting plaque clearance and reducing pro-inflammatory mediators. More recent results show that curcumin improves the TREM2 and related innate immune network hub gene expression implicated in AD. Despite these and other neuroprotective activities and promising anecdotal reports, initial clinical trials with curcumin as organic solvent extracts of turmeric failed to reach biomarker or clinical endpoints and failed to produce effective plasma levels of free curcumin despite high levels of glucuronidated curcumin. Since AD pathogenesis is a decades long process, effective prevention should begin early but cannot be credible without target biomarker validation. New formulations of curcumin that do produce target plasma levels of free curcumin and label retinal plaques in AD patients are now in biomarker targeted clinical trials in subjects with age-related memory impairment and AD.

AGFD 3 Neuroprotective effects of the extra-virgin olive oil component oleocanthal in Alzheimer's disease Amal Kaddoumi, kaddoumi@ulm.edu. Univ. of Louisiana at Monroe, Louisiana Alzheimer's disease (AD) is the most common cause of dementia in older people. To date, no treatment for AD is available, and available medications only provide some symptomatic relief with no clear effect on the disease, which necessitates an intense search for therapeutic agents that can prevent or delay its progression. AD is a complex disorder associated with multiple pathological processes; thus to develop an effective therapy it is preferred to be multifunctional that targets multiple processes. Studies from our laboratory and others showed that extra-virgin olive oil (EVOO) have several protective effects against AD. Oleocanthal is a naturally occurring phenolic secoiridoid isolated from EVOO. Our results from in vitro and in vivo studies in wild type and AD models demonstrated the potential of oleocanthal to prevent and/or hold the progression of AD by targeting multiple pathological processes associated with the disease including amyloid-b (Ab) reduced clearance across the blood-brain barrier and degradation, Ab aggregation, astrogliosis, synaptic loss and neuroinflammation. These findings suggest oleocanthal as a novel molecule that targets multiple mechanisms that play critical roles in the development or progression of AD. Understanding oleocanthal mechanism of action will help optimizing its clinical use and future drug development by providing new drug targets and possible mechanisms involved in AD pathology.

AGFD 4 Maple syrup extract inhibits the beta-amyloid and tau oligomerization of Alzheimer's disease Donald F. Weaver1,3, donald.weaver@uhnres.utoronto.ca, Cassandra Hawco1,3, Yan- Fei Wang2,3, Marcia Taylor2,3. (1) Chemistry, Toronto Western Research Inst., Toronto, Canada (2) Biology, Toronto Western Research inst., Toronto, Canada (3) Univ. of Toronto, Canada Alzheimer's disease (AD) is the most common type of dementia, arising from oligomerization of beta-amyloid (Abeta) and tau peptides; there are no disease stabilizing drugs for the treatment of AD. Since several natural products (resveratrol, ferulate) have anti-oligomeric properties, we sought to identify novel plant products with potential anti-AD efficacy. During our systematic search for natural product-based anti- protein misfolding agents for the putative treatment of AD, we investigated maple syrup. Maple syrup is produced by thermal evaporation of the sap from maple (Acer) trees, a process which concentrates the contained sugars as well as producing a variety of chemical reactions responsible for the distinct taste of the syrup. In addition to sugars, the collected sap contains a wide range of oligosaccharides, amino acids, polyphenols and phytohormones. Three separate extracts of maple syrup were sequentially isolated: Extract A – ethyl acetate soluble; Extract B – n-butanol soluble, methanol insoluble; Extract C – n-butanol soluble, methanol soluble. Each of these three extracts was then evaluated for anti-protein misfolding activity in three separate assays: [i] biotinylated Abeta ELISA-based anti-oligomerization assay, [ii] Abeta thioflavin T anti-aggregation assay (ThT), and [iii] tau thioflavin S anti-aggregation assay (ThS). Extract A demonstrated significant Abeta anti-oligomeric and Abeta anti-aggregant activities as well as the ability to prevent tau aggregation. Extract A inhibited Abeta aggregation by 47% at 100 microM, and demonstrated concentration-dependent activity in the ThT assay. Extracts B and C did not exhibit any activity. This trend was also demonstrated in the Abeta oligomerization assay with A demonstrating significant activity, while both Extracts B and C showed no difference from control ($p = 0.05$). Extract A also prevented aggregation of tau by 41% at 100 microM; extracts B and C had no activity in the ThS aggregation assay. Thus, an ethyl acetate extract of maple syrup has significant Abeta/tau anti-oligomerization activity. This implications of this finding and the potential role of food products not only as therapeutics, but also as confounding variables in clinical trial design for AD will be considered.

AGFD 5 Withanamides in aswagandha botanical to treat and prevent Alzheimer's disease Muraleedharan G. Nair, nairm@msu.edu. Dept of Horticulture, Michigan State Univ., East Lansing About 5.3 million Americans are diagnosed with Alzheimer's disease (AD) costing about $226 million and expected to reach about 8 million by 2020. This cost is expected to reach $1.1 trillion by 2050. AD is a neurodegenerative disorder resulting in the loss of memory and cognitive abilities and caused by oxidative stress on the neuronal cell membrane by beta amyloid protein (BAP). This protein, generated in the AD patient's brain by unwanted secretase enzyme activity on APP protein, is the root cause of AD initiation and progression. BAP catalyzes the oxidation of water molecules to generate OH free-radical. These free-radicals trigger oxidative stress on neuronal cell membrane leading to the destruction of neuronal cells via numerous mechanisms including the fibrillation of tau proteins and/or aggregation of BAP. Unfortunately, numerous drug candidates aimed to mitigate AD failed in Phase III trials. These drugs have been either antibodies to sequester BAP or secretase enzymes that generate BAP. A food-grade antioxidant that could neutralize the ability of BAP from generating free radicals is another significant approach in mitigating AD. In this regard, we investigated never studied before leaves and fruits of Aswagandha for novel antioxidants. Bioassay- directed studies of its fruits afforded withanamides, a novel class of molecules, with potent lipid peroxidation inhibitory activity. These compounds were therefore tested for inhibition of BAP insult to neuronal cells in cell culture experiments. Results confirmed that withanamides protected neuronal cells from BAP damage before and/or after exposing the cells to BAP. Subsequent in vitro and in vivo experiments demonstrated its strong antioxidant activity, lack of cytotoxicity, ability to pass blood brain barrier and ability to chelate to the active motif of BAP. Therefore, a standardized withanamides containing Aswagandha extract will be a novel botanical drug to test for its clinical efficacy in treating and preventing AD.

AGFD 6 Blueberry fruit supplementation in human cognitive aging Robert Krikorian, krikorr@ucmail.uc.edu. Univ. of Cincinnati Academic Health Center, Ohio Neurocognitive decline with aging and in conditions such as Alzheimer's disease represents a substantial public health concern that will produce suffering in patients and caregivers and enormous expenditures of health care resources. Effective medical treatment for dementia is not available. However, attention has begun to shift to preventive measures, and nutritional intervention represents a potentially potent approach to mitigate risk for late life dementia. We will review the findings of recent human trials examining the effects of blueberry supplementation on cognitive performance and brain function in older adults. These sorts of moderate-term intervention trials have methodological limitations, in particular associated with dose and duration of supplementation and uncertainty about metabolic processes and mechanisms. However, recent findings suggest that supplementation with flavonoid-rich blueberry offers the possibility of significant risk reduction, when practiced in advance of dementia.

AGFD 7 Unraveling the key aroma compounds of different types of beer: Are differences in aroma profiles caused by quantitative or qualitative differences in key odorants? Peter H. Schieberle, peter.schieberle@lrz.tum.de. Technical Univ of Munich, Freising, Germany It is without doubt that aroma is among the important drivers of beer quality, or in other words of consumer acceptance. It is also well established today that during food consumption, a certain set of volatile constituents induces a pattern of neural activity in the olfactory bulb. The complex neural patterns generated at the odorant receptor sites are finally "translated" by our brain into a simple perception telling us, for example, the aroma quality of a given product. However, since the overall aroma of beers can significantly be influenced by the recipe and the processing conditions, there is a clear need to understand the aroma signature of beer on the molecular level in order to steer its quality or its consumer acceptance, respectively. By application of the SENSOMICS concept on the volatiles isolated from a German Pilsner-type beer, a Bavarian wheat beer and a British Guiness beer, differences in the key aroma compounds were elucidated by GC-Olfactometry and a calculation of odor activity values. Finally the results were established by recombining the odorants in the same concentrations as they occurred in the three beers using ethanol/water as the matrix. Correlations to the overall aroma profiles will be discussed.

AGFD 8 Hop, the spirit of the beer Michael C. Qian, michael.qian@oregonstate.edu. Oregon State Univ, Corvallis Hops (Humulus luplus L.) are considered the most important ingredient in brewing. Hop aroma quality directly affects beer quality and style. Hop volatile composition is not only determined by variety, but also by agronomical conditions such as climate, soils types as well as hop maturity and processing. The contribution of hop derived volatile compounds to the aroma of finished beer is further complicated by the brewing process, because the hoping scheme, wort boiling, fermentation, maturation, and packaging can affect hop volatile loss and conversion. Hop volatile composition is extremely complex, more than 300 compounds have been identified in hop oil, with terpenic compounds predominate. Aroma composition of hops and their contribution to beer aroma will be discussed in this work.

AGFD 9 Odor-active compounds in novel special flavor hop cultivars and their impact on beer aroma Martin Steinhaus, martin.steinhaus@lrz.tum.de, Silva Neiens. Deutsche Forschungsanstalt für Lebensmittelchemie (German Research Center for Food Chemistry), Freising Hops are used in brewing to enhance shelf life and bitterness of beer. However, depending on the amount and the point of hop addition, they may also have a vital impact on beer aroma. Mainly driven by craft brewers, a new market for hop cultivars with extraordinary aroma properties has evolved in recent years. New breeds already successfully established in the market include the cultivars Huell Melon, Polaris, Mandarina Bavaria, and Hallertau Blanc. Application of a comparative aroma extract dilution analysis (cAEDA) on the volatiles isolated from the hops by solvent extraction and solvent-assisted flavor evaporation resulted in ~50 odor-active compounds among which myrcene, linalool, (E,Z)-1,3,5-undecatriene, nonanal, 2-methylbutanoic acid, and 3-methylbutanoic acid showed high flavor dilution (FD) factors in all four cultivars. Beyond these compounds responsible for the fundamental hoppy aroma, the cAEDA also revealed odorants that corresponded with the characteristic aroma nuances of the individual hop cultivars. E.g. the cantaloupe-like note of the Huell Melon cultivar corresponded to extraordinary high FD factors of some fruity smelling esters, whereas the fruity-fresh note characterizing Polaris could be ascribed to aroma-active amounts of 3-methylbutyl acetate in combination with 1,8-cineol. Quantitation of the compounds by means of stable isotope dilution assays confirmed the cAEDA data. Brewing trials finally disclosed which of the compounds were transferred into beer in aroma-active amounts.

AGFD 10 Options to mitigate sunstruck-flavor formation in beer Susanne Stingl1, susanne.stingl@lrz.tum.de, Peter H. Schieberle2. (1) Deutsche Forschungsanstalt für Lebensmittelchemie, Freising, Germany (2) Technical Univ of Munich, Freising, Germany Due to its nice golden color there is a certain demand in the brewing industry to sell beer in white glass bottles. However, because the commonly used brown glass acts as an effective UV stabilizer, beer quickly develops an unpleasant, so-called "sunstruck- flavor" when filled in white glass. Literature data suggest that this off-flavour is predominantly caused by the extremely potent odorant 3-methyl-2-butene-1-thiol (MBT). Because, in particular isohumulone in the presence of cysteine and riboflavin, is discussed as the key precursor of the mercaptan in some countries hydrogenated hops are used to prevent the formation of MBT. This approach is legally not permitted in Germany and other countries, and thus the only option is to reduce the hop dosage in beer production. However, because some hop constituents are discussed as bioactive components, this approach may lead to a lower nutriceutical value. By application of the Sensomics concept, first, the aroma compounds MBT, but also methane thiol, 3-(methylthio)propanal and phenylacetaldehyde were found to be newly formed after exposure of beer to light. To elucidate their role in off-flavor development, stable isotope dilution assays had to be developed, in particular for the trace compound MBT, and odor activity values were calculated. In a second series of experiments, aimed at clarifying the mechanism of MBT formation, single hop constituents were irradiated in the presence of cysteine and riboflavin. The results revealed humulone besides iso-humulone as precursor of the carbon chain in MBT. Furthermore different compounds could be identified as sources of the mercapto group. Additional model systems undertaken to elucidate ways to mitigate MBT formation showed a strong influence of the pH and the addition of certain polyphenols.

AGFD 11 Characterizing aroma components of rum Chelsea Ickes, Keith R. Cadwallader, cadwlldr@illinois.edu. Dept. Food Sci. Human Nutr., Univ. of Illinois, Urbana Rum is produced by fermenting sugar cane juice, syrup, or molasses, which is then distilled and aged for a number of years. This distilled spirit is unique in that its only standard of identity is that it must originate from sugar cane or sugar cane byproducts. All other manufacturing processes are variable, including type of sugar cane starting material, distillation method, and type of barrel used for maturation. Currently over 1000 different rums are produced, comprising categories such as white, gold, and aged. Even

though variability among rums is high, rum as a distilled spirits class is readily distinguishable from other traditionally aged spirits such as Scotch, whiskey, Bourbon, rye and Tequila. Odorants in rum may originate from the sugar cane, or may be produced during the fermentation, distillation or aging processes. Among these, there is a certain subset necessary to create the characterizing or distinguishing aroma of rum. The purpose of this talk is to identify the components responsible for this spirits' distinctive "rummy" character.

AGFD 12 Cachaça flavour André R. Alcarde2, andre.alcarde@usp.br, John Piggott1. (1) Snowdon Place, Stirling, United Kingdom (2) Escola Superior de Agricultura 'Luiz de Queiroz', Univ. de São Paulo, Piracicaba, SP, Brazil Cachaça is a spirit distilled from sugar cane juice. It is the most important distilled spirit in Brazil and the fourth most consumed in the world. Aging is not mandatory for cachaça, but may be carried out in wood from various sources. Volatiles arise from the raw material used, and from the steps in the process. Some preprocessing and standardisation of the cane juice may be carried out, followed by fermentation, which may be either spontaneous or with a cultured yeast. Volatile compounds produced at this stage are derived from metabolism of yeast and bacteria present. Distillation may be single or double in s simple pot still, or in a column still. The manner of distillation and the materials of the still have a major effect on the composition of the distillate. The distillate may be bottled at this stage, or may be filled into casks for maturation, typically for a few years but possibly up to 10 years. The changes occurring during maturation depend on the alcohol concentration on filling, the wood species, previous use of the cask, and any treatment it has been subjected to. Research has been directed primarily at understanding how existing knowledge of fermentation, distillation, and maturation applies in the case of cachaça, and at improving the consistency of the product by better control of undesirable flavour compounds.

AGFD 13 Bioproduction and anti-inflammatory activity of delta-tocotrienol enriched extracts from hairy roots of annatto Jarrod Creameans1,2, jarrod.creamean@smail.astate.edu, Krishna Vellanki1,2, Maureen Dolan1,2, Fabricio Medina-Bolivar1,2. (1) Biological Sciences, Arkansas State Univ., Judsonia (2) Arkansas Biosciences inst., Jonesboro Annatto (Bixa orellana) is a plant native to South America that has been used as a traditional medicine to treat multiple diseases. The highest natural level of delta tocotrienol, one of the eight E-vitamers, has been found in annatto. Hairy root cultures of annatto were established to study the bioactive compounds in this species. The hairy roots were cultured in liquid medium under either continuous light or dark conditions for 30 days. Root tissue and culture medium extracts collected every 3 days are being analyzed for tocotrienols using high performance liquid chromatography. Our preliminary results indicate that annatto hairy roots produce mainly delta-tocotrienol and trace amounts of gamma-tocotrienol. The anti-inflammatory capacity of the culture extracts is being assessed using a cytokine assay with 3T3-L1 cells. We propose that hairy root cultures of annatto can be developed as a sustainable source of delta tocotrienol.

AGFD 14 Quinone intermediate mediates the cytotoxicity effects of tert-butylhydroquinone (TBHQ) Elvira Sukamtoh, esukamto@umass.edu. Food Science, Univ. of Massachusetts Amherst Tert-butylhydroquinone (TBHQ) is a widely used antioxidant in food products. Previous studies have shown that TBHQ at high doses has cytotoxic and genotoxic effects. However, the underlying mechanisms are not well understood. Here we found that the cytotoxic effect of TBHQ was mediated by its oxidative conversion to a quinone metabolite, tert-butylquinone (TBQ). In MC38 mouse colon cancer cells, co-addition of Cu2+ enhanced the effects of TBHQ on cellular proliferation and cell cycle progression, whereas co-addition of ethylenediaminetetraacetic acid (EDTA) decreased the effects. HPLC analysis showed that co-addition of Cu2+ increased ~80% of oxidative conversion of TBHQ to TBQ, while co-addition of EDTA inhibited ~20% of this process. Together, these results suggest that the oxidative formation of quinone metabolite, TBQ, mediates the cytotoxic effects of TBHQ in cells.

AGFD 15 Selectivity of separation of natural antioxidants in gradient reversed-phase liquid chromatography Michela Palmieri2, 85830@studenti.unimore.it, Petr Cesla3, Federica Pellati1. (1) Univ. of Modena and Reggio Emilia, Italy (2) Life Sciences, Univ. of Modena and Reggio Emilia, Italy (3) Univ. of Pardubice, Czech Republic Polyphenols are a large family of compounds widely distributed in plants. Many of them, are natural antioxidants, which have beneficial effects on human health. The polyphenols can be easily analyzed using liquid chromatography in reversed-phase mode; however, the optimization of separation selectivity is usually required especially for structurally similar or isomeric compounds. The aim of the thesis was to develop a systematic approach to the selection of columns and mobile phases suitable for separation of natural phenolic antioxidants, based on the correlations between the gradient retention times and molecular structure-descriptors of representative phenolic acid and flavonoid standards. For this aim, 14 compounds belonging to the group of phenolic acids and flavonoids were chosen and were subjected to the study. Multiple linear regression, cluster analysis and window–diagram optimization strategies were combined for data evaluation. The gradient retention data for a set of phenolic compounds obtained using six different columns packed with porous shell particles with non-polar chemically bonded stationary phases were used to establish the retention model. The retention factors were then applied for evaluation of selectivity using linear free energy relationship concept, which enables comparison of selectivity of separation among different stationary phases used.

AGFD 16 Effect of elemental sulfur and yeast strain on hydrogen sulfide production in wine post-bottling Elle Friedberg2, efriedbe@wellesley.edu, Gavin L. Sacks1. (1) Food Science, Cornell Univ., Ithaca, New York (2) Dept. of Chemistry, Wellesley College, Massachusetts Volatile sulfur compounds, particularly hydrogen sulfide (H2S), are a common cause of wine faults. H2S, characterized by low threshold "rotten egg" aromas, is of special interest to winemakers because the compound is often absent during wine bottling, but can reemerge after storage. This study was undertaken to investigate the effect of elemental sulfur and Saccharomyces cerevisiae yeast strain variety on "latent" H2S (TCEP-releasable) production in post-fermentation samples of wine. "Latent" H2S was quantified by using a modified developed assay (Kwasniewski 2011) using an H2S Gastec detection tube. Analytical replicates were produced by assaying each sample in triplicate. Data was run through a Multiple Analysis of Variance statistical test in conjunction with a Tukey HSD test. Data collected showed that statistical differences exist between "latent" H2S concentrations produced by varying yeast strains. This data was used to estimate a maximum recommendation of 7 µg/g S0 spray use in the vineyard.

AGFD 17 Structure-property study of the selective Raman spectroscopy detection of fusaric acid and analogs Edgard Martinez Rosado2, edgard.martinez1@upr.edu, Michael Appell1, Lynette E. Orellana3. (1) USDA-ARS, Dunlap, Illinois, US (2) Chemistry, Univ. of Puerto Rico - Mayaguez, Isabela, (3) Programa de Ciencia y Tecnología de Alimentos, Univ. of Puerto Rico – Mayaguez Food security can

benefit from the development of selective methods to detect toxins. Fusaric acid is a mycotoxin produced by certain fungi found sporadically in agricultural commodities. Raman spectroscopy allows selective detection of analytes associated with certain spectral characteristics related to chemical structure. Furthermore, selective Raman detection can be enhanced and tuned through intermolecular interactions, such as Surface Enhanced Raman Scattering (SERS). Raman spectroscopy was carried out to compare the spectral properties of fusaric acid and structurally related analogs picolinic acid, picolinamide, and kojic acid. Conformational analysis was conducted using density functional theory at the B3LYP/6-311+G(2df,2p) level of theory. Aided by the density functional study, the vibrational modes were assigned and unique characteristics of the Raman spectra were identified between the analogs. This study provides a convenient label free approach to distinguish fusaric acid from other related analogs.

AGFD 18 Determination of the effect of dissolved oxygen on the rate of oxidation presented by trans-2-nonenal in beer Daniel Kazal, dkazal@ycp.edu, William H. Steel. Physical Sciences, York College of Pennsylvania, York One of the major contributors to the stale flavors that can develop in beer is trans-2- nonenal. Some of its potential precursors are hydroperoxides found in spent grain and raw materials, but the leading suspect of its origin is the auto-oxidation of free linoleic acid. If this suspicion is correct, then the dissolved oxygen content in beer will impact the presence of this flavor-altering derivative as well as how quickly it develops in beer. This work describes the findings of a two-part, blind study designed in cooperation with Victory Brewing Company. Victory supplied commercially brewed and bottled beer, half of which had been exposed to air in order to increase the dissolved oxygen content. The rate at which trans-2-nonenal appeared in the beer was analyzed by gas chromatography coupled with flame ionization detection and results were compared 'real-time' with beer samples from the same batch that were placed into Victory's daily tasting panels.

AGFD 19 Actions of bioactive phytochemicals in neuropathology Richard Hartman, rhartman@llu.edu. Dept. of Psychology , Loma Linda Univ. California Phytochemicals are broadly defined as compounds produced by plants, many of which have pigment, odorant, and/or irritant properties that may provide biochemical defenses against metabolic byproducts (e.g., reactive oxygen species, protein misfolding) and environmental insults (e.g., pathogens, insects, ultraviolet radiation). Consumption of plants or their phytochemicals may confer some of these beneficial properties and modulate biological pathways including inflammatory, enzymatic, neurotransmitter systems, apoptosis, and neurogenesis. This talk will present data from our laboratory describing the effects of dried fruit, fruit juice, and polyphenol extracts on drosophila and mouse models of Alzheimer's disease, traumatic brain injury, epilepsy, and irradiation. Additionally, data from human studies of open heart surgery and stroke will be presented. Experiments with transgenic mouse models of Alzheimer's disease suggest that these compounds can improve behavioral performance by preventing the production / accumulation of amyloid-beta in the brain. Other mouse experiments suggest that they can reduce lesion size and behavioral deficits associated with mild traumatic brain injury, and that they can upregulate neurogenesis and prevent deficits associated with irradiation. Further experiments with drosophila models of epilepsy and traumatic brain injury are currently underway. In a study of human patients undergoing open heart surgery, we showed that pre- and post-treatment with pomegranate polyphenols not only prevented the occurrence of post-operative cognitive deficits, but improved memory above pre-surgery baselines. Another study of treatment with pomegranate polyphenols following stroke in humans is currently underway. Given the low cost and relative safety associated with dietary interventions, such preventative strategies may ultimately prove more helpful than reactive treatment with pharmaceuticals that have extensive side effect profiles. Together, these data suggest that diets consisting of a wide variety of brightly colored and spicy foods can provide a broad degree of chronic background protection against the deleterious effects of aging and other insults to the brain.

AGFD 20 Phenolic-enriched maple syrup extract shows neuroprotective effects in murine microglial cells and delays β-amyloid aggregation induced neurotoxicity and paralysis of Caenorhabditis elegans Hang Ma1, mahangees@gmail.com, Weixi Liu2, Pragati P. Nahar1, Nicholas DaSilva1, Zhengxi Wei1, Priscilla P. Pharm3, Dhiraj A. Vattem3, Navindra P. Seeram1. (1) Biomedical and Pharmaceutical Sci., College of Pharmacy, Univ. of Rhode Island, Kingston (2) Dept. of Chemistry, Univ. of Rhode Island, Kingston (3) Nutritional Biomedicine & Biotechnology, Texas State Univ., San Marcos Published data supports the neuroprotective effects of several phenolic-containing plant foods, including certain fruits, berries, spices, and nuts, but there is limited data on phenolic-containing natural sweeteners such as maple syrup. Our group has previously reported on the chemical characterization and in vitro anti-inflammatory effects (against RAW 264.2 macrophages) of a phenolic-enriched maple syrup extract (MSX). Herein, we sought to investigate the neuroprotective effects of MSX against Alzheimer's disease using a combination of in vitro and in vivo studies. Based on biophysical data (circular dichroism and zeta sizer), MSX reduced β1-42 amyloid fibrillation similar to the neuroprotective polyphenol, resveratrol (66.7 vs. 69.5%, respectively; both at 200 μg/mL). MSX also showed neuroprotective effects against oxidative and inflammatory stress in BV-2 murine microglial cells. MSX (100 μg/mL) decreased the level of reactive oxygen species in BV-2 cells by 16% compared to control, and downregulated the production of inflammatory markers, nitric oxide and prostaglandin E2, by 24 and 75%, respectively, compared to lipopolysaccharide-stimulated control cells. MSX (10 μg/mL) imparted in vivo protective effects on β1-42 amyloid aggregation induced neurotoxicity and paralysis in Caenorhabditis elegans. The current study adds to the growing body of data supporting the neuroprotective effects of certain phenolic-containing plant foods including maple syrup. Further studies to evaluate the neuroprotective effects of MSX in animal models of Alzheimer's disease are warranted.

AGFD 21 Back to the future: Using phenotypic screening to identify Alzheimer's disease (AD) drug candidates Pamela Maher, pmaher@salk.edu. Salk inst., La Jolla, California There are no disease-modifying drugs for any old age-associated neurodegenerative diseases or stroke. This is at least in part due to the failure of drug developers to recognize that the vast majority of neurodegenerative diseases arise from a confluence of multiple, toxic insults that accumulate during normal aging and interact with genetic and environmental risk factors. Thus, it is unlikely that the current single target approach to drug discovery based upon rare dominant mutations or even a few preselected targets is going to yield useful drugs for these conditions. Therefore, the identification of drug candidates for neurodegeneration should be based upon their efficacy in phenotypic screening assays that reflect the biology of the aging brain, not a single preselected target. We have identified a set of cell-based assays that define molecular toxicity pathways relevant to age-associated neurodegeneration. These include assays for protection against cell death induced by endogenous oxidative stress, energy loss, neurotrophic factor withdrawal and intracellular amyloid beta peptide toxicity. An additional assay for anti-inflammatory activity is also included. We require our drug candidates to work in all of these assays. We identified two polyphenols that were effective in most or all of these assays and used structure

activity relationship-driven iterative chemistry to improve their potency and physicochemical properties. We now have several drug candidates that greatly reduce cognitive and other behavioral deficits in multiple animal models of AD and therefore have great potential for the safe and effective treatment of the disease.

AGFD 22 Potential beneficial effects of a diet with walnuts in Alzheimer's disease Abha Chauhan, abha.chauhan@opwdd.ny.gov, Ved Chauhan. NYS Inst. for Basic Research in Developmental Disabilities, Staten Island, New York Amyloid beta-protein (Aβ) is the major protein of amyloid deposits in the brain of patients with Alzheimer's disease (AD). Extensive evidence suggests neurotoxic effects of soluble oligomers of Aβ, and the role of oxidative stress and inflammation in AD. Walnuts are rich in components that have antioxidant and anti-inflammatory properties. Previous in vitro studies have shown that walnut extract inhibits Aβ fibrillization, solubilizes its fibrils, and has protective effects against Aβ-induced oxidative stress and cell death. In the Tg2576 transgenic mouse model of AD (AD-tg), we have reported the beneficial effects of dietary supplementation of 6% (T6) or 9% walnuts (T9) [equivalent to 1 or 1.5 oz of walnuts per day in human] on the memory, anxiety and learning skills. The diets for the experimental and control mice were comparable as regards to total calories and the contents of protein, carbohydrate and fat. AD-tg mice on control diet without walnuts (T0) showed memory deficit, anxiety-related behavior, and severe impairment in spatial learning ability, position discrimination learning ability and motor coordination compared to the wild-type (Wt) mice on the same diet. AD-tg mice on diet with walnuts (T6, T9) showed a significant improvement in memory, learning skills, anxiety and motor development compared to AD-tg mice on diet without walnuts (T0). Recently, we have also analyzed Aβ levels in the brain and blood samples of these mice at the ages of 4 months (before starting diet with walnuts), 14.5 and 19 months. At the age of 4 months, Aβ levels (brain and blood) were similar in T0 and Wt mice. At the age of 14.5 and 19 months, T0 mice had significantly higher Aβ levels than Wt mice. In the brain, T6 and T9 mice had significantly lower levels of soluble Aβ oligomers compared to T0 mice. In the blood samples, the levels of Aβ 1- 40 and 1- 42 were increased in T6 and T9 mice compared to T0 mice, suggesting that walnuts in the diet can increase the clearance of Aβ from brain to the blood. These findings suggest that dietary supplementation with walnuts may have a beneficial effect in reducing the risk, delaying the onset, or slowing the progression of AD because it can (a) inhibit Aβ fibrillization, Aβ-induced oxidative stress and Aβ-mediated cytotoxicity, and (b) reduce the levels of soluble Aβ oligomers in the brain and increase Aβ clearance.

AGFD 23 Bioactive compounds in dairy products and their relation to neurodegenerative disease Michael H. Tunick, Michael.Tunick@ars.usda.gov, Diane L. Van Hekken, Peggy M. Tomasula. USDA ARS, Wyndmoor, Pennsylvania, US Enhancement of nervous system function and cognitive ability may be aided by bioactive compounds found in dairy products, including calcium-binding phosphopeptides and peptides derived from casein and β-lactoglobulin. These peptides inhibit angiotensin-converting enzyme I, scavenge radicals, reduce blood pressure, and impede lipid peroxidation. Our laboratory subjected processed milk to simulated digestion and identified a number of bioactive peptides, which shows that these compounds form and survive in gastric and intestinal conditions. Other bioactives in dairy products include lactoferrin, a protein that sequesters iron necessary for bacterial growth and controls the balance between reactive oxygen species and their elimination rate, which would protect against oxidative stress injury of cells. Dairy products are the primary dietary source of calcium ion, the altered regulation of which may be related to brain aging and Alzheimer's disease. Early-stage Alzheimer's disease has been related to high insulin concentrations, but regular dairy product consumption is associated with a significantly lower incidence of the insulin resistance syndrome. Research is showing that brain function and cognitive ability are improved with ingestion of some of the components of dairy products.

AGFD 24 Assessment of the ability of dietary soy to impact age-related neurodegeneration Jessy Deshane1, Sreelatha Meleth2, Landon Wilson3, Stephen Barnes3,4, Helen Kim3,4, helenkim@uab.edu. (1) Dept. of Medicine, Univ. of Alabama at Birmingham (2) RTI International, Durham, North Carolina (3) Targeted Metabolomics and Proteomics Laboratory, Univ. of Alabama at Birmingham (4) Dept. of Pharmacology and Toxicology, Univ. of Alabama at Birmingham Beneficial actions of dietary soy (either whole soy protein, or soy isoflavones) on learning and memory have been reported in both animal and human studies. We report here results of proteomics analyses of brain proteins in rodent brain following dietary soy intake that complements these behavior studies. We hypothesized that the behavioral benefits of soy involved changes at the protein level either in abundance or post-translational modifications that could be detected by 2D gel proteomics, and that identification of such proteins would provide insights for specific signaling or enzyme networks that would enable deeper understanding of whether dietary soy has neuroprotective actions, and whether such actions could be extrapolated to prevention of age-related neurodegeneration. In this study, we administered over 12 months a defined diet AIN-76A where the casein protein had been replaced by either soy protein, or soy protein depleted of the isoflavones, to a transgenic mouse model of Alzheimer's (AD). The amyloid precursor protein is overexpressed in this mouse model, and the amyloidogenic Ab fragment, Ab1-42, accumulates over time as in the brains of AD patients. After 12 mo, 2D gel proteomics analysis revealed that there were proteins that were differentially expressed and/or modified in the brains of mice depending on whether the soy protein had the isoflavones or had been depleted of the latter. Mass spectrometry identified proteins, the majority of which had been shown to be aberrantly expressed in AD brain, and in other mouse models of neurodegeneration. Moreover, the changes in these proteins were for the most part in the opposite direction to those observed in AD brains, and in animal models of neurodegeneration. These results are consistent with the hypothesis that ingestion of soy protein is protective against neurodegeneration, and that the isoflavones may be the bioactive components of soy.

AGFD 25 Non-volatile profiling of cask aged spirits using UHPLC/QTOF-MS Thomas S. Collins, tom.collins@wsu.edu. Viticulture and Enology Program, Washington State Univ., Richland While the composition of unaged clear spirits consists of compounds of sufficient volatility to be carried over during the distillation process, the composition of cask aged spirits is more complex and is dependent on the types of cask in which the spirit was aged as well as the aging practices of the producer. Wood derived compounds represent the majority of non-volatile components in aged spirits. The specific wood related compounds associated with cask aged spirits depend on how long the spirit was aged, as well as whether the spirit was aged in new casks or previously used casks. Ultra-high pressure liquid chromatography (UHPLC) coupled with quadrupole time of flight (QTOF) mass spectrometry was used to analyze the non-volatile composition of cask aged spirits, including American, Irish, Japanese and Scotch whiskies, French and American brandies, rums from multiple countries and añejo Tequilas. Analysis was performed using an Agilent 1290 UHPLC/6545 QTOF-MS system; MS data was collected both in scan mode and in a data dependent automated MS/MS mode. Data analysis was done using Agilent MassHunter and Mass Profiler Professional software. The

non-volatile composition of the aged spirits was analyzed using principal component analysis to identify compounds correlated with each spirit type. Additionally, the data for each spirit type was examined for the presence of wood derived compounds which had previously reported in one or more of the spirit types to assess commonalities in wood extractives across the spirit types. The use of UHPLC/QTOF-MS to profile wood related components extracted from casks during aging may be a complementary technique to GC/MS profiling for verification of authenticity of aged spirits.

AGFD 26 Unraveling differences in key aroma compounds of a commercial American bourbon whiskey und a scotch single malt whisky by means of the sensomics concept Veronika Mall1, veronika.mall@Lrz.tum.de, Peter H. Schieberle2,1. (1) Deutsche Forschungsanstalt fuer Lebensmittelchemie, Freising, Germany (2) Technical Univ of Munich, Freising, Germany Aquavite, later known as whisky, was mentioned for the first time in tax documents in Scotland in 1494. Scottish and Irish settlers brought the knowledge on whisk(e)y manufacturing to "new world" America. Over the centuries, differences in making the spirit showed up e.g., due to available raw products and different kilning procedures. While Scotch whisky is produced solely from barley malt, American distilleries use at least 51 % corn next to rye, wheat or barley malt. Furthermore, American whiskey is always stored in freshly burnt casks. In order to decode the unique aroma of whisk(e)y on a molecular basis and to elucidate the impact of the different processes on aroma compound formation, a single malt Scotch whisky and an American bourbon whiskey were studied by means of the sensomics concept. The important aroma compounds identified by mass spectrometry based on results from GC-O and aroma extract dilution analysis, were then quantitated by stable isotope dilution assays. Odor activity values were then calculated considering their odor thresholds in 40 % ethanol ABV. The results were verified by preparing aroma recombinates to mimic the original whisky aroma profile. In detail, the bourbon whiskey featured up to 18-fold higher odor activity values (OAV) for both, the vanilla-like 4-hydroxy-3-methoxybenzaldehyde and the coconut-like cis- whisky lactone than the Scotch spirit. On the other hand, the traditional Scottish kilning process added a strong smoky or "peaty" aroma to the Scotch whisky, which was caused by a specific set of phenolic compounds showing high OAVs. These odorants were mostly absent in the American whiskey.

AGFD 27 From the fruit to the spirit: Changes of key aroma compounds in pears and pear brandy Michael Granvogl1, michael.granvogl@tum.de, Bianca Willner1, Peter H. Schieberle2. (1) Tech Univ. of Munich, Freising Bavaria, Germany (2) Technical Univ of Munich, Freising, Germany In a previous study, 37 key aroma compounds of Bartlett pear brandy were characterized using the Molecular Sensory Science Concept (Sensomics Concept) resulting in an aroma recombinate eliciting the typical aroma of pear brandy. It is a well-known experience that the manufacturing process, which is divided into mash fermentation, distillation, and maturation, clearly influences the final aroma of Bartlett pear brandies. Thus, the aim of the actual study was the analysis of the key aroma- active compounds in Bartlett pears and the fate of the aroma components during the process. Therefore, we elucidated the key odorants in Bartlett pears, in fermented, diluted Bartlett pear mash as well as in the unstored and, finally, in the stored distillate by application of the Sensomics Concept. Thereby, 23 odor-active compounds in Bartlett pears and 32 odor-active compounds in the fermented mash were detected in a flavor dilution (FD) factor range of 8-8192. 28 of these compounds have been identified in Bartlett pears or in fermented pear mash for the first time, among them 3-(methylthio)propanal (cooked potato-like aroma), (E)-β-damascenone (cooked apple- like), and trans-4,5-epoxy-(E)-2-decenal (metallic), all of them showing the highest FD factors in Bartlett pears. Already in the fermented, diluted Bartlett pear mash, the aroma profile has clearly changed showing ethyl (S)-2-methylbutanoate (fruity), acetic acid (vinegar-like), (S)-2-/3-methylbutanoic acid (sweaty), and 2-phenylethanol (flowery, honey-like) with high FD factors. Next, up to 42 aroma-active compounds were quantitated during the manufacturing process (pears, fermented mash, unstored distillate, and stored distillate) using stable isotope dilution assays revealing an essential influence of each step on the aroma development of the final product. Quantitation experiments of the most important aroma-active compounds, such as ethyl (S)-2-methylbutanoate, (E)-β-damascenone, ethyl (E,Z)-2,4-decadienoate, and ethyl (E,E)-2,4-decadienoate, revealed considerable changes during the process. Possible formation pathways as well as degradation reactions will be discussed.

AGFD 28 Identification of compounds that contribute to trigeminal burn of alcoholic spirits Smaro Kokkinidou, kokk0013@umn.edu, Devin G. Peterson. Food Science and Nutrition, Univ. of Minnesota, Saint Paul The smoothness of alcoholic beverages is a general descriptor often associated with product maturity and considered a desirable trait. This work examined the chemical drivers that influence the trigeminal burn of distilled spirits. The influence of carbonyl species on the trigeminal burn intensity of distilled spirit model systems was investigated. Quantities of carbonyl compounds such as hexanal, heptanal, octanal, nonanal, decanal, benzaldehyde and 2-heptanone were significantly changed using two methods; (1) increasing or decreasing the pH from to basic or acidic region, to either induce hemiacetal formation and acetal stabilization or increase aldehyde species, respectively and (2) utilizing a carbonyl scavenger sulfonyl hydrazine polymer treatment to successfully remove carbonyls. Sensory evaluation of samples with reduced carbonyl concentrations had significantly lower perceived trigeminal burn intensity. Recombination experiments revealed that addition of a carbonyl mixture increased trigeminal burn perception in model systems; confirming causality. Individual carbonyls compounds were also examined and octanal, nonanal, benzaldehyde and 2-heptanone were revealed as the strongest potentiators of trigeminal responses. Results suggest that carbonyl species in combination with ethanol activate nociceptors and elicit trigeminal responses. These findings provide a better understanding of the molecular basis of trigeminal burn and a foundation to develop ingredient and/or processing technologies to improve palatability of a wide range of alcoholic products.

AGFD 29 Grape pathogenesis related proteins (PRPs) – a factor responsible for low tannin extraction during winemaking Gavin L. Sacks1, gls9@cornell.edu, Lei-An Chen1, Lindsay F. Springer2. (1) Food Science, Cornell Univ., Ithaca, New York (2) Food Science and Technology, Cornell Univ, Dundee, New York Grape-derived condensed tannins (CT) are critical to the astringent perception of red wines, but the extraction of CT during fermentation or following addition to finished wines is highly variable. The factors limiting tannin extraction or retention across wines are still poorly understood. We have recently shown that differences in CT retention following its addition to wines are well predicted by the concentration of grape pathogenesis-related (PR) proteins, and can be modeled by a Freundlich isotherm. In a subsequent harvest, we produced wines in triplicate from16 site-variety combinations under identical winemaking conditions and observed greater than 100-fold difference (<0.5-50%) in the amount of tannin extracted. The relation between tannin extractability and juice PR protein concentration could be well-modeled by a sigmoidal function (EC50= 52 mg/L, r2 = 0.58), indicating that the poor tannin extractability of some grapes may be due to high PR proteins. Existing approaches to remove protein from wines or juices, e.g. bentonite, may therefore be useful in increasing CT extractability from high PR protein grapes.

AGFD 30 Anti-obesity and anti-hyperlipidemic effect of Gynostemma pentaphylla saponins and the possible mechanisms Jie Liu1, liujiefantasy@163.com, Haiming Shi1, Xiangjun Sun1, Liangli L. Yu2. (1) Shanghai Jiao Tong Univ., Shanghai, China (2) Univ of Maryland, College Park Gynostemma pentaphylla (Jiaogulan in Chinese) has been used as food and beverage ingredients worldwide. Saponins were believed to be responsible for the anti-obesity and anti-hyperlipidemia of G. pentaphylla, but the underlying mechanisms and active components remained unclear. The first objective of this study was the isolation and characterization of the Jiaogulan saponins with the potentials to reduce the risk of obesity and hyperlipidemia. Nine saponins, including six ones reported for the first time, were obtained from G. pentaphylla using an activity-guided isolation approach and elucidated for their chemical structures by 2D NMR and HR-MS data. Moreover, the second objective was to investigate the anti-obesity effect and possible mechanisms of jiaogulan saponins in vivo and in vitro. Compared with that in C57/BL6 mice fed high-fat diet, the overweight, inflammation and insulin resistant in hepatic and adipocyte tissue of test group were alleviated in at the dose of 300 mg/kg/d Jiaogulan saponins. These beneficial effects were the results of a increased energy expenditure partially modulated by a significant improvement of liver mitochondrial activity accompanied with subcutaneous and visceral white adipocyte browning and sustained β-catenin so as to inhibit adipocyte cell cycle and adipogenesis in mitotic clonal expansion. In addition, the third objective was to illuminate the effect and possible mechanisms behind its anti- hyperlipidemic activities. Both decreased intestine absorption of cholesterol and increased total bile acid excretion should be responsible for the reduction of hepatic triacylglyceride and plasma cholesterol(TC), triacylglyceride(TG) and LDL-c compared with that in hamster fed high-fat diet supplemented with 500 mg/kg/d Jiaogulan saponins. In conclusion, the results from this study may be used to promote the value- added utilization of G. pentaphyllum and the use of the extracts or its components in dietary supplements showing the potential as a nutraceutical for reducing the risk of high-fat diet induced metabolic syndrome.

AGFD 31 Kafirin protein and its applications in nano-encapsulation, pickering emulsion and electrospinning fiber Jie Xiao1, xiaojieacademic@gmail.com, Qingrong Huang2. (1) Food Science, Rutgers, The State Univ. of New Jersey, New Brunswick (2) Food Science, Rutgers Univ, New Brunswick, New Jersey Kafirin, the major prolamine protein form sorghum grain, has the potential to serve as a novel building block for food grade delivery vehicles. However, research efforts in clarifying its functionality related properties as well as fulfilling its application potentials were scarce. My Ph.D thesis extends in four specific objectives: 1) Investigate the structure, morphology and self-assembly behavior of kafirin to guide the formulation design thereafter. 2) Assemble kafirin nanoparticles for encapsulation and enhance cellular uptake of hydrophobic nutraceutics. The formation mechanism as well as its cellular uptake fate during oral consumption will be elucidated. 3) Formulate kafirin nanoparticles as a novel Pickering emulsion stabilizer. The microstructure, rheology, stability as well as oral digestion profile of as-prepared emulsions will be fully investigated. 4) Electrospinning of kafirin protein will be carried out and polycarprolactone will be blended to obtain fiber mats with tunable mechanical, swelling and release properties.

AGFD 32 Physicochemical modification of an immunostimulatory gluten peptide and the potential implications for Celiac disease Charlene Van Buiten, charlene.vanbuiten@gmail.com. Food Science, The Pennsylvania State Univ., Univ. Park Dietary polyphenols have been shown to exert anti-nutritional properties in humans through their interaction with other dietary components (e.g., minerals, proteins), despite the fact that their health benefits have been the focus of many studies in recent years. As proteins are often the immunostimulatory agents for food allergies and intolerances, the anti-nutritional effects of polyphenols may be beneficial to some individuals through the binding and sequestration of those proteins. Through structural and thermodynamic characterization of the interactions between polyphenols and a physiologically stable, immunostimulatory fragment of gluten, this present work explores the potential role for a diet rich in polyphenols as a strategy to mitigate the effects celiac disease. At present, the only treatment for celiac disease is adherence to a lifelong gluten-free diet; however, the findings presented here provide foundational support for a nutraceutical approach to ameliorating the symptoms and autoimmune response associated with this disease.

AGFD 33 Chemical modification of poultry feather keratin for biobased wood adhesive applications Nandika Bandara, bandara@ualberta.ca, Jianping Wu. Dept. of Agricultural, Food and Nutritional Science, Univ. of Alberta, Edmonton, Canada Value addition to agricultural waste and byproducts is a key in increasing economic return to farmers and processing industries. Soy meal, canola meal and poultry feathers are some of the agricultural byproducts that require value added applications. North America alone, produces more than 4 billion pounds of poultry feathers which contain ~90% protein, called keratin. Wood adhesives are mainly produced using petroleum byproducts; however, environmental and human health concerns regarding emission of formaldehyde and other volatile organic compounds and non-renewability in synthetic adhesives are prompting the industry to seek alternative bio-based polymers such as proteins. However, protein based adhesives have poor water resistance and adhesion strength compared to traditional wood adhesives. Keratin contains ~7% cysteine in its amino acid composition, which creates strong disulfide bonds among protein molecules making most functional groups unavailable to react with wood surface. However, the same unique structure of keratin provides a potential to use chemical modification in improving its functionality. We hypothesise that chemical modification with reducing agents will improve water resistance and functionality of keratin based wood adhesives; therefore the objective of this study is to improve adhesion strength and water resistance of keratin adhesives using chemical modification. Extracted keratins were modified using optimized concentrations of dithiothreitol (DTT) and Na2SO3. Adhesion strength was measured using Instron tensile loading according to the ASTM standard methods and data were analyzed using ANOVA followed by Duncan's multiple range test to identify the effects of reducing agents. Adhesives were characterized using XRD, FTIR, SEM and DSC for compositional, structural and thermal properties. Adhesion strength of keratin was significantly improved up to ~6-7 MPa and ~4-4.5 MPa for dry and wet adhesion strengths respectively under optimized conditions for DTT, without any delamination which was observed in control samples and some of Na2SO3 modified adhesives. Decrease in β-sheets and α-helix, increase in unordered structures in keratin secondary structure, change in keratin crystallinity and shift in thermal transitions were observed with modification. Chemical modification proved to have the potential for developing value added adhesive products from feather keratin with significantly improved functionalities.

AGFD 34 Advanced analytical techniques for the phytochemical investigation of essential oils Roberta Tardugno, roberta.tardugno@unimore.it, Federica Pellati, Stefania Benvenuti. Dept. of Life Sciences, Univ. of Modena and Reggio Emilia, Italy Essential oils (EOs) are very complex mixtures composed of natural volatile constituents. They are produced by aromatic plant specialized

glands as defensive secondary metabolites. Due to the EOs complexity, deep qualitative and quantitative investigations are necessary to explore their composition, to guarantee their genuineness and to allow a rational investigation about their potential biological activities. In this context, a broad-spectrum method was developed to investigate EOs from different plant genera and species by means of GC-MS and GC-FID techniques. The chemical characterization developed in this work had a key role in classification, selection and explanation of the possible biological activity of the each EO, which was evaluated on several microorganisms and cancer cell lines. The study was focused on autochthonous EOs obtained from plants cultivated in Italy or in other countries, with particular attention to Lavandula angustifolia P. Miller, Lavandula x intermedia Emeric ex Loisel., Thymus vulgaris L. and Cedrelopsis grevei H. Baillon.

AGFD 35 Colorimetric detection of Escherichia coli in drinking water based on bacteriophage infection Juhong Chen3, juhong@foodsci.umass.edu, Vincent M. Rotello1, Sam R. Nugen2. (1) Univ of Massachusetts, Amherst (2) 246 Chenoweth Laboratory, Univ. of Massachusetts , Amherst (3) Food Science, Univ. of Massachusetts, Amherst In this degree research, phage-based colorimetric methods were developed to detect viable Escherichia coli (E. coli) concentration in drinking water. During the phage infection cycle, phages can specifically recognize target E. coli cells and release intracellular β-gal enzyme. Using our proposed novel biosensor strategies, the β-gal enzyme activity as the indictor for the present of E. coli in drinking water was detected. Firstly, T7 phage covalently conjugated to magnetic beads were used to capture, separate, and purity E. coli cells in drinking water. The released β-gal was detected using commercial colorimetric substrates. Next, a novel enzyme-induced metallization multi-colorimetric assay was developed to monitor and measure β-gal activity, which was further employed for high-resolution colorimetric phage-enabled detection of E. coli. In order to improve the limit of detection and decrease the effect of the β-gal vary of in different E. coli strains, engineered phage (T7lacZ) carrying lacZ gen was furthermore built to force overexpression of β-gal in E. coli cells during phage infection. The uses of phage T7lacZ have been demonstrated to become a rapid, sensitive, and reliable colorimetric detection of viable E. coli.

AGFD 36 Dietary bioactives and neurocognitive function: The case for curcumin Andrew Scholey, andrew@scholeylab.com, Kate Cox. Centre for Human Psychopharmacology, Swinburne Univ., Melbourne, Victoria, Australia Cognitive processes involve multiple mechanisms which interact in complex, and possibly idiosyncratic ways. Monopharmacological treatments for brain disorders (including cognitive decline and dementia) have therefore had little impact on the disorders. There is increasing evidence that certain dietary components can impact positively on cognitive function during aging. It may be that by affecting multiple systems, bioactive nutrients, including widely consumed plant flavonoids such as curcumin may offer a more promising approach. This talk will draw on specific examples from a ten year systematic assessment of the behavioural effects of dietary interventions focusing on a recent trial on the cognitive effects of LongvidaTM a highly bioavailable curcumin preparation. In a double-blind, placebo-controlled trial, a cohort of healthy older individuals (n = 60, aged 60- 85 yrs) underwent a series of standardised tests of mood and cognitive function both acutely and following 28 days curcumin supplementation (400 mg LongvidaTM extract containing 80 mg curcumin). Acute effects of curcumin included improved working memory and attention. Following the 28-day intervention, the working memory effect was maintained and there was a significant reduction in fatigue (as measured using standardised self-report measures) and cholesterol. Undertaking the cognitive test battery itself acted as a psychological stressor, increasing negative mood. The curcumin group were significantly protected against this effect, specifically showing significantly reduced fatigue and increased calmness and contentment compared with the placebo group. Dietary flavonoids from a number of sources are capable of improving neurocognitive functioning both acutely and chronically. The RCT demonstrating benefits to mood and cognition add to a growing body of evidence of a number of health benefits following oral curcumin consumption. The mechanisms underlying the effects are not currently known but may relate to documented blood flow, anti-oxidant status and anti-inflammatory effects. Further work is needed to both replicate the behavioral effects and to explore the underlying mechanisms.

AGFD 37 Identifying ache inhibitors as bioactives from Chinese herbal medicine Jun Xu, xujun9@mail.sysu.edu.cn. Sun Yat-Sen Univ., Guangzhou, China The Buzhongyiqi decoction (BD), a Chinese herbal medicine compound, have been used to treat myasthenia gravis (MG) and Alzheimer's disease (AD). Both diseases are associated with acetylcholinesterase (AChE). We hypothesized that the bioactives were AChE inhibitors. To validate the hypothesis, a chemical structure database containing a total of 1,198 chemical structures were built from literature for the herbs (classified into Jun, Chen, Zuo, and Shi herbs, meaning sovereign, minister, assistant, and courier herbs) in BD. With ligand based and structure-based data mining technologies and molecular dynamic simulations, we found that the bioactives of the Buzhongyiqi decoction mainly existed within the Jun and Shi herbs. These bioactive were flavonoid derivatives that act as AChE inhibitors. The molecules of the Chen and Zuo herbs within the Buzhongyiqi decoction may have different functions, and need further investigation. Twenty-four phenylbenzofuran-like compounds were acquired based upon the data mining results, and tested with Ellman assays. We discovered five new AChE inhibitors with novel scaffolds with IC50 values ranging between 2.3 and 11 mM. Our work demonstrated that the bioactives of natural products could be identified by data mining technologies, and novel AChE inhibitors could be discovered by learning from the Nature.

AGFD 38 Evaluation of three tropical fruits on lifespan and experimentally induced neurodegeneration in Caenorhabditis elegans Katia C. Borges2, Juliana C. Azevêdo2, Maria F. Bezerra2, Rebecca Crews1, Roberta T. Correia2, Dhiraj A. Vattem1, dv11@txstate.edu. (1) Nutritional Biomedicine & Biotechnology, Texas State Univ., San Marcos (2) Laboratory of Food Bioactive Compounds and Dairy Technology, Chemical Engineering Dept., Federal Univ. of Rio Grande do Norte, Campus Lagoa Nova, Natal, Brazil Increased risk of neurodegenerative diseases (NDG) and reduced lifespan (LS) are liked to Type-2 diabetes mellitus (T2DM), dyslipidemia (DL) and inflammation (IF). Dysregulation in insulin/insulin-like growth factor-1 (IGF-1) (IIS) signaling, forkhead box O transcription factor (FOXO) and Silent Information Regulators or Sirtuins (SIRT) have been implicated as common etiological factors. We investigated the effect of three tropical fruits Jambolan (Eugenia jambolana Lam.), camu-camu (Myrciaria dubia HBK McVaugh) and Pitanga (Eugenia uniflora L.) fruit in Caenorhabditis elegans model for lifespan (LS) and NDG. For Alzheimer's disease (AD), time to thermally induced amyloid b1-42 (Ab1-42) mediated paralysis was evaluated in transgenic C. elegans. For Parkinson's Disease (PD), MPP+ (1-methyl-4-phenylpyridinium) induced neurodegeneration was quantified by loss in motility due to paralysis. Effect of fruit extracts and their respective fractions on modulating critical genes involved signaling pathways important in IIS, antioxidant response (AR), LS and NDG in transgenic C. elegans were quantified using fluorescence microscopy. Results suggest a statistically significant increase in lifespan coupled with a delay in Ab1-42 and MPP+ induced paralysis. Green fluorescent protein (GFP) tagged expression studies indicated a differential modulation of C. elegans homologs of

genes relevant to IIS, AR and NDG by individual fruits and their fractions. In our preliminary evaluation, these tropical fruits conferred neuroprotection and prolonged lifespan in C. elegans. Further studies on elucidating the molecular mechanism of action and bioactive principles from these fruits are currently underway.

AGFD 39 Experimental and theoretical studies toward the development of new amyloid inhibitors against amyloid-β aggregation
Jie Zheng, zhengj@uakron.edu. Chemical and Biomolecular Engineering, The Univ. of Akron, Ohio The misfolding and aggregation of amyloid-β (Aβ) peptides into amyloid fibrils is regarded as one of the causative events in the pathogenesis of Alzheimer disease (AD). Searching for inhibitors that can inhibit Aβ aggregation would provide alternative therapeutic opportunity for treating AD. Herein, we offer two examples to illustrate the design and screen of Aβ aggregation inhibitors. The first example is tanshinones that are extracted from Chinese herb Danshen and traditionally used as anti-inflammation and cerebrovascular protection drugs. We found that Tanshinone I (TS1) and Tanshinone IIA (TS2) exhibit different inhibitory abilities to prevent unseeded amyloid fibril formation, disaggregate preformed amyloid fibrils, reduce Aβ-induced cell toxicity. But, TS1 shows better inhibitory potency than TS2. The second example is peptide- based Aβ inhibitors. A hybrid high-throughput computational method is developed to efficiently screen and design peptide-based inhibitors against Aβ aggregation and toxicity from the first principle, followed by experimental validation. We propose and demonstrate a proof-of-concept of the "like-interacts-like" design principle that the self- assembling peptides are able to interact strongly with conformationally similar motifs of Aβ peptides and to competitively reduce Aβ-Aβ interactions, thus preventing Aβ aggregation and Aβ-induced toxicity. Hopefully, this work provides structural-based design principles for different types of Aβ aggregation inhibitors beyond those available today.

AGFD 40 Neuroprotective effects of urolithins, pomegranate ellagitannin-gut microbial derived metabolites: In silico, in vitro, and in vivo studies Daniel B. Niesen1, dan_niesen@my.uri.edu, Tao Yuan1, Hang Ma1, Nishan Shah1, Weixi Liu1, Rebecca Crews2, Dhiraj Vattem2, Navindra P. Seeram1. (1) College of Pharmacy, Biomedical and Pharmaceutical Sciences, Univ. of Rhode Island, Kingston (2) Texas State Univ., San Marcos Emerging data supports the neuroprotective effects of several natural products, including compounds from fruit, berries, spices, and nuts, against Alzheimer's disease (AD). Among these, the pomegranate (Punica granatum) fruit has been reported to show anti-AD responses in several transgenic animal models ranging from decreased brain deposition of the amyloid-β peptide to improvements in learning related tasks. From a pomegranate extract (PE), previously reported by our group to have anti-AD effects in an aged transgenic animal model, twenty-one compounds, which were primarily ellagitannins, were isolated and identified (by HPLC, NMR and HRESIMS). However, it is well known that ellagitannins are not bioavailable but rather are converted by gut microflora into colonic derived metabolites, namely, urolithins (dibenzopyranone derivatives), which reach physiologically relevant concentrations in vivo. Therefore, we hypothesized that urolithins are the relevant brain absorbable compounds contributing to the anti-AD effects of pomegranate. Indeed, computational studies, used to predict blood brain barrier permeability, revealed that none of the PE constituents, but the urolithins, fulfilled criteria required for brain penetration. Urolithins prevented β-amyloid fibrillation in vitro and methylated-urolithin B, but not PE or its predominant ellagitannins, had a protective effect in Caenorhabditis elegans post induction of amyloid β1-42 induced neurotoxicity and paralysis. Additionally, the urolithins were screened using Autodock Vina to evaluate ligand-receptor binding affinity. Further in vivo studies to investigate the brain permeability and anti-AD potential of urolithins are warranted.

AGFD 41 Metabolomics of urinary metabolites as well as in grape seed bioactives that may have a role in postmenopausal neurodegeneration John Cutts1, Landon Wilson1, Stephen Barnes1,2, Helen Kim1,2, helenkim@uab.edu. (1) Dept. of Pharmacology and Toxicology, Univ. of Alabama at Birmingham (2) Targeted Metabolomics and Proteomics Laboratory, Univ. of Alabama at Birmingham Rats that have undergone surgical ovariectomy (OVX) (a rodent model of menopause) have impaired cognitive function, presumably due to the loss of circulating 17b- estradiol, which when restored has been shown to have behavioral benefit. Dietary intake of grapeseed extract (GSE), enriched in polyphenols, attenuated cognitive impairment in ovariectomized rodents. We examined the urinary biomolecule composition following OVX, as well as GSE polyphenols, to complement our understanding about behavioral dysfunction following OVX, as well as the actions of GSE in OVX rats. We used nano-liquid chromatography tandem mass spectrometry (nano-LC-MS/MS) to examine urinary metabolites from spontaneously hypertensive rats, since the GSE behavioral benefits were previously demonstrated in these rats. The rats were OVX or sham-OVX, and given GSE daily for 4 days, after which 24 h urines were collected. All urine samples were deproteinated then extracted with ethyl acetate, dissolved in water and filtered through a 0.22 mm filter, and finally subjected to LC- MSMS. Positive ion spectra were collected and uploaded to the Scripps XCMSonline server, where they were analyzed using METLIN software. Over 5,500 peaks with unique retention times were resolved in a gradient of acetonitrile. 0.2% had $p < 0.001$. A striking difference was that selected phospholipids were 10-15 fold lower in the OVX group. Ongoing informatics analysis will reveal identities of peaks not initially identified, due to limitations in the existing databases. In complementary studies, targeted LC- MS/MS revealed that selected GSE polyphenols, namely epicatechin and 3-O-methyl- epicatechin, were more glucuronidated in the urines of OVX rats, although the total amounts of the polyphenols were similar between sham and OVX rats. We hypothesize that understanding the metabolomics differences resulting from OVX will enhance our understanding of the neurodegeneration resulting from OVX. Furthermore, the higher glucuronidation of GSE polyphenols indicates that postmenopausal women may need higher doses of bioactives such as GSE.

AGFD 42 Typicity of great Chardonnay wines, evidence for new potent markers Jacques Gros1, jacques.gros@u-bordeaux.fr, Axel Marchal1, Valérie Lavigne2, Virginie Moine3, Philippe Darriet1. (1) Oenology, Wine and Vine Sciences inst. - Université de Bordeaux, Villenave d'Ornon, France (2) Seguin Moreau France, Cognac (3) Laffort group, Bordeaux, France Vigorous and flexible, Chardonnay vine is the world most planted white grape variety. The derived wines have their own sensory properties, distinctly recognized by tasters (Ballester et al., 2005). Researches focused on the most encountered "yellow fruit", "butter" and "honey" characters, leading to the evidence for non specific odorant markers (Moio et al., 1994; Lee and Noble, 2003; Jaffre 2009). However, for the finests Chardonnay wines models, experts describe a more complex bouquet, poorly studied until now. This paper exposes the investigation on molecular determinants of those specific and rare odorant characters. Chardonnay wines coming from different origins were assessed for their level of typicity. The main odorant attributes were collected among the panelists. Besides the recurrent descriptors such as "butter", "gunflint" or "yellow fruit", the terms "hazelnut", "almond", "bergamot", "white flowers" and "verbena" emerged as important descriptors, in accordance with the tells of experts. To investigate the molecular determinants of these notes, gas chromatography olfactometry experiments were conducted on the corresponding wine extracts. Odorant Zones (OZ) "Hazelnut" and "almond" have been specifically perceived in the high typical

Chardonnay wines extracts. High resolutive multidimensional GC-GCMS analysis has been focused on each of these specific OZs. Two nutty-like carrying a 5-membered ring heterocycle were evidenced. By seeking specific ions in the chromatograms, three more compounds sharing the same moiety were evidenced. Despite occurring at levels below their individual odor threshold, their occurrence in typical Chardonnay wines was significantly more abundant than in bad Chardonnay wine examples and non Chardonnay wines. This result is noticed regardless of oak aging. The paper deals with the odorant behavior of a single family of volatile markers present in combination. A new model of compounds entering into the composition of Chardonnay model wines is proposed. Those results open up new prospects for a more accurate monitoring of Chardonnay winemaking.

AGFD 43 Unravelling fruitiness in Vitis vinifera cv. Carmenere red wines Eduardo Agosin1, agosin@ing.puc.cl, Carolina Pavez2, Maria Inés Espinoza2. (1) Chemical and Bioprocess Engineering, Pontificia Universidad Catolica de Chile, Santiago, (2) DICTUC SA, Centro de Aromas y Sabores, Santiago, Chile Consumer wine preferences are increasingly oriented towards more fruity wines. Odorant compounds related to fruitiness are primarily fermentative ethyl esters, such as ethyl isobutyrate and ethyl hexanoate, among others. Varietal aroma compounds also contribute to this character, particularly C13-norisoprenoids and thiols. The latter are highly reactive and normally present at very low concentrations. They are responsible for grapefruit and exotic fruity aroma notes in white wines; and contribute in red wines with red- and black-berry-like aroma notes, as well. The quantitative analysis of these compounds is quite difficult, particularly due to the wine matrix effect and their low concentrations in wine. In this work, we developed - and optimized - a SPME extraction method of volatile compounds in red wines to identify and quantify thiols - 3-sulfanyl-1-hexanol (3SH), 3- sulfanylhexyl acetate (3SHA), 4-sulfanyl-4-methyl-2-pentanone (4SMP), phenylmethanethiol (PhMT) and 2-furanylmethanethiol (FFT)); C13-norisoprenoids (β- damascenone, α- and β-ionone) and ethyl esters present in wine. Quantitation was carried out by CG-MS in negative ionization mode. Recovery values ranging from 94% to 119% in red wines were achieved. Repeatability and reproducibility for all analytes, expressed in RSD, were below 15%. The proposed method was applied to several Vitis vinifera cv. Carmenere varietal red wines of the 2013 vintage from Colchagua and Cachapoal Valleys (Southern Chile). Thiol content in the selected wines was variable, particularly for PhMT, 3SHA and 3SH. Sensory profiling by a trained panel showed fruity attributes in these samples correlate well with the concentration of the quantified compounds. Wines with the highest concs. of 3SH (3100 ng/L) and 3SHA (95 ng/L) exhibited strong cassis, blackberry, raspberry, strawberry and cherry attributes.

AGFD 44 Synergistic effects of copper and pH - wine making variables that significantly impact reductive aromas in wines Marlize Z. Bekker, marlize.bekker@awri.com.au, Mark E. Smith, Agnieszka Mierczynska-Vasilev, Paul A. Smith, Eric Wilkes. The Australian Wine Research inst., Adelaide, South Australia, Australia Winemakers have the ability to influence a range of components during the winemaking process. Managing wine pH and remedial treatments such as Cu2+ fining, are two of these variables that can be controlled post-fermentation before bottling, helping winemakers to instill their unique style and signature to wines. The role of Cu2+ in the formation of H2S has been well established, however, the synergistic effect of wine pH and Cu2+ addition on the formation of volatile sulfur compounds (VSCs) associated with 'reductive' aromas in wines has not yet been studied. Four VSC compounds were significantly influenced by pH effects, with lower wine pH associated with decreased H2S, MeSH, DMS, and CS2 concentrations in both Chardonnay and Shiraz wines. Treating wines with Cu2+ resulted in significantly increased H2S (Figure 1), however, at lower wine pH the total produced H2S 2+ concentration was significantly decreased. This suggests the availability of Cu catalyze the formation of H2S was inhibited by lowering the pH of the wines. The interaction between H2S and variable pH concentrations on Cu2+-complex particle sizes was subsequently studied in a model wine matrix using nanoparticle tracking analysis. It was found that different wine pH levels as well as H2S addition significantly impacts the particle size and concentrations. This suggest that the pH of the wine affects the type of Cu2+-complexes produced which may subsequently impact on the reactivity of Cu2+ and its ability to interact with wine compounds and be involved in the catalytic formation of VSCs. These results confirm that formation of VSCs post-bottling is regulated by a complex range of variables. Some, such as pH and Cu2+ treatment, are within winemakers' ability to manipulate to reduce the overall impact of VSCs on wine aroma.

AGFD 45 Impact of vineyard exposure to smoke on wine composition and sensory properties Lieke van der Hulst1, Chris Ford1, Rachel Burton1, Renata Ristic1, Natoiya Lloyd2, Yoji Hayasaka2, Paul Boss3, Kerry Wilkinson1, kerry.wilkinson@adelaide.edu.au. (1) Wine Science, The Univ. of Adelaide, South Australia (2) The Australian Wine Research inst., Glen Osmond, South Australia (3) CSIRO Plant Industry, Adelaide, South Australia Taint in grapes and wine as a consequence of vineyard exposure to bushfire smoke has resulted in significant financial losses for grapegrowers and winemakers in Australia, Canada, South Africa and the USA. Several volatile phenols have been identified in wines made from fruit harvested from smoke-affected grapevines; but the accumulation of smoke-derived volatile phenols in glycoconjugate precursor forms has also been demonstrated. The taint, characterized by objectionable 'smoky', 'smoked meat', 'dirty' and 'ashy' aroma and flavor attributes, is thought to be influenced by the duration and phenological timing of smoke exposure. However, the concentration of smoke taint marker compounds and intensity of smoke-related sensory attributes in wine might also depend on cultivar, and fruit maturity at harvest. This paper describes trials undertaken to determine to the extent to which smoke taint develops in wines made from smoke-affected grapes (i) from different grape varieties and (ii) harvested at different maturity levels (i.e. at total soluble solids of 16-20 °Brix vs. 22-25 °Brix). Three white grape varieties (Chardonnay, Sauvignon Blanc and Pinot Gris) and four red grape varieties (Shiraz, Cabernet Sauvignon, Merlot and Pinot Noir) were exposed to smoke under experimental conditions (for 1 hour) at approximately 7 days post-veraison. The impact of smoke exposure on wine sensory properties was evident, irrespective of grape variety, and descriptive sensory analysis readily differentiated control (unsmoked) and smoked wines. In a related trial, grapevines from two white grape varieties (Chardonnay and Sauvignon Blanc) and two red grape varieties (Shiraz and Merlot) were exposed to smoke at two levels of maturity. Smoke-related sensory attributes were more apparent in Sauvignon Blanc wine made from early-harvested fruit and in Chardonnay wine made from late-harvested fruit, only; whereas Merlot and Shiraz wines exhibited smoke taint irrespective of fruit maturity. The implications of these research findings for industry, with respect to detecting and assessing smoke tainted grapes and wine, will also be presented.

AGFD 46 Relating sensory attributes, notably 'tropical fruit' flavour and volatile chemical composition in Chardonnay wines Dimitra L. Capone, dimitra.capone@awri.com.au, Alice Barker, Patricia Williamson, Leigh Francis. Research, AWRI, Adelaide, South Australia The Chardonnay wine variety is one of the top selling white varieties around the world and its wine style can vary quite significantly in both taste and aroma. Aromatically the aromas can vary between 'tropical', 'grapefruit', 'pineapple', 'stonefruit', 'lime', 'green apple' to 'pungent' and 'green'. In order to investigate the diversity of this wine style a set of 20 grape juices was sourced from

vineyards across multiple regions in Australia, selected on the basis of historical knowledge regarding likelihood of producing the 'tropical fruit flavour' (passionfruit, pineapple). The juices were fermented under standardised conditions, with no oak treatment, and the varietal thiol compounds involved in the tropical fruit character were quantified in the wines using a recently developed LC-MS/MS method, together with other key aroma compounds. The sensory profiles of the wines were assessed through a trained descriptive analysis panel, and multivariate relationships were determined between the sensory profile and the chemical composition in the data sets. Additionally varietal thiol data was quantified and will be presented from a survey of commercially available Chardonnay wines to investigate the importance of these compounds to Chardonnay wines.

AGFD 47 Role of selected microbial dehydrogenases in the synthesis of flavor compounds Selim Kermasha, selim.kermasha@mcgill.ca. Food Science Agr. Chemistry, McGill Univ., Sainte-Anne-de-Bellevue, Quebec, Canada The presence of selected dehydrogenases, including alcohol dehydrogenase (ADH-YL) and aldehyde dehydrogenase (ALDH-YL), in Yarrowia lipolytica JMY 861, and their potential role in the synthesis of flavor compounds were investigated. The experimental findings showed that using reduced form of nicotinamide adenine dinucleotide (NADH) as cofactor, the ADH-YL activity in-vitro was 6-fold higher than that with reduced form of nicotinamide adenine dinucleotide phosphate (NADPH); however, the results indicated the absence of any ALDH-YL activity. The in-situ reduction of hexanal into n-hexanol was found to be instantaneous; however, when the yeast cells suspension was diluted by 150-time, the initial relative hexanal concentration was increased by 84.1%. Using the diluted yeast cells suspension, the in-situ hexanal reduction reaction was achieved within 70 min of reaction, with a 95.4% relative n-hexanol concentration. The in-situ relative n-hexanol concentration decreased steadily with a concomitant increase in the hexanal concentration. The optimum pH of 6.7 for the biomass production of Y. lipolytica was shown to favor the hexanal reduction over the n-hexanol oxidation. The chromatographic analyses indicated the conversion, in-situ, of linoleic acid hydroperoxides (HPODs) into volatile C6-compounds, mainly 2-hexanone, hexanal, 3- hexanol and 2-hexenol, after 60 min of HPODs addition to the yeast cells suspension.

AGFD 48 Building a subdivision at the ACS: Sowing the seeds of change Ezra M. Pryor3, ezra.pryor@gmail.com, Jahan Marcu2, Melissa J. Wilcox1. (1) Grace Davison Discovery Sciences, Bannockburn, Illinois (2) Green Standard Diagnostics, Inc., Brooklyn, New York (3) Ez Chem Consulting, Ontario, California This presentation of the AGFD symposium offers a unique perspective on the evolution of the cannabis chemistry movement being the founding member of the nascent CANN subdivision. Learn how it all started and what have been challenges along the way. Ezra will discuss the challenges of building a volunteer base, working with a very large parent organization, overcoming stigmas, and the benefits of getting involved.

AGFD 49 Potency trends in confiscated cannabis and analytical methods Mahmoud A. Elsohly1,2, elsohly@elsohly.com. (1) Elsohly Labs Inc, Oxford, Mississippi (2) Nat'l Ctr for Natural Products Research, Sch of Pharmacy, Univ. of Mississippi, Oxford Cannabis is the most widely abused drug in the world due the psychological activity of its major constituent (of the drug type) Δ9-tetrahydrocannabinol (THC). The drug contains over 500 constituents belonging to over 20 different chemical classes the most important of which is the cannabinoids with 104 components, most prominent of which are THC and CBD (cannabidiol). We have been monitoring the levels of these two predominant cannabinoids along with 5 other cannabinoids existing in much lower levels but significant enough to monitor. With the much interest in cannabis for therapeutic purposes and the two major cannabinoids (THC for the drug type and CBD for the fiber type), this presentation will give some insights into the changes in the levels of these cannabinoids, over the last few years in confiscated products. GC-FID was used throughout the study and therefore only the total cannabinoid levels are given. However, we have recently developed HPLC, UPLC, and SFC methods, which could provide levels for the major neutral and acidic cannabinoids. These methods will be presented as well as the kinetics of the decarboxylation process by which the acidic cannabinoids are converted to the neutral, pharmacologically active components. Supported by the National inst. on Drug Abuse (NIDA) contract # N01DA-10-7773.

AGFD 50 Responsible cultivation policy: Preserving personal cultivation rights while regulating commercial cultivation as agriculture Kristin Nevedal2, kristin@patientfocusedcertification.org, Jahan Marcu1. (1) Green Standard Diagnostics, Inc., Brooklyn, New York (2) Patient Focus Certification, Washington, DC This presentation will cover the following topics Overview of Cultivation policy nationally, Cultivation Techniques or Methods used Nationally , Plant Count vs. Square Footage Regulatory Models, Environmental Considerations, Cultivation Bans, Responsible Solutions Within the thirty-five states referenced in the States Report, various types of cultivation techniques, or methods, are allowed depending on the State and possibly the locality in which the cultivation is taking place. While the vast majority of States with medical cannabis programs require that cannabis be cultivated indoors, a few states also allow for open air, greenhouse and row cover methods of cultivation. All cannabis cultivation poses risk to the environment relating to the use of mediums, nutrients, water, and pesticides. Indoor cultivation poses additional environmental concerns due to the necessary and intensive electricity use associated with the high intensity discharge lighting systems, ventilation systems, heating and cooling systems, etc. In 2011, Dr. Evan Mills released a report on the carbon footprint of indoor cannabis cultivation entitled Energy Up in Smoke. Dr. Mills estimated that cannabis cultivated using national average grid electricity, results in the emission of approximately two pounds of greenhouse gas per cannabis cigarette produced. Throughout the US two different methods are used for regulating cannabis cultivation. The most popular method is to restrict the number of plants allowed to be cultivated, referred to as a plant count based regulatory system. The most responsible regulatory method however, is to regulate based on the square footage of mature plant canopy. Square footage based regulatory systems are used in some States and within California depending on local regulatory ordinances. It is important to note that the Dept. of Food and Agriculture utilizes a square footage based model to regulate crops produced for human consumption. Based on the information presented in this workshop, the conclusion can be drawn that utilizing a square footage based model for regulating cannabis cultivation provides not only the most accurate means of estimating yields but also allows farmers to utilize cultivation techniques that vastly reduce the potential for adverse environmental impacts. Therefore regulating cannabis cultivation in a manner that is analogous to other crops produced for human consumption provides the most responsible means of regulation.

AGFD 51 Improving quality control methods for cannabis using flash chromatography Jahan Marcu3, James P. Kababick1, Melissa J. Wilcox2, melissa.wilcox@grace.com, Mark Jacyno2. (1) Flora Research Laboratories, Grants Pass, Oregon (2) Grace Davison Discovery Sciences, Bannockburn, Illinois (3) Green Standard Diagnostics, Inc., Brooklyn, NY The American Herbal Pharmacopeia (AHP) recently

published a Cannabis monograph, setting standards for identification, analysis, and quality control. Additionally, the American Herbal Products Association (AHPA) issued basic product safety guidelines for cultivation, manufacturing, dispensing, and laboratory operations for medical Cannabis. The recommendations from the AHP and AHPA are steadily being adopted and are implemented in US states through a 3rd party oversight program called Patient Focused Certification. However, a number of significant hurdles must be overcome to reach higher levels of product safety. Among the issues facing laboratories are access to high purity reference standards, transportation of samples for pesticide or contaminant analysis, having flexibility to efficiently quantify several compounds from a variety of complex matrices in a high throughput manner, dependency on the use of high amounts of toxic solvents, and a shortened life span of expensive analytical equipment used in the routine analysis of viscous and particulate samples. Flash chromatography can help overcome some of the issues facing laboratories engaged in quality control of Cannabis medicines by offering a more efficient way to isolate cannabinoids and other compounds of interest from complex matrices, enhancing potency testing and characterization techniques. Our data was obtained by analyzing complex matrices, i.e., edibles (gummy candy, chocolate, brownies, oil) and topicals (lotion) spiked with known amounts of cannabinoids. We also demonstrate how flash technology can be used to isolate individual canabinoids that can be used as reference standards.

AGFD 52 Cannabis: Taxonomy and secondary metabolism Justin Fischedick, justin@excelsioranalytical.com. Excelsior Analytical Laboratory, Richmond, California, US The taxonomy of the genus Cannabis has often been the subject of legal and scientific debate. Traditionally this debate has centered on how to legally distinguish cannabis used for its fiber / seed commonly called hemp and cannabis used for its intoxicating / medicinal effects known commonly in North America as ‘marijuana’. Currently as more countries and states legalize the use of medical marijuana the need to classify cannabis based on its therapeutic properties has emerged. The secondary metabolites found in cannabis have been extensively characterized. Over 100 terpenophenolic compounds known as cannabinoids have been identified. Cannabis also produces numerous terpenoids, flavonoids, and nitrogenous compounds. In this lecture I will discuss the chemical diversity, biosynthesis, and biological activity of the various compounds found in cannabis. Furthermore I will discuss how these compounds especially cannabinoids and terpenoids can be used to chemically classify cannabis cultivars. Specifically, I will highlight the research my colleagues and I have done in this area over the past decade.

AGFD 53 Laboratory preparations of vinaxanthone and xanthofulvin, natural products enhancing CNS regeneration Dionicio Siegel, drsiegel@ucsd.edu. Skaggs School of Pharmacy and Pharmaceutical Sciences, Univ. of California, San Diego, California, US The natural products vinaxanthone and xanthofulvin have been shown to have remarkable regenerative effects in animal models of spinal cord injury. After complete severing of the spinal cord continuous delivery of either compound leads to a number of beneficial effects including; enhanced axonal regeneration, remyelination, decreased apoptosis, and enhanced angiogenesis at the site of injury. These compound driven effects all led to an improved outcome following injury. We have developed synthetic routes to both natural products, providing the first laboratory synthesis of xanthofulvin and second of vinaxanthone. To access derivatives of vinaxanthone a new ynone coupling reaction has been developed providing expedited syntheses of chemically edited derivatives. The coupling reaction allows rapid access to new derivatives, wherein n ynone precursors generate n2 vinaxanthone analogs. Testing these compounds for the ability to promote neuronal regrowth by severing axonal connections in C. elegans using laser axotomy has provided preliminary structure-activity relationships for vinaxanthone.

AGFD 54 Salvia divinorum: A unique CNS active plant Thomas E. Prisinzano, prisinza@ku.edu. Medicinal Chemistry, Univ. of Kansas, Lawrence Salvia divinorum Epling & Játiva (Lamiaceae) is a mint plant native to Oaxaca, Mexico that has been used for centuries for its vision-inducing and analgesic properties. Although the sacramental use of S. divinorum by indigenous people dates back hundreds of years, an understanding of the psychoactive effects by American and European drug users dates back only about 20 years. Since the finding that the major active component, salvinorin A, exerts its potent psychotropic actions through the activation of opioid receptors, the site of action of morphine and related analogues, there has been much interest in elucidating the underlying mechanisms behind its effects. These effects are particularly remarkable, because (1) salvinorin A is the first reported non-nitrogenous opioid receptor agonist, and (2) its effects are not mediated by serotonin receptors, the classical target of hallucinogens such as LSD and mescaline. This talk will outline our recent progress in developing novel treatments for CNS disorders by targeting opioid receptors. In particular, our efforts to develop drug abuse medications through a better understanding of the chemistry and pharmacology of salvinorin A will be described.

AGFD 55 Discovery of anti-Alzheimer agents from Chinese herbal medicine Qiong Gu, guqiong@mail.sysu.edu.cn, Jun Xu. Research Center for Drug Discovery, School of Pharmaceutical Sciences, Sun Yat-Sen Univ., Guangzhou, China Salvia genus plants have been used as multiple functional agents in Chinese herbal medicine for many years. These plants contain structurally diverse molecules, including sesquiterpenoids, diterpenoids, polyphenols, triterpenoids, and steroids et al. According to clinic data, one of the therapeutic functions of these plants is aromatic resuscitation, which is associated with treating neurodegenerative diseases including Alzheimer disease (AD). To identify the active ingredients of the herbs as anti-Alzheimer agents, we investigated Salvia miltiorrhiza Bunge with phytochemistry, bioassay experiments, and cheminformatics. The studies revealed that salvianolic acid derivatives were the anti-AD agents with multiple functions. The compounds inhibited amyloid beta (Aβ) aggregation, chelated metal ions that induced Aβ aggregation, blocked reactive oxygen species formation in SH-SY5Y cells, and alleviated Aβ-induced paralysis in transgenic Caenorhabditis elegans. Salvianolic acid-like fragments exist in many molecular structures discovered from S. miltiorrhiza Bunge plants. Our observation indicated that salvianolic acid like fragments are privileged scaffolds for anti-AD agents. This discovery may help to identify more active anti-AD agents from Chinese herbal medicine.

AGFD 56 Fungal metabolome as a rich resource for tau aggregation inhibitors Smita R. Paranjape1, Yi-Ming Chiang2, Clay C. Wang2,3, Berl R. Oakley1, Truman C. Gamblin1, gamblin@ku.edu. (1) Dept. of Molecular Biosciences, Univ. of Kansas , Lawrence (2) Dept. of Pharmacology and Pharmaceutical Sciences, School of Pharmacy, Univ. of Southern California, Los Angeles (3) Dept. of Chemistry, Univ. of Southern California, Los Angeles The abnormal aggregation of the microtubule-associated protein tau is closely linked to neuronal death and subsequent cognitive deficits in Alzheimer’s disease and other related neurodegenerative diseases. The inhibition and reversal of tau aggregation is believed to be a significant target for the development of therapeutic strategies to treat such disorders. In our efforts to identify tau aggregation inhibitors (TAIs), we have sought to explore the secondary metabolome of the fungus Aspergillus nidulans for unique compounds with anti-tau aggregation properties. Fungal natural products have historically been a rich source of biologically

important compounds ranging from anti- cholesterol medications to antibiotics. By screening just a small library of A. nidulans natural products, we were able to identify three lead compounds capable of inhibiting tau aggregation. One of these, asperbenzaldehyde, represented a novel class of TAI. Because asperbenzaldehyde is a precursor to the chemical class of azaphilones, we subsequently generated and analyzed the TAI activity of 11 azaphilone derivatives in vitro. We found that all azaphilone derivatives tested inhibited tau aggregation. Four of the compounds also caused the disassembly of pre-formed filaments in a dose- dependent fashion by reducing both the length and number of tau filaments. Tau also retained significant microtubule-stabilization activity even in the presence of the most potent TAI, indicating that azaphilone scaffold may be a very promising structural core for future development of tau therapeutics and that the A. nidulans secondary metabolome is a rich resource for the further discovery of TAIs.

AGFD 57 Disaggregation of amyloid beta peptides by tabersonine and related compounds: Biophysical, bioanalytical, and cytotoxicity studies Tianhan Kai1,2, Lin Zhang3, Gargey B. Yagnik1, Aihua Jing1, Bingqing Zhao1, Feimeng zhou1, fzhou@calstatela.edu. (1) Dept. of Chemistry, California State Univ., Los Angeles (2) College of Chemistry and Chemical Engineering, Central South Univ., Changsha, China (3) College of Food Science and Technology, Central South Univ. of Forestry and Technology, Changsha, China Aggregates of amyloid beta (Aβ) peptides are believed to be responsible for the neuropathology of Alzheimer's disease and effective inhibition of the Aβ peptide aggregation should be a viable modality for treating AD. In this presentation, we will describe the inhibition of Aβ fibril formation by tabersonine, an ingredient extracted from the bean of Voacanga Africana. Tabersonine at 10 μM can inhibit the formation of Aβ(1- 42) fibrils or convert mature fibrils into largely innocuous amorphous aggregates. A variety of biophysical methods (surface plasmon resonance, ThT assay, circular dichroism, and size exclusion chromatography) are used in conjunction with cytotoxicity assays and molecular dynamics calculations to elucidate the interaction between Aβ peptides and tabersonine. We will also present other studies that address and detect Aβ aggregates formed in vitro and in vivo. We will show that surface plasmon resonance is a useful technique for detecting biomarkers of neurological significance in cerebrospinal fluids. Techniques, such as voltammetry and chromatography combined with electrochemical detection, demonstrated to be powerful for studying the inhibition of Aβ peptide aggregation by curcumin.

AGFD 58 Efficient synthesis and neuroprotective activity of CN2097: A cyclic disulfide polyarginine peptidomimetic binding PDZ domain of PSD-95 Rakesh K. Tiwari1, rakeshtiwarisir@gmail.com, Siva R. Kotla1, John Marshall2, Dennis J. Goebel3, Keykavous Parang1. (1) Biomedical and Pharmaceutical Sciences, Chapman Univ. School of Pharmacy, Irvine, California (2) Dept. of Molecular Pharmacology, Physiology, and Biotechnology, Brown Univ., Providence, RI (3) Dept. of Anatomy and Cell Biology, School of Medicine, Wayne State Univ., Detroit, Michigan PDZ domains are an adaptor or scaffold proteins involved in protein-protein interactions and modulation of numerous cellular process. The PDZ3 domain of the postsynaptic density-95 protein (PSD-95) is important in the development of neurobiological diseases, such as stroke associated with ischemic brain damage, psycho-stimulant addition, and Angelman syndrome (AS). A peptidomimetic CN2097 consists of a polyarginine peptide linked through a disulfide linker with a PDZ cyclic peptide containing a lactam ring and a β-alanine linker (R7-Cs-sC-YK[KTE(β-Ala)]V) was used to understand the function of PSD-95. The peptide forms unique contacts outside the canonical PDZ binding pocket. The limitation of current synthetic methodology prompt us to design efficient synthesis of CN2097 to provide sufficient amounts of CN2097 for preclinical studies. The PDZ domain cyclic peptide was synthesized by using Fmoc/tBu solid phase chemistry followed by cleavage of the peptide from the resin with in situ sulfur activation. This methodology provided a high yield of the peptide with activated cysteine that formed a disulfide linkage with polyarginine peptide containing a cysteine residue in the water to afford CN2097 in 6 h with 90% yield. CN2097 was used to evaluate neuroprotective activity against AS. AS characterize with a serve cognitive impairment and autism due to loss of expression of the maternally inherited allele of the Ube3A ubiquitin gene. The mice deficient of Ube3A gene produce low long term potentiation (LTP) which related with high activity-regulated cytoskeleton-associated protein (Arc/Arg3.1). The high level of arc interfer with brain-derived neurotrophic factor (BDNF) TrkB receptor signaling which induce LTP induction and maintenance. We found that CN2097 binds to PDZ domain of PSD-95 which decrease the interaction of Arc with PSD-95 to restore BDNF-induced TrkB/PSD-95 complex formation, signaling, and facilitate the induction of LTP in AS mice.

AGFD 59 Applied peptidomics and digestomics to guide protein nourishment in infants for optimal gut health David Dallas, dcdallas@ucdavis.edu. Food Science and Technology, Univ. of California, Davis Infants have immature gastrointestinal tracts that are both less capable of protein digestion and more sensitive to potential damage than adults. Premature infants, particularly, have inadequate digestive processes. Working with neonatal intensive care units, we have collected samples from infants, including gastric contents, stool and urine as well as their mother's milk. We have assembled a state-of-the-art mass spectrometry- and computation-based peptidomics platform to identify how proteins are digested in vivo in these infants. Our research has revealed, with sequence-specific detail, that milk contains enzymes that begin to digest milk proteins within the mammary gland and continue to assist in digestion in the infant's stomach. Ongoing research in our lab investigates milk protein digestion in piglet models. Specifically, we are investigating the effects of intact milk proteins vs. hydrolyzed milk proteins vs. milk proteins with an added protease in the context of a high protein weaning diet on protein digestion, the gut microbiome, microbial metabolism and gut inflammation. High protein diets can increase microbial protein degradation (putrefaction) in the colon, which increases the concentration of many inflammatory metabolites associated with gut inflammation. This model will provide insight into best practices for infant feeding of term and premature infants for optimal digestion and gut health.

AGFD 60 Alpha-lactalbumin-catechin conjugates improve the chemical stability of the vitamin A precursor β-carotene in nanoemulsions Jiang Yi2, yijiangjnu@gmail.com, Yuzhu Zhang1, Liqing Zhao2. (1) USDA, Albany, California (2) College of chemistry and environmental engineering, Shenzhen Univ., Shenzhen, Guangdong, China Free radical method was used to prepare α-lactalbumin (ALA)-catechin conjugates and the interaction between ALA and catechin was investigated with SDS-PAGE, ESI-MS, and far UV CD. Covalent binding between ALA and catechin were confirmed with SDS- PAGE, and ESI-MS. Far UV CD results showed that the content of β-sheet decreased with a corresponding increase in unordered structures after grafting. The mean particle sizes of nanoemulsions stabilized with ALA and ALA-catechin conjugates were 158.8 and 162.7 nm, respectively. Both the rate of particle growth and the total BC loss at 50 °C were greater than at 25 °C. The retention rates of β-carotene (BC) in nanoemulsions were 30.9% and 56.7% for ALA and ALA-catechin conjugates, respectively, after 30 days of storage at 50 °C. The BC retention encapsulated in nanoemulsion was significantly improved using ALA-catechin conjugates, compared with BLG alone. The antioxidative properties (reducing power, free radical scavenging activity and free radical scavenging activity) of ALA were improved with catechin conjugation, which possibly led to the increase of BC retention in

nanoemulsions. The results suggested that the milk proteins modified with polyphenols may be widely used in labile bioactive compounds encapsulation delivery system.

AGFD 61 Bioactive peptides generated from plant proteins in relation to molecular structures Lingyun Chen1, lingyun1@ualberta.ca, Zhigang Tian2. (1) Agricultural, Food and Nutritional Science, Univ. of Alberta, Edmonton, Canada (2) Univ. of Alberta, Edmonton, Canada This study has revealed strong antioxidant activities of barley hordein hydrolysate fractions and investigated the relationships between antioxidant properties and structural features of hordein peptides. Barley hordein fractions separated based on molecular weight and surface hydrophobicity demonstrated strong antioxidant bioactivities, especially ferrous ion chelating capacity. Structural studies revealed the poly-L-proline helix, β-turn and β-sheet as the dominant structural elements in the large molecular weight fraction, while most of the small sized peptides assumed unordered random coil conformation accompanied by a large amount of ionized carboxyl groups produced as a result of partial deamidation of glutamine residues during hydrolysis. A study of antioxidant capacity in relation to peptide structure indicated the contribution of hydrophobic residues in radical scavenging and the positive effect of ionized carboxyl groups together with Lys and Met in metal chelation activity. QPYPQ was identified as the most repeated sequence in potent RP-HPLC fractions, which might be a particular structural motif that plays a key role in scavenging free radicals. Cellular models confirmed that the barley peptide effectively inactivate lipid hydroperoxides and intracellular reactive oxygen species. Peptides with alternating residues were also found effective in inhibition of amyloid fibril formation.

AGFD 62 Ovomucin derived peptides as anti-adhesive agents against infectious diseases Xiaohong Sun, xs7@ualberta.ca, Michael Gänzle, Jianping Wu. Agriculture, Food and Nutritional Science, Univ. of Alberta, Edmonton, Canada The majority of infectious diseases are initiated by the adhesion of pathogens and toxins to the host tissues. Agents that can disrupt or inhibit pathogens and toxins attachment to the host tissues, and thus reduce the incidence of infectious diseases are alternatives to antibiotics, which are known the cause of drug-resistant bacteria. Ovomuicn, a glycoprotein accounting approximately for 2-4% of the total egg albumen protein, is a member of mucin family and consists of 33% of carbohydrate content on average. Ovomucin is rich in sialic acids (2.6-7.4%, w/w), which are a family of acylated derivatives of a nine-carbon carboxylated monosaccharide and play important roles in bacteria adhesion (act as glycan receptor on the surface of host tissues). The objective of the study was to study the potential of ovomucin derived peptides as an anti-adhesive agent. Ovomucin was hydrolyzed by 14 kinds of proteases and their anti-adhesive activities were screened using the hemagglutination assay. Nine hydrolysates showed minimum inhibitory concentrations (MIC) ranging from 10 to 0.31 mg/mL for two Enterotoxigenic Escherichia coli strains (ECL13795 and ECL13998). Ovomucin acid protease II hydrolysate showed the best anti-agglutinating activity (MIC: 0.31 mg/mL), and was chosen to further fractionate by ion exchange chromatography and reverse-phase high performance liquid chromatography. Finally, two fractions exerted the most potent activity, with MIC of 0.25 mg/mL and 0.03 mg/mL against strain 1033 and 1032, respectively, were further studied in IPEC-J2 cells (porcine small intestinal epithelial cell line) and characterized by HPLC-MS. Ovomucin derived peptides may have potential application as an anti-adhesive agent to prevent the infectious diseases.

AGFD 63 New tree nut allergens Yuzhu Zhang1, yuzhu.zhang@ars.usda.gov, Wen-Xian Du1, Boram Lee1,2, Yuting Fan1,4, Shu-Chen Lyn3, Kari Nadeau3, Tara H. McHugh1. (1) USDA-ARS Western Regiona Research Center, Albany, California (2) Univ. of Texas Southwestern Medical Center , Dallas (3) Stanford Univ., Stanford, California (4) School of Food Science and Technology, Jiangnan Univ., Wuxi, Jiangsu, China The 7S vicilin and 11S legumin seed storage globulins belong to the cupin protein superfamily and are major food allergens in many of the “big eight” food allergen groups. Korean pine vicilin and pecan vicilin are thus predicted to be food allergens. Recombinant vicilins were expressed in E. coli and purified. Their recognition by food allergy patient sera and the recognition patterns of urea extracts of pine nut and pecan by the same sera were analyzed by western blot. The results indicated that both the recombinant and native vicilins of Korean pine nut and pecan reacted with IgE in sera of patients with pine nut and pecan allergies, respectively. This demonstrated, for the first time, that vicilins of Korean pine and of pecan are indeed food allergens. Further studies are needed to understand the allergenicity of these copper binding seed storage proteins in tree nuts.

AGFD 64 Studies on the mechanism of calcium ion on the allergenic activity of EF-hand domain food-induced allergen Shiwen Han, shiwen0414@163.com, Huilian Che, h05074@cau.edu.cn. College of Food Science and Nutritional Engineering , China Agricultural Univ., Beijing In recent years, food allergy incidence increased year by year, with 3% to 5% of adults and 4% of children in developed countries each year. It is of great significance for finding a potential therapeutic target to preventive and control the occurrence and development of food-induced allergy. Several studies have reported that there is a close relationship between Ca2+ and food-induced anaphylaxis. Among them, the food allergen family of EF-hand domain occurs as a calcium-binding proteins and highly cross-reactive allergens between food and pollen. In this study, the composition, structure, Ca2+-binding and target interaction properties of Calcium-binding food allergens and the hydropathy, flexibility and antigenic index were analyzed by the DNAStar Protean system to predict the mechanism of Calcium-binding domain on the linear epitopes, which to further identify the influence of calcium ions to the IgE binding capacity and allergenic activity of EF-hand domain food allergen. Further researches were carried out by using human serum from patients with a positive case history of IgE-mediated allergy to EF-hand domain food allergen and BALB/c mice model assay to identify the allergen derivative mutated in calcium-binding domain had the lowest allergenic activity. We are hoping to find a new therapeutic to treat food allergy by reducing allergenic activity of food allergen protein.

AGFD 65 Influence of free amino acids, oligopeptides and polypeptides on the formation of pyrazines in Maillard model systems Gustavo Luis Leonardo Scalone2, Prabin Lamichhane2, Tatiana Cucu2, Norbert De Kimpe1, Bruno E. De Meulenaer2, bruno.demeulenaer@ugent.be. (1) Dept of Org Chem Univ Ghent, Belgium (2) Food Quality and Food Safety, Ghent Univ., Zwijnaarde, Belgium Pyrazines are specific Maillard reaction compounds known to contribute to the unique aroma of many products. Most studies concerning the generation of pyrazines in the Maillard reaction have focused on amino acids, while little information is available on the impact of peptides and proteins. The present study investigated the generation of pyrazines in model systems containing whey protein, hydrolyzed whey protein, amino acids and glucose. The impact of thermal conditions, the ratio of the reagents and the aw was measured on the pyrazine formation by HS-SPME-GC-MS. The presence of oligopeptides from hydrolyzed whey protein contributed significantly to an increased amount of pyrazines, while in contrast free amino acids generated during protein hydrolysis contributed to a lesser extent. The

generation of pyrazines was enhanced at low aw (0.33) and high temperatures (>120 C). Additional experiments were considered by using α-dicarbonyl compounds in model experiments in order to further elucidate the different mechanisms of pyrazine formation. As a result, some pyrazines were found to be amino acid specific while others were produced more abundantly in peptide containing systems. This study showed that peptides are very important Maillard reaction precursors, and that their role in the generation of pyrazines in Maillard reaction systems has been dramatically underestimated.

AGFD 66 Cold-adapted β-galactosidase from a psychrotrophic bacterium Rahnella sp. R3: Protein structure and enzymatic properties Yuting Fan2,1, yilin58299@163.com, Yuzhu Zhang1, Ruijin Yang3. (1) USDA, Albany, California (2) Food Science and Technology, Jiangnan Univ., Albany, California (3) jiangnan university, Wuxi, China The cold-adapted β-galactosidase (R-β-Gal) from psychrotrophic bacterium Rahnella sp. R3 is a member of the glycoside hydrolases family 42 and it is a cold-adapted β- galactosidase. It was cloned and expressed in E. coli BL21. The purified R-β-Gal retained 80% of its maximum activity at temperatures as low as 4°C and formed a 225kDa trimeric structure in solution. R-β-Gal was crystalized and its crystal structure was solved. To the best of our knowledge, this is the first cold-adapted protein structure of GH42 enzymes. Each R-β-Gal molecule consists of three domains, an N-terminal catalytic domain that forms a (β/α)8 TIM barrel, a mixed β-sheet and α-helix domain, and a C-terminal β-sandwich domain. R-β-Gal did not require the presence of metal ions to be active and the presence of metal ions, such as Ca2+, Co2+ and Al3+ caused different levels of secondary changes of the enzyme. In consistent with the other structural known β-galactosidases of GH42, there is a zinc atom ligated by four cysteine residues in the second domain of R-β-Gal. Two residues, Glu157 and Glu314, superimposed well with the catalytic residues of other β-galactosidases were predicted to be required for its catalytic activity and this was verified by site-directed mutagenesis.

AGFD 67 Structural modification of an immunodominant gluten peptide upon interaction with (-)-epigallocatechin-3-gallate Charlene Van Buiten1, charlene.vanbuiten@gmail.com, Carlos N. Pacheco2, Emmanuel Hatzakis2, Ryan Elias1. (1) Food Science, The Pennsylvania State Univ., Univ. Park (2) Chemistry, The Pennsylvania State Univ., Univ. Park Tea is one of the most widely-consumed beverages in the world, and has been studied extensively for its putative benefits to human health. (-)-Epigallocatechin-3-gallate (EGCG), a major phenolic constituent of tea, has demonstrated biological activity against major inflammatory pathways and hypersensitivity disorders, as well as the ability to alleviate symptoms of food allergies and intolerances. One proposed mechanism of this effect is sequestration and structural modification of immunostimulatory proteins as a result of direct interactions with EGCG. Recent studies in our lab have demonstrated the ability of dietary polyphenols, including EGCG, to interact with a2-gliadin (57 – 89), a 33-amino acid peptide responsible for the stimulation of the adaptive immune response associated with celiac disease. The present work characterizes the impact of these interactions on the structural confirmation of the 33- mer, which adapts a natively unfolded structure with polyproline II helix motifs. This characteristic structure allows recognition and preferential binding of the peptide by antigen presenting cells in individuals with celiac disease, initiating the onset of the adaptive immune response associated with the disease. Circular dichroism experiments show that the 33-mer undergoes conformational changes in the presence of excess EGCG. This response is corroborated by NMR data wherein chemical shift perturbation of both 1H and 13C signals allows for the elucidation of interaction sites on the peptide. The size and stability of the 33-mer/EGCG complexes formed were also characterized by dynamic light scattering and differential scanning calorimetry.

AGFD 68 Navigating the ever changing regulations and rules of the cannabis industry Cynthia Ludwig, cynthia.ludwig@aocs.org. AOCS, Boulder, Colorado, US With 23 states having approved Medical Marijuana and 4 states having approved Adult Usage and several other relaxing the criminal charges associated with possession of small quantities, it is difficult to know if possession is legal and how much you can have and what testing you need to do to satisfy requirements for selling. Unlike any other medicine, medical marijuana has not undergone the scrutiny of FDA approval, is not federally approved and each state has its own set of rules and regulations. This has lead to chaos in the industry and confusion as to what a dispensary must do in order to comply. Analysis of metadata from states like Washington show just how wide spread the inaccuracies of testing can be. Analysis of the requirements from different states reveals that not only that the rules are incredibly variable but that some states obviously didn't understand the implication of the words and numbers they were writing. I will review the current issues of some of the key states and outline needs across the industry as related to analytical testing and regulation compliance. The good news is that there are some great scientists out there trying to help educate the governmental agencies and hopefully reasonable regulations and laws can be put in place that will ensure patient and consumer safety across the US.

AGFD 69 Review of Bedrocan science: Patient-inspired and science-based Arno Hazekamp, a.hazekamp@bedrocan.nl. Bedrocan, Leiden, Netherlands In 2003 The Netherlands became the first country to make standardized herbal cannabis available on prescription. Under this program, Bedrocan has acquired more than 13 years of experience, becoming an international producer of pharmaceutical- grade cannabis. Today, our products are used by patients in The Netherlands as well as Canada, Italy, Germany, Finland and the Czech Republic. We provide a range of fully standardized cannabis products to patients, each with a reproducible cannabinoid profile and independently analyzed for quality by experienced laboratories. As Bedrocan strains are used by patients, as well as qualified for use in clinical research, they have become a preferred choice for scientists and physicians who wish to study the pharmacological effects of cannabis . Over the years, Bedrocan has grown from a small cultivator of medicinal cannabis into a leading organizer of cannabis research. By teaming up in 2005 with Leiden Univ. - The Netherlands' oldest university - Bedrocan gained access to state-of-the-art research facilities and a network of experts in a wide range of research fields. Our current network includes over 15 professional institutes, academic departments, and pharmaceutical companies worldwide. This makes the city of Leiden an important hub for cannabis-related research, ranging from fundamental chemical research and receptor-binding studies, to performing fully compliant clinical trials with herbal cannabis. Bedrocan strives to bridge the gap between patients' needs for cannabis and the quality standards of modern medicine. We do this through an active research program, a commitment to sharing our knowledge through scientific publications, and by developing research tools which provide a platform to further the independent study of cannabis. Standardization, accurate dosing, and strict safety standards are the cornerstones of medicine today. We believe herbal cannabis can, and should, meet these standards of modern medicine. Simultaneously, we use input from those who use cannabis for medical purposes to identify topics that are most important to address in this time of rapidly expanding availability of cannabis products. We call this patient-inspired research. In all we do, our challenge is to make the best choices based on patients',needs and preferences, while using scientific data to support our final decisions on research methodology and product development.

AGFD 70 Consumer safety and an accredited laboratory Susan A. Audino, susan.audino@gmail.com. Laboratory Accreditation Auditor, Oreint, Ohio Product safety is not new to analytical testing labs. State, federal, and private laboratories exist across the country to ensure food and feed products are appropriately labeled and commodities are safe for consumption. We are learning that cannabis and its applications in food and feed products should not be exempt from a consumer's expectation of safe products, which is leading legislators to include "testing" as part of state regulations for cultivators and dispensaries. Unfortunately, analytical laboratories are limited by the lack of Official Test or Standardized Test Methods. The quality of these analytical laboratories can range from exceptionally good to exceptionally poor, yet most will likely declare themselves "good" laboratories producing scientifically sound results. This session will demystify the idea of "laboratory accreditation" by discussing the appropriateness of the ISO/IEC 17025 standard to cannabis-testing laboratories and the inherent benefits of laboratory accreditation.

AGFD 71 Results from auditing medical cannabis operations in the US Jahan Marcu1, jahan.marcu@gmail.com, Steph Sherer2, Kristin Nevedal3. (1) Green Standard Diagnostics, Inc., Brooklyn, New York (2) Americans For Safe Access, Washington, DC (3) Patient Focused Certification, Washington, DC Regulation is becoming mandatory in states that allow medical cannabis. The producers, manufacturers, dispensaries, and laboratories involved in this industry can operate legally in their states but function without much regulation or oversight. Due to increasing concerns over the need to standardized medicinal cannabis preparations, the American Herbal Product Association (AHPA) has created industry guidelines on manufacturing, producing, dispensing, and laboratory operation standards. Additionally, the American Herbal Pharmacopeia (AHP) completed the Cannabis monograph, a guide for the standardization of cannabis. The work of AHPA and AHP laid the foundation for a certification body called Patient Focused Certification (PFC) a project of Americans for Safe Access. AHPA and AHP guidelines are being incorporated into state level regulations as mandatory product safety standards in new state programs. PFC launched in early 2014 with facilities in several states having successfully completed the auditing process. Over a dozen operations have been certified in over 8 states. Results from over a year of auditing of medical cannabis facilities will be discussed, including data on corrective actions with research on the impact of such regulations on patients, facilities, government, universities, and neighborhoods.

AGFD 72 Understanding cannabis diversity in today's medical applications Jeffrey C. Raber, jeff@thewercshop.com. The Werc Shop, Inc., Bellevue, Washington Cannabis sativa L. is an exceptionally diverse plant which is rapidly rising in popularity as a physiologically useful tool in alleviating a number of chronic ailments and disease states. An analytical perspective within California and Washington has shown a vast number of different plant cultivars are currently being brought to market, sometimes being misnamed and misidentified, which makes selection of the right product a unique challenge with respects to this botanical medicine. Additional complexity in making the proper medical selection comes from a plethora of consumption methods and product types, all leading to different metabolic rates and ultimately to physiological responses. An overview of cannabis chemistry, cannabis analysis and infused products currently present on the market will be provided.

AGFD 73 Beyond cannabis and anandamide Raphael Mechoulam, Mechou@cc.huji.ac.il. Pharmacy School, Hebrew Univ., Jerusalem, Israel Nearly 50 years ago, Gaoni and I isolated the psychoactive constituent of Cannabis, Delta 9- tetrahydrocannabinol (THC), elucidated its structure and synthesized it. Although a huge amount of research was done on THC its mechanism of activity remained obscure for almost 20 years, when Allyn Howlett in the US, found a specific brain receptor, named CB1, whose stimulation led to the well known marijuana effects. Then, in the early and mid 1990's, we identified the endogenous cannabinoids, anandamide and 2-arachidonoyl glycerol (2-AG) that act on CB1. The biosyntheses and metabolism of these endocannabinoids were clarified by efforts of many groups in the US and Europe. Thus, the endocannabinoid system became a reality and was found to be involved in a large number of physiological processes. I shall discuss 2 major aspects of endocannabinoid activity: 1. Specific CB2 receptor agonists. These agonists do not cause marijuana-type activity, but act as major novel protective entities in a variety of pathological conditions. The activity of a novel, camphor-resorcinoid HU-910 in lowering the formation of pro- inflammatory cytokines and in protection of brain trauma will be discussed. 2. Endogenous N-acyl amino acids and related constituents. Anandamide is the amide of arachidonic acid with ethanolamine. It can be viewed as the forerunner of a many additional fatty acid – amino acid (or amino acid-derived) molecules in the brain, as well as in the periphery. The activity of most of these novel entities remains to be elucidated. Exploratory work on this family of endogenous constituents has however revealed that some of these N-acyl-amino acids play a role in diverse biochemical systems. A few examples from our research: Arachidonoyl serine – causes vasodilation and is .neuroprotective after traumatic brain injury by reducing apoptosis. Oleoyl serine (OS) - In a mouse ovariectomy model for osteoporosis we have shown that OS effectively rescues bone loss by increasing bone formation and markedly restraining bone resorption. Conclusion. Synthetic specific CB2 agonists and endogenous N-acyl-amino acids (and related moieties) seem to be major groups of cannabinoid-like compounds with a wide spectrum of physiological activities.

AGFD 74 Metal oxide nanoparticles for destructing dyes and bacteria Yuanbing Mao, ybmao@yahoo.com. Dept. of Chemistry, Univ. of Texas- Pan American, McAllen, Texas Nanostructured photocatalysis has attracted great attention as a promising method of water and air cleaning as well as photocatalytic killing of a wide spectrum of pathogenic microorganisms including bacteria, viruses, fungi and algae. The main drawbacks of low quantum yields and lack of visible-light utilization hinder their practical applications. Hence, intense research has been done to enhance their photocatalytic efficiency and visible-light utilization. Here nanocomposites were synthesized and characterized in details in terms of their structure and morphology using XRD, SEM, EDX, and TEM among others. Their photocatalytic properties for destruction of toxic dye molecules and bacteria were studied. We also will present our studies on establishing the basic photodegradation and photokilling mechanisms, identifying the effective disinfection factors, and investigating the disinfection kinetics for practical purposes.

AGFD 75 Applications of nanoporous cyclodextrin polymers to prevent exposure to mycotoxins Michael Appell, michael.appell@ars.usda.gov, Michael A. Jackson, Kervin Evans. (1) NCAUR ARS USDA, Peoria, Illinois. As a continued effort to maintain a safe food supply, new strategies and technologies are developed in order to reduce human and animal exposure to contaminants. Agricultural commodities are occasionally contaminated by certain species of fungi that produce mycotoxins at levels that are health risks. We have developed and characterized a series of nanoporous beta-cyclodextrin-polyurethane polymers capable of improving the analysis of toxin levels and also the removal of toxins from contaminated beverages. Atomic force microscopy analysis indicated the polymers exhibit irregular surface morphologies. Analytical methods were developed to detect the toxin patulin in apple juice using the cyclodextrin

polyurethane polymers as sorbents in solid phase extraction columns. In addition, suitable cyclodextrin polyurethane materials removed ochratoxins from wine (1-10 ng/L). Sorption assays indicated the affinities of the mycotoxins patulin, citrinin, ochratoxin A, and zearalenone were influenced by the cross-linking agents and suggest the binding properties of the cyclodextrin polyurethane polymers could be tuned for applications.

AGFD 76 Enzyme nanotechnology: Moving towards next-generation biocatalytic materials for food applications Julie M. Goddard1, Joey Talbert2, jotalber@iastate.edu. (1) Food Science, Univ. of Massachusetts Amherst (2) Food Science & Human Nutrition, Iowa State Univ., Ames Enzymes have long been utilized for the processing and analysis of food and agricultural products. However, stability, solubility, activity, and economic restrictions have limited the use of these catalysts. The application of nanotechnology has provided new insight into how enzymes function and has fostered the creation of next-generation biocatalytic systems. Our investigations have focused on the use of nanotechnology as a means to overcome challenges related to enzyme immobilization for food applications. This work has led to a better understanding of enzyme-material interactions in addition to the development of new biocatalytic materials. In this presentation, recent research conducted in our labs will be discussed alongside future applications.

AGFD 77 Comparative study of b- and g-cyclodextrin as ionophores in potentiometric sensors for naltrexone and some applications of ionophore in chemical sensors Gamal A. Mostafa, gamal_most@yahoo.com. Pharmaceuitcal Chemistry Dept., College of pharmacy, Riyadh, Saudi Arabia The construction and developed of membrane sensors for naltrexone are described. The sensing membranes incorporate molecular recognition components b- or g- cyclodextrin as ionophores. Sensor 1 was fabricated using b- cyclodextrin, while sensor 2 was used g- cyclodextrin in presence of ion additive, poly vinyl chloride as matrix and dioctylphthalate as plasticizer. The sensors display fast, stable and the sub-Nernstian response over a relative wide naltrexone concentration range over a wide variety of pH range. The sensors show good selectivity for naltrexone, with high degree of precision and accuracy for both sensors. The proposed sensors have been applied for determination of naltrexone in some pharmaceutical preparation and as indictor sensors for some potentiometric titrations. Ionophore-based membrane sensors are well known as electro-active materials used in formation of many membrane sensors, which are used for the measurement of a wide variety of different samples in complex biological and environmental matrixes. The advantage of the proposed sensors are mainly due to simple design, low cost, adequate selectivity, low detection limit, high accuracy, and wide concentration range.

AGFD 78 Colorimetric detection of Escherichia coli based on the enzyme-induced metallization of gold nanorods Juhong Chen3, juhong@foodsci.umass.edu, Angelyca Jackson3, Vincent M. Rotello1, Sam R. Nugen2. (1) Univ of Massachusetts, Amherst (2) 246 Chenoweth Laboratory, Univ. of Massachusetts, Amherst (3) Food Science, Univ. of Massachusetts, Amherst A novel enzyme-induced metallization colorimetric assay was developed to monitor and measure beta-galactosidase (β-gal) activity, and was further employed for colorimetric bacteriophage (phage)-enabled detection of Escherichia coli (E. coli). This assay relied on enzymatic reaction-induced silver deposition on the surface of gold nanorods (AuNRs). In the presence of β-gal, the substrate p-aminophenyl β-D-galactopyranoside (PAPG) is hydrolyzed to produce p-aminophenol (PAP). Reduction of silver ions by PAP generates a silver shell on the surface of AuNRs, resulting in the blue shift of the longitudinal localized surface plasmon resonance (LSPR) peak and multicolor changes of the detection solution from light green to orange-red. Under optimized conditions, the detection limit for β-gal was 0.128 nM, which was lower than the conventional colorimetric assay. Additionally, the assay had a broader dynamic range for β-gal detection. The specificity of this assay for the detection of β-gal was demonstrated against several protein competitors. Additionally, this technique was successfully applied to E. coli detection in combination with bacteriophage infection. Due to the simplicity and short incubation time of this enzyme-induced metallization colorimetric method, the assay is well suited for the detection of bacteria in low-resource settings.

AGFD 79 Functionalization of biopolymer silver nanosubstrates for pathogen detection Jing Chen, jing.chen@ars.usda.gov, Bosoon Park. USDA, ARS, Athens, Georgia, US Pathogenic bacteria are one of the leading causes of foodborne outbreaks in the US. Timely detection of foodborne pathogens are among the top priorities from both public health and food industry. Alternative rapid methods are being developed to replace traditional microbiological methods which take several days to complete for confirmation. Surface enhanced Raman spectroscopy (SERS) as a rapid, non- destructive optical method has shown to be promising in pathogen detection, but in order to specifically detect pathogens from complex matrices, antibodies are normally used to functionalize the SERS-active substrates. As single stranded oligonucleotides, aptamers have emerged as a promising alternative to antibodies for their superior affinity, stability and lower cost. Nevertheless, their successful application in SERS detection relies on functionalization of the SERS-active nanostructures. In this research, we have developed a method for functionalizing biopolymer encapsulated silver nanoparticles (BeSNs) with anti-Salmonella Typhimurium aptamers. The BeSNs were first labeled with a Raman reporter, 4-mercaptopyridine (4MP), and encapsulated by a thin layer of silica, which serves to contain the 4MP molecules and increase biocompatibility of the BeSN substrate. The aptamer molecules were then attached to the silica layer for specificity. The amounts of silane coupling agents, 4MP, and aptamer were optimized to obtain stable SERS substrates. Using aptamers targeting at different pathogens, the obtained SERS probes can potentially be used as a SERS label for specifically identifying various pathogenic bacteria in foods.

AGFD 80 Short history of mycotoxin research John Pitt, John.Pitt@csiro.au. CSIRO Food and Nutrition, North Ryde, New South Wales, Australia As soon as man began to store grains, about 10,000 years ago, we can be certain that spoilage fungi and mycotoxins were already present, lowering grain quality and causing sickness. We know from relatively recent research that egotism and Fusarium mycotoxins caused havoc among human populations all down through the Middle Ages, and no doubt during previous periods of human history as well. We now understand that the yellow rice syndrome which killed young, healthy Japanese people before 1915 was due to a mycotoxin and that alimentary toxic aleukia that killed hundreds of thousands of Russian people in the 1940s was also a mycotoxicosis. The first experimental evidence of a common mould producing a toxic compound was published in 1911, and the American veterinarians Forgacs and Carll introduced the term “mycotoxicosis” for toxic compounds in animal feeds in 1952. But serious research on the toxicity of common foodborne fungi only occurred after the outbreak of “Turkey X disease” in the United Kingdom in 1960. Research that eventually led to the understanding that many common fungi produce very toxic compounds whenever they grow in highly nutritious substrates such as human foods and animal feeds. This paper will describe some of the milestones that have led us to our current extensive understanding of the important mycotoxins, and of the specific fungi that produce them.

AGFD 81 Climate variability and mycotoxin exposure J. David Miller, david_miller@carleton.ca. Chemistry, Carleton Univ., Ottawa, Ontario, Canada The number of people exposed to the mycotoxins aflatoxin and fumonisin often greatly in excess of the tolerable limits has increased and the costs of managing these toxins as well as deoxynivaleol exposure has increased for others. This is due to three basic factors, food insecurity, changing crop patterns and weather driven increases in prevalence and geographic distribution of mycotoxins. Further, there is a fairly long list of rare toxicoses that have occurred in the past but became uncommon. For example, in recent years, cropping and weather patterns have conspired to increase the prevalence of ergot in parts of western Canada. For those highly exposed in the developing world, more aggressive efforts at crop diversification are required along with better capacity to minimize exposure to toxins in the most vulnerable populations. For the fully developed market economies, increasing the cost effectiveness and reliability of toxin prediction and monitoring strategies is indicated. Central to these goals will be innovation in the analysis of the common mycotoxins, a goal often stated but now is becoming essential for global food safety.

AGFD 82 Worldwide occurrence of mycotoxins in foods Dojin Ryu2, dryu@uidaho.edu, Hyun Jung Lee1. (1) Food Science, Agr Bldg 129A, Univ. of Idaho , Moscow, Idaho, US (2) School of Food Science, Univ. of Idaho, Moscow Among all known mycotoxins to date, aflatoxins, ochratoxins, fumonisins, deoxynivalenol, and zearalenone are of greatest concern in public health mainly due to their prevalence and toxicity. These toxic secondary metabolites are produced mainly by three fungal genera of Aspergillus, Fusarium, and Penicillium. The levels of contamination may vary widely depend on the mycotoxin, commodity, and other factors including environment. According to surveys conducted in the last decade, total aflatoxins detected in cereals, nuts, and dried fruits ranged 0.02 µg/kg - 4.32 mg/kg. Though most mycotoxins occur at low levels, they can cause serious adverse effects in different organs including the liver, kidney, and immune system in humans. Consequently, many countries regulate mycotoxins with their maximum levels in various commodities. While cereal grains are most commonly contaminated, one or more mycotoxins can be found in virtually all agricultural commodities and their processed foods due to their heat stability. In farm animals, the intake of feed contaminated with mycotoxins may result in the contaminated animal products such as a milk, meat, and eggs. Mycotoxins may occur in various combinations by a single or multiple fungal species in food matrices. Therefore, more information on co-occurrence of mycotoxins in foods and its interactive toxicity in humans are needed.

AGFD 83 Emerging mycotoxins: Beyond traditionally determined food contaminants Franz Berthiller, franz.berthiller@boku.ac.at, Elisabeth Varga, Michael Sulyok, Rudolf Krska. IFA-Tulln, Univ. of Natural Resources and Life Sciences, Vienna, Austria, Tulln, Austria Mycotoxins are defined as toxic secondary metabolites of molds. The term “emerging mycotoxins”, while often used nowadays, is not so clearly defined. One approach defines these compounds as “mycotoxins, which are neither routinely determined, nor legislatively regulated; however, the evidence of their incidence is rapidly increasing” (Vaclavikova et al., Food Chemistry 136, 2013). It is the belief of the authors that the reasons for the increasing incidence of certain mycotoxins can be grouped into the following categories: a) improved analytical techniques (e.g. multi-mycotoxin methods), which allow the determination of a large number of mycotoxins at a very high sensitivity b) newly detected toxins (e.g. NX-toxins, or masked mycotoxins) c) “neglected” mycotoxins (e.g. enniatins or moniliformin), which have been discovered already some time ago, but not ranked as the most important toxins and therefore are not (yet) regulated d) “surprising” finding of known mycotoxins in parts of the world, in which they were not encountered before (e.g. due to climate change) All of the above categories have in common that liquid chromatography – mass spectrometry (LC-MS) based methods play a major role in their discovery or in the reliable determination of their occurrence. The rapid development of analytical techniques allows to obtain a broad picture regarding fungal contamination of food. By far not all of the detected compounds are toxicologically relevant and therefore of little or no health concern to consumers. The aim of this presentation is to highlight recent discoveries regarding emerging mycotoxins and discuss their potential impact.

AGFD 84 Aflatoxin and child growth: The critical first 1000 days of life in underdeveloped world regions Paul C. Turner, pturner3@umd.edu. Environmental Health, Univ. of Maryland, College Park Childhood stunting has long term consequences on both later morbidity and mortality. In many developing regions of the world insufficient nutrition and gastrointestinal infection in the first few years of life are significant drivers of stunting. However, only about 50% of the poor growth is explained by these risk factors. A number of studies from Sub- Saharan Africa reveal strong associations between aflatoxin exposure and poor infant growth. Aflatoxins, secondary toxic metabolites of certain Aspergillus fungi, are frequent contaminants of dietary staples in many subsistence farming populations, and cause both acute and chronic disease. In high risk regions more than 90% of the population have chronic aflatoxin exposure at moderate to high levels; while globally several billion persons live in regions with some risk of exposure occurring. The studies in infants also highlight the critical role of weaning in aflatoxin exposure, thus offer a potentially simple approach to delay exposure. In this presentation I will review some of these data, including maternal and infant aflatoxin exposure; provide suggestive mechanisms, and introduce novel studies that seek to improve our understanding of the multiplicative contributions of aflatoxin, poor hygiene and nutrition on child health. While aflatoxin exposure dominates the mycotoxin issue on growth we are increasingly aware of exposure to additional mycotoxin families including the fumonisins and the trichothecenes. The possible contribution of these mycotoxins will be considered in these novel investigations.

AGFD 85 Effects of mechanical strain on average orientation and packing of polymeric constituents in onion epidermis cell walls Kabindra Kafle1, kuk188@psu.edu, YongBum Park1, Shixin Huang1, Daniel Cosgrove1, Seong H. Kim2. (1) Penn State Univ., State College, PA (2) Penn State Univ., Univ. Park, PA The organization of polymeric constituents in plant cell walls and bio-based polymeric films is of importance to understand their biomechanical properties. The change in average orientation of cell wall polymers upon mechanical strain was monitored using polarized transmission infrared (IR) spectroscopy, and the packing of cellulose microfibrils (CMFs) was studied with vibrational sum frequency generation (SFG) spectroscopy. A never-dried onion abaxial epidermis of the second scale of an onion bulb showed an anisotropy in mechanical stretch. The epidermal cell wall can be considered as a fiber reinforced composite, where CMFs assume the role of load bearing fibers. The analysis of infrared dichroism of the glycosidic linkage of cellulose and the ester carbonyl group of pectin showed that the average orientations of both cellulose and pectin chains change along the stretch direction by ~8° from their initial distributions upon 14% mechanical strain along the vertical bulk axis and by ~3o upon 12% strain along the horizontal bulk axis. This appears to be accompanied by changes in CMF packing especially when the cell walls are stretched along the vertical bulk axis.

AGFD 86 Swine odor removal with biochar Okhwa Hwang2, hoh1027@korea.kr, Sung Back Cho2, Deug Woo Han2, Kyoung Ro1. (1) USDA-ARS, Florence, South Carolina (2) Animal Environment Division, Korean RDA NIAS, Chunju, Korea Thermo-chemical treatment of natural biomass feedstock, such as pyrolysis, can produce value-added biochar, a carbonaceous solid product. The biochar has been used as a soil amendment to improve soil quality and sequester carbon. Biochar can also be used as an adsorbent to reduce malodorous emissions from livestock operations. The objective of this study was to evaluate the odor removal potential of various biochars, made from different biomass feedstocks and process conditions. Both plant- and animal manure-based biomass feedstocks were pyrolyzed at 350 oC and 500 oC. Some of these were also partially activated with steam at 700 oC. The biochar samples were then analyzed for their chemical elemental compositions, volatile matter, fixed carbon, ash contents, density, and surface areas. Sorption capacities of these biochar were evaluated using a continuous flow sorption column system. Odorous volatile organic compounds, phenolic, and indoles along with S containing compounds were analyzed with GC/MS. Headspace gas from a tank containing raw swine manure was introduced at 300 mL/min into a sorption column containing 10g of biochar. Sorption capacities of these biochar samples for each different compound will be presented.

AGFD 87 Thermally reprocessible polylactic acid grafted cellulose nanocrystal films through reactive extrusion process Prodyut Dhar, prodyut@iitg.ac.in, Debashish Tarafdar, Amit Kumar, Vimal Katiyar. Chemical Engineering, Indian inst. of Technology Guwahati, Guwahati, Assam, India In this paper, we demonstrate grafting of polylactic acid onto cellulose nanocrystals (PLA-g-CNC) using dicumyl peroxide (DCP) as cross-linking agent via reactive extrusion process. PLA-g-CNC nanocomposite films showed improved compatibilization between hydrophobic PLA and hydrophilic CNCs alongwith interesting property of recyclability. The maximum fraction of PLA chains grafted on CNC surface was found ~66% with the highest grafting efficiency (40.7%) and gel yield (74.2%) achieved at 1wt%CNC loadings. During the reactive extrusion process, it was found that complex viscosities of PLA-g-CNC nanocomposites were higher (50-70 Pa.s at various CNC loadings) in comparison to neat PLA (40 Pa.s), probably due to the formation of branched and cross-linked structures. NMR and FTIR spectroscopic studies confirm the grafting between the methine (-CH) groups of PLA with the methylene groups of CNC by establishing C–C bridge using DCP as grafting agent. Due to the chain extensions and formation of branched structures, the weight and number average molecular weight of PLA-g-CNCs increased significantly (~40%). Interestingly on thermal recycling of PLA-g-CNC gels at similar extrusion conditions, the molecular weight didn't showed any significant deterioration. Both PLA-g-CNC and rPLACNC (obtained after further recycling) are capable of forming transparent films with improved adhesion and dispersion of CNCs. Due to formation of the C–C bonds with the CNCs, both the thermal stability and the mechanical properties of PLA-g-CNC nanocomposites improved significantly. The tensile strength and young's modulus improved by 41and 490% respectively, whereas the filler effectiveness coefficient (CFE) values decreased, suggesting that the grafted CNCs act as an efficient reinforcing agent. The E' increased on incorporation of CNC in presence of DCP due to formation of cross-linked structure and better interfacial adhesion with the polymer matrix. XRD and DSC studies shows improvement in crystallinity, possibly due to grafting of the amorphous PLA chains onto the crystalline CNC segments which act as nucleating agent. This novel reactive extrusion-based strategy can be implemented for industrial scale fabrication of PLA-g-CNC recyclable biocomposite films for potential applications in packaging.

AGFD 88 Chitosan-based multilayer nanocoatings that exhibit high gas barrier and flame retardant behavior Jaime C. Grunlan, jgrunlan@tamu.edu. Texas A M Univ, College Station Chitin, extracted from crustacean shells, is the second most abundant polysaccharide after cellulose. Despite its abundance, unmodified chitin's usefulness is very limited, because of its poor solubility in most solvents. Alkaline deacetylation of chitin produces chitosan (CH), which is soluble in acidic aqueous solutions because of the protonation of its amino groups at pH < 6. In addition to its solubility, chitosan is biodegradable, biocompatible, and benign. Thin films prepared via a layer-by-layer (LbL) assembly were prepared with cationic CH and anionic montmorillonite (MMT) clay nanoplatelets. Thin-film assemblies prepared with CH at high pH are thicker, because if the low polymer charge density. A 30-bilayer nanocoating (~100 nm thick) reduces the oxygen permeability of a 0.5-mm-thick polylactic acid film by four orders of magnitude. In an effort to create an environmentally-friendly flame retardant system for foam and fabric, thin films were assembled layer-by-layer (LbL) using "green" materials obtained from completely renewable sources. Ten bilayers of pH 6 chitosan (CH), as the cationic layer, and pH 10 montmorillonite (MMT) as the anionic layer, were deposited on flexible polyurethane foam (30 nm thick and added 4 wt%). When cut open after direct flame from a propane torch for 10 seconds, white undamaged foam was revealed under a thin black char layer. In related work on foam, vermiculite (VMT) clay was layered with CH, followed by layers of an intumescent system comprised of CH and APP (or polysodium phosphare [PSP]). This 'stacked' FR system (i.e., intumescent layers on top of clay layers) reduced the foam's peak heat release rate by 66%. Just two clay layers provide enough support to the foam during heating to allow intumescence to occur prior to collapse, creating our best result to-date. Another recipe, involving layers of poly(vinylsulfonic acid sodium salt) and CH, completely extinguishes the flame from a butane torch on this same foam. This exciting result is due to a 'gas blanket' effect in which the coating releases small amounts of NH3, SO2 and H2O that prevent oxygen from reaching the foam surface. These environmentally-benign nanocoatings could prove beneficial for new types of food packaging or a replacement for environmentally persistent antiflammable compounds.

AGFD 89 Investigation of solvent systems and potential applications of soy proteins Gang Sun1, gysun@ucdavis.edu, Abolfazl Aghanouri2. (1) Textiles and Clothing, Univ. of California, Davis (2) Univ. of California, Davis, Richmond Soy proteins are by-products of soy oil productions in forms of soy flour or soy protein isolates. The US is the number one producer of soy bean, one of the most important vegetable proteins, in the world. Utilization of the proteins in different products has been a long term goal of many research teams with many progresses. Different from cellulose polymer, the dissolution of soy proteins and also control the configurational and conformation structures of the proteins in solutions and during formation of products are the key issues, which have been partially solved by using inorganic materials and other polymers such as urea alkaline solutions and poly(vinyl alcohol) blends. However, these approaches are rather limited on producing products with less soy protein contents and low mechanical properties. In the past few years we have been working on investigating on how to identify proper organic solvent systems for soy proteins, instead of urea or polymers, so as to make the polymers easily processable into suitable products. Here the focus was on finding organic solvents that can control the configuration and conformation of the proteins. The Hansen solubility parameter theory was employed in the study. Solvent systems developed based on the theory were able to provide proper dissolution and denaturing performance of the proteins. In addition, the proper applications of the soy proteins were explored.

AGFD 90 Ammonia and hydrogen sulfide removal using biochar Kyoung Ro2, kyoung.ro@ars.usda.gov, Isabel M. Lima1, Gudigopura Reddy3. (1) USDA Ars SRRC, New Orleans, Louisiana (2) USDA-ARS, Florence, South Carolina (3) NC A&T State Univ., Greensboro, North Carolina Reducing ammonia and hydrogen sulfide emissions from livestock facilities is an important issue for many communities and livestock producers. Ammonia has been regarded as odorous, precursor for particulate matter (PM), and contributed to livestock mortality. Hydrogen sulfide is highly toxic at elevated concentrations, causing death at high level of exposure and headaches and eye irritation over a long period of low level exposure. Biochar has the potential to serve as a sorbent for removing gaseous pollutants such as ammonia and hydrogen sulfide. In this research, ammonia and hydrogen sulfide sorption capacities of biochars made from pyrolyzing wood shavings and chicken litter at 250 oC and 480 to 500 oC were determined via sorption column experiments. Steam, phosphoric acid, and potassium hydroxide activation techniques were employed to activate some biochar samples. The bed depth service time model was used to calculate the maximum sorption capacities of various biochar samples. Non-activated biochar samples had maximum sorption capacities ranging from 0.15 to 5.1 mg NH3-N/g biochar, comparable to that of commercial activated carbons. Sorption capacities of other biochars will be presented.

AGFD 91 Effects of processing conditions on the structure of enzymatic modified soy protein isolate-based bioplastics Elham Zadeh, elham88@vt.edu. Sustainable Biomaterials, Virginia Tech, Blacksburg, Virginia Plant-based biopolymer materials are becoming attractive as an alternative to animal- based biopolymers through recent technical improvement and rising social-cultural and hygienic concerns. Soy protein isolate (SPI) with more than 90% protein purity, was enzymatically modified with activated and deactivated transglutaminase, which consist of 99% stabilizers, and fabricated with glycerol as a plasticizer at three different enzyme incubation times (1h, 2h & 3h) and two protein denaturation temperatures (80 & 90 °C). Tensile strength, percent elongation, and surface hydrophobicity of the films were characterized comparing to the films with the deactivated enzyme and a control film which was not treated with the enzyme. The viscosity of the film forming solution was measured by concentric rheometer as a function of enzymatic incubation times. Modified films with the enzyme and the deactivated enzyme showed significant increase in mechanical properties and initial contact angle of the films comparing to the control film. However, the viscosity profile of the film forming solution treated with the enzyme was significantly increased as the incubation time increased compare to those with the deactivated and without the enzyme, which is an excellent evidence of enzymatic treatment to biopolymeric film. Increasing enzyme incubation time boost tensile strength and reduced percent elongation of films prepared at 80 °C, however, it did not have a significant effect on the films prepared at 90 °C ($p>0.05$). Based on above observations, the enzymatic treatment to protein based polymer can be a useful way to control the physical properties of protein based biopolymeric film and this treatment can be applied to the wide spectrum of business areas such as packaging, food, pharmaceutical, and agricultural industries.

AGFD 92 Mountain beetle pine infestation: Characterization of the polar components for Lodge pole pine (pinus contorta) acetone extractives Roderquita K. Moore, roderquitamoore@fs.fed.us. USDA, Madison, Wisconsin Mountain pine beetle infestation of lodge pole pine is a major concern. The morality of the tree once attacked is within one year. These dead trees in the forest put the forest at resist for out of control forest fires. The ultimate focus of this research is to identify tree derived high value chemicals. Characterizing the chemicals from unutilized wood is apart of the biorefinery concept to produce fuels, power, and chemicals from biomass. The polar component was separated from the infected and uninfected lodgepole pine acetone extractives. GC-MS was used however GCxGC was use identify chemical that ordinary would not be identified due to co-eluting and highly concentrated chemicals. Silivchemicals which are chemicals derived from trees are used in comestic, paints and oils. The sap and heartwoods of the infected and uninfected woods were solvent extracted and separated into non-polar and polar components. This study focuses on comparing and identifying chemicals in the polar component which known for carrying toxic chemical which can be used for drug development.

AGFD 93 Innovative technologies for anti-flammable cotton fabrics Sechin Chang, sechin.chang@ars.usda.gov, Brian D. Condon. USDA- ARS- SRRC, New Orleans, Louisiana Due to its environmentally friendly properties, supercritical carbon dioxide (scCO2) is considered in green chemistry as a substitute for organic solvents in chemical reactions. In this presentation, innovative approaches for preparation of flame retardant fabrics were obtained by utilizing supercritical carbon dioxide with minimum amount of co- solvent. Our attempts at flame retardant cotton fabrics treated with low cost inorganic formulations or a novel environmentally friendly phosphorus-nitrogen containing small molecules in scCO2 were done successfully. Furthermore, the flame retardant fabrics have been prepared by the layer-by-layer method of branched polymer containing phosphorus-nitrogen, clay, and inorganic formulations on cotton fabric. The evidence of flame retardant chemical penetrations or surface modification of cotton fabrics were confirmed by the Fourier transfer infrared spectroscopy (FT-IR), elemental analysis (EA) and scanning electron microscope (SEM), and the treated cotton fabrics were evaluated flammability tests such as 45 degree angle (clothing textiles test -- ASTM D1230-01; 16 CFR 1610) and vertical (ASTM D6413-08; 16 CFR 1615, 1616). In addition to the thermal properties of desired products will discuss by thermogravimetric analysis (TGA) and micro-scale combustion calorimeter (MCC).

AGFD 94 Ultra-small-angle x-ray scattering study of zein self-assembly Suzan Uzun2, susan071986@hotmail.com, Graciela Padua1. (1) Univ. of Illinois, Urbana, Illinois, US (2) Food Science and Human Nutrition, Univ. of Illinois, Urbana The self-assembly/aggregation of zein in ethanol-water solutions of high solids mass fraction was studied by ultra-small-angle x-ray scattering (USAXS). Ethanol content of solutions was 70-90% (v/v), zein concentration 30-60% (w/v), and oleic acid 0 or 14% (w/w zein). USAXS analysis revealed that depending on ethanol content and protein concentration three or four structures of different sizes may coexist in zein solutions. Structures in the high q region exhibited a rod shape with radius of gyration (Rg) below 50 Å. Intermediate structures were found in the range of 300 – 900 Å, where corresponding Porod slope (P values) of ~3 suggested an irregular shape. In the low q region, the unified fit model predicted P=4 for structures of Rg, 3,000 – 6,000 Å indicating the presence of larger spherical structures with smooth surfaces. The absence of mass fractals suggested that zein structures were formed through self- assembly, rather than by clustering of primary particles. The addition of oleic acid notably affected the size and shape of structures formed in zein solutions. The impact of oleic acid on the smallest structures (Rg < 30 Å) was seen in their disk-like shape, different from corresponding structures in zein only solutions. At low q vectors, the size of aggregated/self-assembled oleic acid-zein structures was much larger than those in zein only solutions. Larger Rg values suggested oleic acid facilitated the assembly process, perhaps playing a surfactant role. P values suggested oleic acid promoted an earlier structure development by forming discs and spheres faster than samples without it. According to our results, self-assembly of zein develops various structures in concentrated solutions. Oleic acid facilitates the assembly process.

AGFD 95 Isolation, characterization and anti-proliferative activities of Picroside compounds present in Picrohiza kurroa, (kutki) extract Bishambar Dayal1, dayalb77@gmail.com, Trinava Roy1, Michael A. Lea5, Sagar Patel2, Shaheir Ali3, Shaogang Li4. (1) Medicine, Rutgers Univ. New Jersey Medical School, Princeton Jct (2) Medicine, Microbiology, Biochemistry and Mol.genetics, Rutgers Univ., Newark, New Jersey (3) Medicine, Microbiology, Biochemistry, and Mol.genetics, Rutgers Univ., Newark, New Jersey (4) Pharmacology, Rutgers Univ., Newark, New Jersey (5) Microbiology, biochemistry, and mol. genetics, Rutgers Universtiy New Jersey Medical School, Newark Picrorhiza kurroa is an herb that is well known for its medicinal properties and grown in the Himalayan region. P. kurroa is known to contain Iridoid glycosides such as Picrosides 1, 2 and 3. Picrohiza kurroa (Kutki) has several medicinal properties including treatment of hepatitis, jaundice, anemia, asthama, anti-arthritic and hepato- protective activities. We have initiated a systematic study to isolate, characterize and carry out biological studies of different picrosides present in Kutki extract. The picrosides present in Kutki extract were isolated using sequential extraction of solvents (hexane, acetone, ethyl acetate and methanol), separated, resolved and analyzed via analytical and preparatory thin-layer chromatography in the solvent system: CHCl3, : CH3OH : CH3COOH; (18:4:0.5, v/v/v). Picroside I (Rf 0.25), Picroside II (Rf 0.60), and Picroside III (Rf 0.77). Characterization of compounds was accomplished by a characteristic NanoDrop UV visible (Rf=0.77) λ max. 254 nm, and Rf=0.60, λ max. 264 nm. LC-MS/MS analysis of Picroside 1, (ES-API, +ion mode) did not show molecular ion peak but a major peak at m/z 147 characteristic of a loss of cinnamic acid side-chain residue indicative of general Picrolive structure. Picroside 2 exhibited M/Z at 167 in the (ES-API +ion mode) a loss characteristic of vanilloyl side chain. Other prominent ions in the (ES-API -ion mode) showed a molecular ion peak at M/Z=511/512 (60%, 25%) and 477 (M-2H2O 100% and its derivative M/Z 639 indicative of its glycosidic derivative. Picroside 3 in the (ES-API -ion mode) showed a molecular ion peak at [M- H]=537,100%), [M+] 538 and [M+H]=539 respectively. The anti-proliferative activity of the different compounds present Kutki extract was tested in the Caco-2 human colon cancer cell line. Cancer cells, according to the Warburg effect, metabolize glucose into lactic acid; thus causing a decrease in pH. This was monitored by lower absorbance of phenol red at 560 nm, and reflected significant anti-proliferative activity. Growth was monitored using staining of cells with sulforhodamine B and measurement of absorbance at 510 nm in 96 well plates. The results showed inhibition of proliferation of Caco-2 human colon cancer cells that was found to be concentration dependent. Chemically engineered Kutki extract compounds may provide another source of natural products which could be useful for studying nanoparticle drug delivery therapeutics.

AGFD 96 Development and characterization of functionalized TiO2/polylactic acid nanocomposite films for food packaging applications Naerin Baek1, nbaek@vt.edu, Susan Duncan 1, Young Kim2, Joseph Marcy1, Sean F. Okeefe1. (1) Food Science and Technology, Virginia Tech , Blacksburg, Virginia (2) Sustainable Biomaterials , Virginia Tech , Blacksburg, Virginia TiO2 nanoparticles (T) have beneficial properties in food packaging applications, but low compatibility between T and polylactic acid (PLA) causes T to agglomerate, making materials opaque and decreasing efficiency. A surface modification of TiO2 nanoparticles with oleic acid (OT) was introduced in this study to enhance compatibility between T and PLA matrices. This study focused on fabrication of oleic acid modified TiO2/PLA nanocomposite films (OT-PLA) by using a solvent casting method and its characterization, compared with unmodified TiO2/PLA nanocomposite films (T-PLA) and pure PLA films. Surface modification of TiO2 nanoparticles with oleic acid (OT) was confirmed by X-ray diffraction (XRD), FTIR, transmission electron microscopy (TEM) and thermogravimetric analysis (TGA). Scanning electron microscopy (SEM), UV-Vis and oxygen transmission rate (OTR) analyzer were used to characterize properties of the films. T and OT were identified as anatase phase with sizes ranging of 3-10 nm by XRD and TEM. In FTIR spectrum of OT, stretching vibrations of oleate anions at (1506 cm-1 and 1423 cm-1) and C-H at (2910 cm-1 and 2843 cm-1) were shown due to the surface modification. Weight loss of OT was 13% higher than T by TGA. It implied T was successfully modified by oleic acid. Higher transparency and better dispersion of OT-PLA were obtained due to improvement of compatibility between OT and PLA matrices. SEM showed irregular agglomeration of T in T-PLA, yet there was no agglomeration shown in OT-PLA. OTR of OT-PLA (183.05 ± 18.19 ml/m2/day) was significantly lower than the T-PLA (337.75 ± 42.5 ml/m2/day) or PLA films (401.28 ± 10.11 ml/m2/day). Both OT-PLA and T-PLA showed significantly higher UV-Vis absorption than PLA films. Absorption rate of OT- PLA was higher than T-PLA in the region of 280-350 nm. OT-PLA can potentially be used as an innovative food packaging material as an economical, functional and environmentally friendly alternative.

AGFD 97 Targeted delivery system based on chitosan and sulfated β-glucan for the colon Cigdem Yucel1, cigdem@food.ku.dk, Javier Sotres3, Ana Rascon2, Jens Risbo4, Marite Cardenas5,3. (1) Food Science, Univ. of Copenhagen, Denmark (2) Aventure AB, Lund, Sweden (3) Biomedical Science, Malmo Univ., Malmo, Sweden (5) Chemistry, Univ. of Copenhagen, Denmark The layer by layer (LbL) technique leads generation of tailorable coatings and has broad range of applications. We aimed at employing the LbL for a targeted delivery system using sequential adsorption of oppositely charged chitosan and derivative of oat β- glucan. A coating based on such system can be used to protect its content against acidic stomach and release it to the human colon i.e. by enzymatic degradation. The use of sulfated β-glucan in LbL coating allows combining the prebiotic effect of β-glucan with protection ability of chitosan under acidic conditions. Oat β-glucan was modified by sulfation reaction in order to introduce negative charges and chitosan was used as positively charged biopolymer below pH 6.5. The bio-coatings were investigated via in situ QCM-D and AFM for their ability to form assembled multilayers and material properties i.e. structure and rigidity as well as resistance to simulated gastrointestinal environment and degradation with model chosen bacterial enzyme, β-glucanase. Results showed reproducible and non-rigid multilayer formation. Bio-coatings were resistant to gastric stress when exposed to simulated gastric fluid. Moreover, coatings were partially degraded with simulated intestinal fluid as a result of interactions with bile salts and β-glucanase. Partial degradation can potentially release the coated molecules i.e. probiotic bacteria to the intestine or favor access of microflora to prebiotic coating material. Therefore, a delivery system based on LbL coating of chitosan and sulfated β- glucan can be utilized as carriers releasing bioactive molecules. Since this system will be applied for coating of probiotic bacteria in the frame of our research, related results will also be presented.

AGFD 98 Dual-enzyme nanobiocatalyst for the cascade conversion of cellulose to fructose via a glucose pathway Cheng-Yu Lai2, cylai@desu.edu, Daniela R. Radu1, Gulnihal Ozbay2. (1) Delaware State Univ., Hockessin (2) Delaware State Univ., Hockessin There are various forms of biomass resources in the world, including agriculture residues, dedicated energy crops, wood product wastes, and municipal solid waste. These biomass resources seem to be the largest and most promising future resources for biofuels and valuable chemicals production from non-fossil fuel. Cellulose (from wood, agricultural residues, waste sulfite liquor from pulp, and paper mills) must be converted into sugars, generally by the action of acids or cellulolytic enzymes. Cellulose is converted into glucose trough hydrolysis.

Enzymatic hydrolysis is the key to cost- effective ethanol production from lignocellulosic substrates in the long run, as it is very mild process, gives potentially high yields, and the maintenance costs are low compared to acid or alkaline hydrolysis (Kuhad et al. 1997). The process is compatible with many pretreatment methods, but materials poisonous to the enzymes need to be removed or detoxified when chemical pretreatment precedes enzymatic hydrolysis. Process efficiency would increase tremendously if the need for such pretreatment would be eliminated. Our research focuses on porous materials as high-surface area scaffolds utilized as solid support for catalytic purposes. The synergy created at the nexus of enzymatic catalysis and porous silica materials is owned to the ability of porous scaffolds not only to host a large number of catalytic units but to also protect them from degradation. In addition, the substantial benefit of the porous silica nanomaterials is that they enable placement of multiple enzyme in close proximity, which opens the horizon of cascade bio catalyzed reactions. We aim to transformation of cellulose to D-fructose in one step by using a porous silica nanosphere (PSN) with pores > 10 nm as support for: i). A cellulase enzyme, which converts cellulose to D-glucose; and ii). Glucose isomerase enzyme, which converts (isomerizes) D-glucose to D-fructose. Current work demonstrates the proof-of-concept of dual-enzyme immobilization to achieve the aforementioned steps. Silica materials scaffolds synthesis and characterization for porosity, surface area and composition will be presented, along with enzyme immobilization and assessment of the efficiency of the cascade reaction.

AGFD 99 Urinary biomarkers for human multi-mycotoxin exposure Michele Solfrizzo, misolfr@tin.it, Lucia Gambacorta, Antonio Francesco Logrieco. inst. of Sciences of Food Production, National Research Council, Bari, Italy Deoxynivalenol (DON), zearalenone (ZEA), aflatoxin B1 (AFB1), fumonisin B1 (FB1), and ochratoxin A (OTA) are the main mycotoxins frequently co-occurring in food/beverage worldwide. They are mainly produced by Fusarium graminearum (DON, ZEA), Aspergillus flavus and A. parasiticus (AFB1), F. verticillioides and F. proliferatum (FB1), Penicillium verrucosum and A. carbonarius (OTA). These fungi can colonize plants and agricultural products and produce mycotoxins either in the field, at harvest and during storage. Since the complete elimination of these contaminants from agricultural commodities is practically impossible they can be find in food/feed derivatives with negative effects on animal and human health. It is therefore important to identify and measure the amount of mycotoxins ingested daily with the diet in order to establish if the exposure is below or above the tolerably daily intake (TDI) established for each mycotoxin. The use of modern methodologies based on LC-MS/MS have demonstrated that foods are often contaminated with a cocktail of mycotoxins. LC-MS/MS is also used to determine urinary mycotoxins and their key metabolites that can be used to calculate the daily mycotoxin ingestion. We have developed a sensitive UPLC-MS/MS method which is capable to determine urinary mycotoxin biomarkers at concentrations usually occurring in humans living in developed countries. This method was used to detect and measure incidence and concentrations of the above mentioned mycotoxins and relevant key metabolites in urines of 52 volunteers resident in South Italy. The presence of ZEA + ZOLs, OTA, DON, FB1 and AFM1 were detected in 100%, 100%, 96%, 56% and 6%, of urines, respectively. All samples contained biomarkers of two or more mycotoxins. The mean concentrations of biomarkers ranged from 0.055 ng/mL (FB1) to 11.89 ng/mL (DON). Urinary biomarker concentrations were used to estimate human exposure to multiple mycotoxin. For OTA and DON, 94% and 40% of volunteers, respectively exceeded the TDI for these mycotoxins whereas for FB1 and ZEA all volunteers were largely below the TDI. These results highligh the importance of using sensitive methods to determine urinary mycotoxin biomarkers and suggest to conduct epidemiological studies to assess multi-mycotoxin exposure in human and animal populations with different food/feed diets.

AGFD 100 Risk of exposure to multiple mycotoxins from maize based complementary foods in Tanzania Analice Kamala1,2, Martin Kimanya3, martin.kimanya@nm-aist.ac.tz, Carl Lachat1, Liesbeth Jacxsens1, Johana Ortiz4, Geert Haesaert5, Patrick Kolsteren1,6, Bendantuguka Tiisekwa7, Bruno E. De Meulenaer1. (1) Food Quality and Food Safety, Ghent Univ., Belgium (2) Tanzania Food and Drugs Authority, Dar es Salaam, Tanzania, United Republic of (3) School of Life Sciences and Bio-Engineering, The Nelson Mandela African inst. of Science and Technology (NM-AIST), Arusha, Tanzania, United Republic of (4) Faculty of Chemical Sciences, Cuenca Univ., Ecuador (5) Dept. of Applied Biosciences, Faculty of Bioscience Engineering, Ghent Univ., Belgium (6) inst. of Tropical Medicine, Antwerpt, Belgium (7) Faculty of Agriculture ,Sokoine Univ. of Agriculture, Morogoro, Tanzania, United Republic of Children receiving maize based complementary foods in Tanzania are at a high risk of exposure to multiple mycotoxins. We estimated consumption of maize based complementary foods and contamination of multiple mycotoxins in 300 households (100 from each of 3 three agro-ecological zones) of Tanzania. Complementary food consumption was estimated, for children aged 6 to 12 months, using two 24 h dietary recalls. Mycotoxins in the foods were analysed using an ultra high performance liquid chromatography / time-of-flight mass spectrometry (UHPLC/TOFMS) method with a QuEChERS-based procedure for sample extraction. The risk of exposures above limits of health concern, such the tolerable daily intake of 2µg/kg/body weight/day (TDI) for Fumonisin B1 (FB1), was estimated for each of the mycotoxins, using the probabilistic approach. Maize based food consumption levels ranged from 13 - 185g/child/day (Average 59g/child/day). Contaminations were estimated for eleven mycotoxins at levels ranging from 3 - 1081µg/kg for aflatoxin B1, 12 -177µg/kg for aflatoxin B2 , 2.2 - 39µg/kg for aflatoxin G1 , 16 -73 µg/kg for ochratoxin A, 68 - 2196µg/kg for deoxynivalenol, 18 - 18,184 µg/kg for FB1, 178 - 38,217µg/kg for fumonisin B2 , 15 -25 µg/kg for HT-2 toxin and 651 -1464µg/kg for zearalenone (ZEN). Aflatoxin G2 was detected in one sample at 3µg/kg. The children were at a risk of exposures above the limits of health concern. The risk ranged from 18% for HT-2, through 35% for DON to 100% for total aflatoxins. These findings demonstrated that consumption of maize or its use in complementary foods in Tanzania possess very high risk of health effects. Strategies targeting more than one mycotoxin are urgently needed to minimize mycotoxin exposures from maize in Tanzania.

AGFD 101 Fumonisin exposure in women linked to inhibition of an enzyme that is a key event in farm and laboratory animal diseases Ronald T. Riley1,2, ronriley.usda@gmail.com, Kenneth Voss1, Jency L. Showker1, Trevor Mitchell1, Olga Torres3, Jorge Matute4, Simon G. Gregory5, Allison E. Ashley- Koch5, Joyce R. Maddox6, Janee Gelineau-van Waes6. (1) Toxicology & Mycotoxin Research Unit, USDA-ARS, Athens, Georgia (2) Environmental Health Sciences, Univ. of Georgia, Athens (3) Laboratorio Diagnostico Molecular S.S., Guatemala City, Guatemala (4) Centro de Investigaciones en Nutricion y Salud, Guatemala City, Guatemala (5) Dept. of Medicine, Duke Univ. Medical Center, Durham, North Carolina (6) Dept. of Pharmacology, Creighton Univ., Omaha, Nebraska Fumonisin B1 (FB1) is a toxic chemical produced by molds. The molds that produce fumonisin are common in corn. Consumption of contaminated corn by farm animals has been shown to be the cause of animal disease. The proximate cause (key event) in the induction of diseases in animals is inhibition of the enzyme ceramide synthase. Inhibition of de novo ceramide biosynthesis in animals results in a global disruption of sphingolpid metabolism. Fumonisin has been hypothesized to be an environmental risk factor for diseases in humans in countries where corn is a dietary staple and infection with the mold, Fusarium verticillioides, is likely. In order to determine if fumonisin contributes to disease in

humans, methods were developed to measure changes in the urine and blood levels of chemicals that are indicators of changes indicative of pre- disease states in animal studies. The human studies have focused on populations in Guatemala where corn is a dietary staple. Intake of fumonisin in these populations can be very high. Corn, urine and blood were sampled from over 1500 women and the results show that fumonisin intake and changes in a unique class of fats (sphingoid base 1-phosphates) in the blood are correlated in a manner that mimics the effects of fumonisin in laboratory animals. The findings are consistent with the hypothesis that ingested fumonisin inhibits the same enzyme, ceramide synthase, in humans as it does in farm and laboratory animals consuming diets high in fumonisin. These findings are the basis for development of biomarker-based studies in humans designed to identify possible human diseases where fumonisin could be a contributing factor and will provide an incentive to reduce fumonisin exposure in developing countries where corn is a dietary staple. These studies were supported by USDA-ARS and Award RC4HD067971-01 from the Eunice Kennedy Shriver National Inst. of Child Health and Development.

AGFD 102 DNA Adduction by ochratoxin A: Insight for mechanism of action and aptasensor development for mycotoxin detection Richard A. Manderville, rmanderv@uoguelph.ca. Chemistry, Univ. of Guelph, Ontario, Canada Ochratoxin A (OTA) is a naturally occurring chlorophenolic mycotoxin that contaminants a wide range of food products and poses a human cancer threat. Studies on the effects of OTA in mammalian tissue have shown that it causes deletion mutations through the induction of double-strand DNA breaks. The toxin also undergoes metabolism to generate reactive intermediates that covalently attach to DNA to generate DNA adducts that serve as biomarkers for OTA exposure. Because DNA adduct formation is strongly correlated with mutagenicity and carcinogenicity, OTA-mediated DNA adduction may be at the root of its carcinogenic potential. Our studies have shown that OTA, like other chlorinated phenols, undergoes metabolism to generate radical species that attach to the C8-position of 2′-deoxyguanosine (dG) to form carbon-linked (C-linked) and oxygen- linked (O-linked) C8-dG adducts. To gain an understanding of the biological impact of such DNA adducts, model C- and O-linked C8-dG adducts have been incorporated site- specifically into DNA substrates and studied using primer-elongation assays with DNA polymerase enzymes. Our studies demonstrate that bulky C-linked and O-linked C8-dG lesions structurally related to the authentic OTA C8-dG adducts are strong blocks of DNA replication. The implications of these model studies to OTA-mediated mutagenicity will be discussed. C-Linked C8-dG adducts also exhibit fluorescent properties and act as effective G mimics in antiparallel G-quadruplex structures when placed in syn-G positions. An aptamer that binds OTA selectively folds into an antiparallel G-quadruplex. Our studies demonstrate how emissive C8-dG adducts can serve as probes for OTA detection. Selective placement of C-linked C8-dG adducts within the OTA aptamer can enhance aptamer affinity for the toxin and provide a fluorescent response to OTA binding.

AGFD 103 Mycotoxins at the blood-brain barrier: Metabolism, toxicity, barrier integrity and transfer to the brain Matthias Behrens1, mattbehrens@wwu.de, Sabine Hüwel2, Hans-Joachim Galla2, Hans-Ulrich Humpf1. (1) WWU Münster, inst. of Food Chemistry, Germany (2) WWU Münster, inst. of Biochemistry, Germany Fungi of the different genera produce toxic secondary metabolites. To induce adverse effects in the brain after consumption of contaminated food, these mycotoxins would require to penetrate or weaken the blood-brain barrier. Although neurotoxic effects have been described, a systematic study investigating the effects of mycotoxins on the blood- brain barrier is still missing. In the present study results of an in vitro cell culture model are presented. Primary porcine brain capillary endothelial cells (PBCEC) form a monolayer with strong intercellular tight junctions, which inhibit the paracellular diffusion of xenobiotics into the brain tissue. Before applying the test compounds in transport studies, they were tested for their effects on cellular viability. The integrity of the barrier in vitro was ensured by transendothelial electrical resistances (TEER) of >600 Ω×cm2 analyzed by cellular impedance spectroscopy. The obtained values are much higher and closer to the barrier integrity in vivo compared to commercial brain capillary endothelial cell lines. To determine the rate of blood-brain barrier permeation, samples from the blood and the brain compartment were analyzed at time points up to 48 h via LC-MS/MS and LC- HRMS. Fumonisins (FB1, HFB1), moniliformin (MON), trichothecenes (DON, 3-AcDON), zearalenon (ZEN), α-zearalenol (α-ZEL), ochratoxin A (OTA), ochratoxin α (OTα), citrinin (CIT) and dihydrocitrinone (DHCIT) were chosen as test compounds to cover a wide range of polarity and molecular size. The data show that DON, 3-AcDON, FB1 and OTA disturb the blood-brain barrier integrity by affecting cellular viability and TEER. Phase I and II metabolites of ZEN and α-ZEL were detected and quantified. HFB1, ZEN metabolites, OTA, OTα, CIT and DHCIT might be substrates of efflux transporters at the blood-brain barrier.

AGFD 104 Renal gene expression changes in mice and rats exposed to dietary ochratoxin A Andree Nunnikhoven, Ivan Curran, Anne Marie Gannon, Zoe Gillespie, Laurie Coady, Cunye Qiao, Virginia Liston, David Lefebvre, Nikia Ross, Rekha Mehta, Genevieve Bondy, bondygenevieve5@gmail.com. Food Directorate, Health Canada, Ottawa, Ontario Ochratoxin A (OTA), a phenylalanyl derivative of a substituted isocoumarin (R)-N-[5- chloro-3,4-dihydro-8-hydroxy-3-methyl-1-oxo-1H-2-benzopyran-7-y1)carbonyl]-L- phenylalanine, is produced by species in the fungal genera Aspergillus and Penicillium that grow on crops during storage. Studies have shown that exposure to OTA can cause renal tumours in rodents and poultry and that OTA is nephrotoxic in rodents, pigs and poultry. Although OTA exposure can lead to DNA damage, there is ongoing controversy about its mode of action in the kidney, and in particular whether renal tumours result from direct interaction of OTA or a reactive OTA metabolite with DNA, or by indirect epigenetic interactions of OTA with non-DNA targets, or both. Clarification of the events associated with nephrotoxicity was sought using global mRNA expression profiling and individual gene expression analyses of kidneys from mice and rats exposed to OTA in the diet. Kidneys were harvested at terminal necropsy from p53+/- mice and their homozygous (p53+/+) counterparts exposed to OTA for 26 weeks, and from juvenile Fischer rats exposed to OTA throughout gestation and lactation. Metabolism and biotransformation pathways were down-regulated in kidneys from mice exposed to OTA. The expression of specific genes associated with cell cycle regulation, DNA damage repair, tumour suppression and apoptosis were also altered in kidneys from OTA-exposed mice. Gene expression analyses will be analysed in relation to phenotypic changes in mice and rats, and putative mode(s) of action for OTA-induced nephrotoxicity will be discussed.

AGFD 105 FlavonQ: An automated data processing tool for profiling flavone and flavonol glycosides with ultra-high-performance liquid chromatography−diode array detection−high resolution accurate mass−mass spectrometry Pei Chen1, pei.chen@ars.usda.gov, Mengliang Zhang2, Jianghao Sun1. (1) USDA, Beltsville, Maryland (2) Food Composition and Methods Development Lab, USDA, Beltsville, Maryland Profiling flavonoids in natural products poses great challenges due to the diversity of flavonoids, the lack of commercially available standards, and the complexity of food matrices. The increasing popular use of ultra high-performance liquid chromatography diode array detection high-resolution accurate-mass mass spectrometry (UHPLC HRAM-MS) for the analysis of flavonoids has made the task easier and more reliable, however, data-mining of the UHPLC HRAM-MS data is very daunting, labor-intensive, and

expertise-dependent process. An automation data processing tool that could transfer field-acquired expertise into the data analysis will be very valuable. FlavonQ is being developed as such an "expert system" for the analysis of flavone and flavonol glycosides, an important subclass of flavonoids. It is capable of automatic data format conversion, peak detection, flavone and flavonol glycosides peaks extraction, flavone and flavonol glycosides identification and semi-quantitation. The system was applied to the determination of flavone and flavonol glycosides in 9 different plant with an average execution time of 43 ± 11 seconds. The analysis results by FlavonQ were manually verified and was in good agreement.

AGFD 106 Taking metabolomics beyond primary metabolism - challenges and opportunities for capturing plant chemical diversity
Bernd M. Lange1,3, lange-m@wsu.edu, Sean R. Johnson2. (1) inst. of Biological Chemistry, Washington State Univ., Pullman (3) M.J. Murdock Metabolomics Laboratory, Washington State Univ., Pullman Plants evolved the ability to synthesize a plethora of small molecules that used to be called "secondary metabolites", because their functions had remained somewhat elusive. Perhaps a better term is specialized metabolites, which indicates that their roles in defense of signaling may be unique to certain species, families or larger taxa, but in terms of importance are clearly not "secondary" to "primary metabolites" of central metabolism. A unique analytical challenge is the chemical diversity of plant specialized metabolites, the assessment of which requires innovative chromatographic, spectrometric and database solutions. An overview of currently available online platforms and application examples from our own research will be presented.

AGFD 107 Second-generation metabolomics in food research: Merging untargeted and targeted data acquisitions for food and exposome analysis Oliver Fiehn, ofiehn@ucdavis.edu. NIH West Coast Metabolomics Center, Univ. of California, Davis At UC Davis, the NIH West Coast Metabolomics Center integrates more than 30 mass spectrometers in six laboratories, focusing on complex lipids, eicosanoids and lipid mediators, primary metabolism, proteomics, genomics and informatics analyses. In addition, identification of novel compounds of unknown structure is part of research advancements and collaboration-based services. The presentation will highlight novel informatics tools how to interrogate mass spectrometry-based metabolomics data, from compound identification to quality controls. These tools include SWATH-type data independent UPLC-QTOF and TripleTOF MS/MS experiments, but also novel software for distinguishing isobaric co- elutions, retention time predictions and isotope ratio matching. As example, we annotated 165 polyphenols in six commercial red wines by MS/MS matching in 5-min chromatography. Multivariate regression analysis linked the profiles of the red wines to tasting scores. In addition, we highlight the power of gas chromatography with TOF and QTOF MS analysis due to its superior chromatographic peak capacity and higher universality compared to more selective LC separations. We will highlight processed for exposome analyses, identification of unknowns through databases, and, importantly, predicting mass spectra through heuristic and ab-initio calculations. We will show expansions of our LipidBlast library of virtual MS/MS spectra, quantum-mechanical modeling of electron ionization GC-MS spectra and application of these tools to identify novel compounds in metabolomics studies. All these tools are used in research and service projects: currently, over 35,000 samples/year are analyzed in our Center, in ranges of studies of plants, microbial, mouse and human clinical samples.

AGFD 108 Breast milk or infant formula: Consequences for the microbiome and metabolome Carolyn Slupsky, cslupsky@ucdavis.edu. Dept. of Nutrition, Univ. of California, Davis The long- and short-term health benefits of breast-feeding have long been recognized. Indeed, breast-feeding is associated with lower incidences of necrotizing enterocolitis and diarrhea in early life, in addition to lower incidences of inflammatory bowel diseases, diabetes, obesity, and cardiovascular disease later in life. The mechanism by which breast-feeding imparts these protective measures is poorly understood. We have previously reported profound differences between breast-fed and formula-fed infants on growth trajectory, immunological development, succession of the gut microbiome and metabolism that suggests that early dietary exposures may influence the risk of chronic disease in adulthood1. It is unknown whether the difference between breast feeding and formula feeding is related to specific formulas, or whether other formulas or additives will cause the same effect. To investigate how the composition of infant formula affects the gut microbiome and host metabolism, fecal microbial ecology, measured through 16s rRNA sequencing, and comprehensive metabolic profiling of serum, urine, and feces measured through 1H NMR metabolomics, were analyzed in the context of high and low protein diets, different carbohydrates and addition of probiotics. These results will be discussed in the context of highlighting the link between diet and health.

AGFD 109 Metabolomics for understanding the plant chemistry: Comparison of lipid extraction methods for lipid profiling in algae
Nutan Kaushik1, kaushikn@teri.res.in, Tobias Kind2, Oliver Fiehn3. (1) The Energy of Resources inst., New Delhi, India (2) Genome Center, Univ. of California, Davis (3) NIH West Coast Metabolomics Center, Univ. of California, Davis Microalgal strains with high oil, or lipid content are of great interest in the search for a sustainable feedstock for the production of biodiesel. Various methods for extraction of lipids have been reported for lipidomic studies. Chloroform/methanol/ water extraction has been reported to extract lipids of all major classes. Matyash et al (2008) proposed methyl-tert-butyl ether (MTBE) based extraction method for faster and cleaner lipid recovery. For cell disruption, previously it was reported that homogenization of cells is performed better with steel ball than with glass bead milling (Lee and Fiehn, 2008) . In present work we compared the lipid extraction efficiency of Chloroform/methanol/ water and methyl-tert-butyl ether (MTBE) and also two cell disruption methods steel ball and sonication for microalgae Chlamydomonas reinhardtii . It was observed that number of metabolites extracted with Chloroform/methanol/ water (2:5:2) were higher than methyl- tert-butyl ether (MTBE). Further steel ball and sonication were found be equally effective in disrupting the cell wall for extraction of metabolites.

AGFD 110 Comparison of volatile compounds in fermented rice broths Hyeon Ji Lim2, hyeonji1224@gmail.com, Sang Mi Lee2, Yoon Jung Roh2, Joo Young Lee2, Byong Wook Eum3, Ji Won Chang3, Young-Suk Kim1. (1) Dept. of Food Science and Engineering, Ewha Womans Univ., Seoul, Korea (2) Ewha womans Univ., Seoul, Korea (3) R&D Center, Sempio Food Company , Cheongju-si, Korea Different rice preparations, which included whole milled rice, ground milled rice, whole brown rice, and ground brown rice, were fermented after inoculation of Lactobacillus paracasei. Volatile compounds in the fermented rice broth samples were extracted using solid-phase microextraction (SPME) before analyzed by gas chromatography- mass spectrometry (GC-MS) to compare the differences in their volatiles profiles. The contents of methyl 2-hydroxybenzoate, diacetyl, 2,3-butanediol, hexanal, nonanal, furan-2-carbaldehyde, ethanol, and 1-octen-3-ol were higher in the fermented milled rice sample than fermented brown rice one. On the other hand, the formation of 2- nonanone, 1-hexanol, 5-hexyldihydro-2(3H)-furanone, acetic acid, 3-methylbutanoic acid, and hexanoic acid were significantly increased in the fermented brown rice sample. The contents of acetoin, ethanol, 3-methylbutanoic acid, and 4- ethenyl-2-methoxyphenol were highest in the fermented

whole rice sample, whereas those of 6-methylhept-5-en-2-one, 2-propylfuran, and 2-butylfuran were higher in the fermented ground rice sample than others. Among the volatile compounds, our study demonstrated that diacetyl, 2,3-butanediol, 5-hexyldihydro-2(3H)-furanone, hexanoic acid, and benzaldehyde were major compounds that differentiated the fermented rice samples according to the raw materials.

AGFD 111 Crystal structure and catalytic mechanism proposal of cellobiose 2-epimerase from Caldicellulosiruptor saccharolyticus DSM 8903 Qiuyun Shen1,3, shenqy@mail.hzau.edu.cn, Yuzhu Zhang2, Ruijin Yang3, Siyi Pan1. (1) College of Food Science and Technology, Huazhong Agricultural Univ., Wuhan, Hubei, China (2) USDA, Albany, California (3) School of Food Science and Technology, Jiangnan Univ., Wuxi, Jiangsu Province, China Cellobiose 2-epimerase from thermophile Caldicellulosiruptor saccharolyticus (CsCE) can catalyze the conversion of lactose into lactulose, a non-digestible disaccharide widely used in food and pharmaceutical industries. Information about the structural bases of the cellobiose 2-epimerase catalysis of lactose isomerization is lacking. Single crystals of wild type CsCE (WT-CsCE) and mutant G4-C5 were obtained by the hanging drop vapor diffusion method and the best crystals diffracted to 1.54 Å and 1.67 Å resolution, respectively. Mutant G4-C5 was obtained through four sequential rounds of random mutagenesis and screening, and had a 2.8-fold increase in specific activity without compromising thermostability. The structure of CsCE demonstrates an (α/α)6 barrel fold, which shows significant structural homology with other enzymes from N- acyl-D-glucosamine 2-epimerase (AGE) superfamily. The (α/α)6 barrel structure consists of 6 outer helices running in roughly the same direction and 6 inner helices oriented in the opposite direction and the formed deep cleft is considered to be a putative active site. Important residues were identified by amino acid sequence alignment and tertiary structure superposition with enzymes from the same superfamily. Site-directed mutagenesis of these residues showed that Arg56, His188 and His377 were strictly required for activity and Glu191, Glu312, Arg380, Trp308 and Trp372 were also essential for high activity. Based on the catalysis properties and structural information, CsCE likely perform a deprotonation/protonation mechanism through a cis-enediol intermediate in a metal-independent manner and His377 and His188 may serve as the acid/base catalytic sites. Structure of mutant G4-C5 showed that three mutations A12S, R5W and K328I were in the different α-helixes at the surface region and far from the putative catalytic center. Amino acid substitution, F231L, was also at the surface of the protein, but it was close to the entrance of the cleft. Mutation I52V located in an inner α- helix and was close to the conserved residues Arg56, Tyr114 and Trp372.

AGFD 112 Inhibition of formation of advanced glycation end-products by an oligosaccharide-enriched fraction purified from cranberry (Vaccinium macrocarpon) Jiadong Sun1, Hang Ma1, hang_ma@uri.edu, Weixi Liu2, Joel Dain2, David C. Rowley1, Navindra P. Seeram1. (1) College of Pharmacy, Univ. of Rhode Island, Kingston (2) Chemistry Dept., Univ. of Rhode Island, Kingston Advanced glycation end-products (AGEs) are a polymorphic group of compounds implicated in several chronic complications including type-2 diabetes and neurodegenerative diseases. Herein, an oligosaccharide-enriched fraction, purified from North American cranberries (Vaccinium macrocarpon), was evaluated for its anti-AGE effects using human serum albumin and D-fructose as the model protein and glycating agent, respectively. The cranberry oligosaccharide-enriched fraction reduced AGE formation in a concentration dependent manner (44, 47, 61 and 65 % at 10, 50, 100, 200 µg/mL, respectively). Interestingly, 65 % inhibition was achieved with the cranberry oligosaccharides at 200 µg/ml while the positive control, aminoguanidine (a synthetic anti-AGE agent) showed 78 % at a much higher concentration of 500 µg/ml. Further studies to evaluate the mechanisms of anti-AGE effects of cranberry oligosaccharides are warranted and are being pursued by our group.

AGFD 113 Advanced glycation endproducts inhibitory compounds from amla (Phyllanthus emblica) Kenneth N. Rose, kenneth_rose@my.uri.edu, Chunpeng Wan, Hang Ma, Weixi Liu, Navindra P. Seeram. College of Pharmacy, Univ. of Rhode Island, Kingston Glycation is the non-enzymatic reaction between proteins and reducing sugars that leads to the formation of advanced glycation endproducts (AGEs). The formation and accumulation of AGEs lead to several chronic human illnesses including type-2 diabetes and neurodegenerative diseases. The traditional Indian Amla (Phyllanthus emblica) fruit (also known as Indian gooseberry) has been linked with a wide variety of biological effects including anti-diabetic effects. Moreover, published data suggest that Amla extracts show anti-AGE effects but the active compounds were not identified. Herein, we report the isolation and structure elucidation (by NMR) of ten (1-10) compounds from a commercial Amla juice powder, which included six gallotannins/gallic acid derivatives and four ellagitannins/ellagic acid derivatives. The anti-AGE effects of the Amla extract and pure compounds were investigated using a combination of in vitro (BSA-fructose assay) and in vivo (Caenorhabditis elegans) assays.

AGFD 114 Antibacterial properties of common herbs and spices Bryce Lipinski, B05lipi@siena.edu, Daniel F. Moriarty, dmoriarty@siena.edu. Dept. of Chemistry and Biochemistry, Siena College, Loudonville, New York Microorganisms resistant to antibiotic drugs have become a larger public concern in recent years. The search for molecules with broad-spectrum activity has led to the investigation of plant material as a potential source for a sufficient and easily obtainable source for these molecules. By extracting peptides and other small molecules from various herbs and spices (focused mainly on Thyme and Cinnamon) the antibacterial activity can be investigated. Multiple solvents were used in order to extract different classes of molecules, and inhibition of bacterial growth is examined by exposing bacterial to the various extracts. Samples showing strong inhibition of bacterial growth are run through a reverse-phase high performance liquid chromatography (HPLC) attached to a diode-array detector to separate out the molecules. Once the various molecules have been separated, each will be tested for antimicrobial activity. Molecules with positive activity will be analyzed using MS in order to confirm the identity.

AGFD 115 Pea protein isolate as a natural nanocarrier for enhanced dispersibility and stability of curcumin Shuo Chen, schen2020@foxmail.com. College of Light Industry and Food Science, South China Univ. of Technology, Guangzhou, China This work reported that as a type of amphiphilic biopolymers, pea protein isolate (PPI) mainly presented in the nanoparticle form with the hydrodynamic diameter of 70-90 nm at pH 7.2 in solutions. Curcumin as a model drug was loaded into pea protein nanoparticles with a low-energy and toxic solvent-free method. PPI nanoparticles did not suffer noticeable changes in particle size and external morphology upon complexation with curcumin, while the surface hydrophobicity markedly decreased. Fluorescence data exhibited that quenching process between PPI and curcumin was primarily due to static quenching by the formation of PPI-curcumin nanocomplex. Fourier transform infrared spectroscopy and Circular Dichroism patterns further confirmed successful complexation and its influence on the secondary structure of pea proteins. After complexation, the solubility and thermal stability (at 25 °C and 100 °C) of curcumin were both considerably enhanced. The results suggest PPI can be utilized as a promising natural nanocarrier for encapsulation and oral delivery of lipophilic compounds in food and pharmaceutical industries.

AGFD 116 New approaches to the preparation and characterization of tormentic acid Edward J. Parish1, Hiroshi Honda2, chrishonda@yahoo.com, Tsao-Yi Wei4, Jin-Bin Wu3, Jinbinwu@gmail.com, Hui-Ya Ho3. (1) Auburn Univ, Auburn, Alabama (2) NPU, Fremont, California (3) Pharmacy, China Medical Univ., Taichung, Taiwan (4) Bioengineering, Northwestern Polytechnic Univ., Fremont, California This paper represents the preparation, isolation and purification of tormentic acid, can inhibit the activity of the matrix metalloproteinase for the decomposition of the collagenase substrate III

AGFD 117 Novel approaches to the chemical synthesis and biological activity of 24- ketolanosterol an inhibitor of HMG-CoA reductase Edward J. Parish2, Jiandao Yin3, yjd0059@163.com, Hiroshi Honda1, chrishonda@yahoo.com, Tsao-Yi Wei5, Hongfei Yin4. (1) Bioengineering, Northwestern Polytechnic Univ., Fremont, California (2) chemistry, Auburn Univ, Auburn, Alabama (3) Environmental Science and Safety, Tianjin Univ. of Technology, Tianjin, China This paper represents a facil synthesis of ketolanosterol to be a potent inhibitor of 3- hydroxy-3-methylglutary coenzyme A reductase activity in mouse cells grown in a serum-free medium

AGFD 118 Facile synthesis and carbon-13 nuclear magnetic resonance spectral properties of cholest-4-en-3,6-dione Edward J. Parish1, Hiroshi Honda2, chrishonda@yahoo.com, Tsao-Yi Wei3, Huey-Lih Shyu4, hlshyu@ctust.edu.tw. (1) chemistry, Auburn Univ, Auburn, Alabama (2) Bioengineering, Northwestern Polytechnic Univ., Fremont, California (4) Medical Technology, Central Taiwan Univ., Taichung, Taiwan This paper represents the chemical synthesis of cholest-4-en-3-one and cholest-4-en- 3,6-dione. The cholesterol derivative cholest-4-en-3,6-dione is a naturally occurring substance found in both plant and animal tissues.

AGFD 119 Novel approaches to the chemical synthesis and spectral characterization of hydroxysterols Yu-Chen Lo2, bennylo@ucla.edu, Huey-Lih Shyu3, hlshyu@ctust.edu.tw, Wan-Yuan Huang5, Hiroshi Honda1, Tsao-Yi Wei4. (1) NPU, Fremont, California (2) Chemistry, Biochemistry and Bioengineering, UCLA, Fremont, California (3) Medical Technology, Central Taiwan Univ., Taichung, Taiwan (5) Bioengineering, Northwestern Polytechnic Univ., Fremont, California This paper represents the facile synthesis of 11α-hydroxysterols and the complete structural characterization of the products and intermediates.

AGFD 120 Chemical synthesis and characterization of lanosterol derivatives, inhibitor of cholesterol biosynthesis Edward J. Parish1, Wan-Yuan Huang3, Hiroshi Honda4, chrishonda@yahoo.com, Tsao-Yi Wei4, Huey-Lih Shyu2, hlshyu@ctust.edu.tw. (1) chemistry, Auburn Univ, Auburn, Alabama (2) Medical Technology, Central Taiwan Univ., Taichung, Taiwan (3) Bioengineering, Northwestern Polytechnic Univ., Fremont, California This paper represents a facile synthesis and characterization of lanosterol derivatives, lanost-8-en-3β-ol-7,11-dione has been found to be a potent inhibitor of sterol biosynthesis in animal cells in culture.

AGFD 121 Novel preparation and characterization of kinsenoside Edward J. Parish1, Jin-Bin Wu3, Hui-Ya Ho3, jlbioaya@gmail.com, Hiroshi Honda2, chrishonda@yahoo.com, Tsao-Yi Wei4. (1) Auburn Univ, Auburn, Alabama (2) NPU, Fremont, California (3) Pharmacy, China Medical Univ., Taichung, Taiwan (4) Bioengineering, Northwestern Polytechnic Univ., Fremont, California This paper represents the preparation, purification, spectral chracterization of kinsenoside, which can inhibit the activation of macrophages, inhibit the formation of osteoclasts, and inhibit the function of osteoclasts.

AGFD 122 Elucidation of changes in non-volatile metabolites of amylolytic yeast, Saccharomycopsis fibuligera, according to the cultivation times JiHye Jeong, 923jjh@gmail.com, Na Kyeom Lee, Young-Suk Kim. Ewha Womans Univ., Seoul, Korea Makgeolli is a traditional Korean alcoholic beverage made from rice by fermentation after addition of nuruk, a microbial starter. Microorganisms and their metabolites influence on the quality of Makgeolli. An amylolytic yeast, Saccharomycopsis fibuligera, was isolated from nuruk and its non-volatile metabolites were analyzed using GC- TOF/MS for the cultivation times of 24 hours. The non-volatile metabolites were extracted with a fast filtration method and then derivatized before GC-TOF/MS analysis. In total, 22 amino acids, 8 carbohydrates, 13 lipids and 12 organic acids were detected in this study. In particular, the contents of glycerol and trehalose were significantly increased, while galactose and oxalic acid were decreased according to the cultivation times.

AGFD 123 Microbial synthesis of myrcene by metabolically engineered Escherichia coli Eun-Mi Kim1, Jin-Hee Eom1, Youngsoon Um1, Yunje Kim1, Han-Min Woo1,2, smsb.lab@gmail.com. (1) Korea Inst. Sci. Tech., Seoul, Korea (2) Green School, Korea Univ., Seoul, Korea Myrcene, a monoterpene (C10), has gathered attention as a starting material for high- value compounds, such as geraniol/linalool and (−)-menthol. Metabolic engineering has been successfully applied to produce monoterpenes, such as pinene and limonene, at high levels in microbial hosts. However, microbial synthesis of myrcene has not yet been reported. Thus, we metabolically engineered Escherichia coli for production of myrcene by introducing a heterologous mevalonate pathway and overexpressing tailoring enzymes, such as geranyl diphosphate synthase (GPPS) and myrcene synthase (MS). Although MSs have broad ranges of functionality for producing various monoterpenes, our engineered E. coli strains harboring MS from Quercus ilex L. produced only myrcene (1.67 ± 0.029 mg/L). Subsequent engineering resulted in higher production of myrcene by optimizing the levels of GPPS in amino-acid-enriched (EZ- rich) defined medium, where glycerol as a carbon source was used. The production level of myrcene (58.19 ± 12.13 mg/L) was enhanced by 34-fold using in situ two-phase extraction to eliminate cellular toxicity and the evaporation of myrcene.

AGFD 124 Structure activity related, mechanistic, and modeling studies of gallotannins containing a glucitol-core and a glucosidase Hang Ma1, mahangees@gmail.com, Ling Wang2,3, Daniel B. Niesen1, Wen Tan3, Qiong Gu2, Jun Xu2, Navindra P. Seeram1. (1) Biomedical and Pharmaceutical Sciences, Univ. of Rhode Island, Kingston (2) School of Pharmaceutical Sciences, Sun Yat-Sen Univ., Guangzhou, China (3) School of Bioscience and Bioengineering, South China Univ. of Technology, Guangzhou Gallotannins containing a glucitol core, which are only produced by members of the maple (Acer) genus, are more potent α-glucosidase inhibitors than the clinical drug, acarbose. While this activity is influenced by the number of substituents on the glucitol core (e.g. more galloyl groups leads to increased activity), the mechanisms of inhibitory action are not known. Herein, we investigated ligand-enzyme interactions and binding mechanisms of a series of 'glucitol-core containing gallotannins (GCGs)' against the α- glucosidase enzyme. The GCGs included ginnalins A, B and C (containing two, one, and one galloyl/s, respectively), maplexin F (containing 3 galloyls) and maplexin J (containing 4 galloyls).

All of the GCGs were noncompetitive inhibitors of α-glucosidase and their interactions with the enzyme were further explored using spectroscopic measurements. The binding regions between the GCGs and α-glucosidase, probed by a fluorescent tag, 1,1′-bis(4-anilino-5-napththalenesulfonic acid, revealed that the GCGs decreased the hydrophobic surface of the enzyme. In addition, circular dichroism analyses showed that the GCGs bind to α-glucosidase and lead to loss of the secondary α-helix structure of the protein. Also, molecular modeling was used to predict the binding site between the GCGs and the α-glucosidase enzyme. This is the first study to evaluate the mechanisms of inhibitory activities of gallotannins containing a glucitol-core on α-glucosidase.

AGFD 125 Anti-glycative, reactive carbonyl scavenging and anti-amyloid fibrillation effects of ayurvedic medicinal plants Weixi Liu2, Hang Ma1, mahangees@gmail.com, Lu Zhang1, Chunpeng Wan1, Joel Dain2, Navindra P. Seeram1. (1) Biomedical and Pharmaceutical Sciences, Univ. of Rhode Island, Kingston (2) Dept. of Chemistry, Univ. of Rhode Island, Kingston Advanced glycation end-products (AGEs) are contributors to several disorders including diabetes and Alzheimer's disease. For centuries, Ayurvedic herbs have been used for the treatment of these diseases. Herein, the anti-glycative and neuroprotective effects of twenty-three Ayurvedic medicinal plants were evaluated. Since elevated glycation level in vivo is caused by multiple factors including hyperglycemia, oxidative stress, and carbonyl stress, the herbs were also evaluated for total polyphenol content, anti- oxidative activities, and carbonyl scavenging properties. All of the samples (at 100 μg/mL), showed anti-AGE effects ranging from 15.1-90.8%. Pomegranate (Punica granatum) peel and flower extracts showed the most potent inhibitory effects of 90.8 and 86.5% which were higher than positive control, aminoguanidine (AG; 67.2%). Amla (Phyllanthus emblica) juice (85.3%) and moringa (Moringa oleifera) fruit (75.6%) extracts were also superior to AG. To evaluate for neuroprotective effects, the inhibitory effects of the herbs on Aβ1-42 fibrillation were tested by the thioflavin T assay. Bacopa (Bacopa monnieri) showed the highest inhibition (63.5%), followed by gotu kola (Centella asiatica; 62.6%) and moringa seed extract (50.5%). Pomegranate peel and flower, and amla juice extracts inhibited Aβ1-42 fibrillation (49.9, 36.6 and 33.7%) higher than the positive control, resveratrol (31.8%). Interestingly, these plant extracts also showed high polyphenol contents, anti-oxidative activities, and carbonyl scavenging properties. Pomegranate peel extract had the highest polyphenol content (41.2%) among the herbs followed by amla juice extract (38.9%). Pomegranate peel and amla juice extracts also exhibited the strongest methylglyoxal (MGO) scavenging activities by reducing MGO content by 87.3 and 78.6%. In addition, both herbs showed strong anti- oxidative activities (IC50 13.7 and 11.1 μg/mL, respectively). Therefore, the activities of pomegranate and amla may be due to their high polyphenol contents which contributes to their anti-oxidative and carbonyl scavenging properties. Further studies on these promising Ayurvedic herbs are being pursued by our group.

AGFD 126 Vapor-Infusion of wine flavor volatiles in specialty dark chocolate and analysis via GC-MS Sydney Richards1, sydr90@hotmail.com, Ryan MacFarland1, Peter J. Iles1, Luther D. Giddings1, Mary Alvarez2, Ron V. Valcarce1, Ryan Holcomb1, Neil R. Bastian3. (1) Salt Lake Community College, Murray, Utah (2) Salt Lake Community College, Bountiful, Utah (3) Salt Lake Community College, Kaysville, Utah Chocolate modified by the inclusion of additional flavor agents (e.g., citrus fruits, berries, coffee, spices & etc.) has become increasingly sought after. Chocolates filled or flavored with wine fit this trend. In this study, wine flavor agents were vapor-infused into single origin artisanal dark chocolate. The vapor-infused chocolates were analyzed using GC-MS. Various methods were used in an attempt to maximize the vapor-infusion of wine flavor agents. Changes in chocolate taste and texture were also subjectively assessed by a panel of volunteer tasters.

AGFD 127 Pesticide mobility in soils: An initial characterization comparing productive vs non-productive soils Giselle A. Querejeta, Erica P. Beiguel, erica@buanzo.com.ar, Enrique A. Hughes, Javier Montserrat, Anita Zalts. Environmental Chemistry, Universidad Nacional de General Sarmiento, Los Polvorines, Buenos Aires, Argentina Traditional horticulture in Argentina is mainly done in small scale enterprises, and involves the intensive use of pesticides; these are xenobiotics whose application may alter soil properties and even the complete ecosystem. Other amendments are used as well, such as organic fertilizers, that could change soil composition. The aim of this work was to evaluate a potential environmental impact of this activity, comparing pesticide mobility in soils from active horticultural units with non-productive soils from the same region. Soils from Moreno district (Bs. As., Argentina) were sampled and sieved. Vertical mobility of trifluralin and chlorpyrifos was determined in glass columns (45 cm long) according to the OECD guide (OECD/OCDE (2004). "OECD Guidelines for the testing of chemicals. Leaching in soil columns." 312), using atrazine as reference because of its intermediate mobility behaviour. After elution and extrusion, pesticides were extracted from soil using cyclohexane:acetone 50:50 and quantified by gas chromatography. In all cases we observed that atrazine had higher mobility in non-productive than in productive soils. Trifluralin showed a similar behaviour, being practically immobile in horticultural soil. Chlorpyrifos was the most displaced pesticide in non-productive soil, reaching 15 cm from the top of the column, while in horticultural soil most of the product remained in the first 10 cm. So, the results show that soil used for horticultural production retained pesticides in higher amounts than non-productive soil. . This was not expected because the non-productive soil had more organic matter than horticultural soil. The first hypothesis was that organic matter would interact strongly with pesticides, so these products would be more retained in non-productive soil than in the soil actually used for horticulture, however the experimental results showed an inverse behaviour for all three pesticides. In conclusion, this preliminary assay indicates that, in this soil, mobility was not directly related to organic matter content; as these samples had been dried, mixed and sieved a possible explanation could be related to the structure of the soil sample. This hypothesis leads to the question of what would happen with pesticide mobility results, if the productive soil is not sieved (i.e. conserves its structure as in the farm), even though organic matter is higher in non-productive soils. This will be addressed in future research.

AGFD 128 Evaluation of immunogenicity of hepatitis b vaccine referred to the clinic Ehsan Rezaei, erezaeii@yahoo.com. medical student, Hormozgan, Iran Introduction: Hepatitis B as a serious viral disease, much of the health and financial resources allocated to the developing countries. One way of preventing it, is vaccination. Unfortunately, the immunity provided by the vaccine is incomplete and factors such as gender, age, body mass index, smoking, and the time elapsed since the last vaccination, the affects. In this retrospective cross-sectional study of all the people from 1388 to 1393 to a private clinic for infectious diseases Hepatitis B Vaccination visited and where they had been registered on the basis of variables derived . Finally, data mining software and SPSS 22 registered using this software as well as tests descriptive statistics (mean, standard deviation, and frequency) as well as statistical tests such as Chi-square analysis and T test were analyzed. A total of 133 people, 75 men (56.4%) and 58 patients (43.6%) were female. People were divided into six groups based on age, 1-10 years, 7 patients (5.3%), 11-20 in 17 patients (12.8%), 21-30 years, 34 patients (25.6%), 31-40 years, 34 patients (25.6%), 41-50 years, 32

patients (24.1%) and more than 50 years, 9 patients (6.8%) has been vaccinated. People pointed to three categories based on the level of antibodies less than 10 IU / L to 24 (18 percent), 10-100 IU / L, 33 patients (24.8%) and greater than 100 IU / L 76 patients (57.1%) have been divided. 42.9% of one to ten years (3) in the 10-100 seat while only 11.8% of 31-40 year-olds (4 people) are at this level. According to the P-value must be said that there are significant differences between age groups in the level of safety. 25.3% of men (n = 19) in the safety level of less than 10, while only 8.6% of women (5 people) are at this level. According to the P-value must be said that there is a significant difference between the sexes in safety. Given that vaccination against HBV immunization in the range of best practices to control HBV infection in iran, the serological tests to evaluate the safety levels after vaccination is recommended. In this study, based on three parameters to assess the safety of hepatitis B vaccination in females than in males. The safety level is reduced with age.

AGFD 129 Effect of pH and xanthan-locust bean mixtures on the physicochemical properties of whey protein-stabilized oil-in-water emulsions Cory Owens1, cory.owens470@topper.wku.edu, Hanna(John) Khouryieh2, Kevin Williams1. (1) Chemistry, Western Kentucky Univ., Bowling Green (2) Food Processing and Technology, Western Kentucky Univ., Bowling Green The effect of pH and xanthan (XG)-locust bean gum (LBG) mixtures on the physical stability of 2 wt% whey protein isolate (WPI) stabilized oil-in-water (O/W) emulsions containing 10% v/v menhaden oil was investigated by measuring particle size, cream stability, viscosity, and microstructure. The O/W emulsions containing .1% XG-LBG mixtures were compared to emulsions with .1% XG and .1% LBG alone along with controls with no gums. The results indicated that creaming is dependent on pH and biopolymer type. At pH 5, all emulsions had similar patterns of phase separation and had no turbidity in the serum phase. The lack of turbidity is likely because at pH 5 the WPI is near its isoelectric point and can be adsorbed more efficiently. This also allows the droplets to aggregate in a similar way and rate in all emulsions at pH 5. Rapid creaming in the XG and XG-LBG emulsions at pH 3 and 5 were a result of flocculation from the complexation of XG-WPI complexes. These complexes were seen to be part of the large floccules in the microstructures. The XG-LBG emulsions at pH 7 showed the greatest resistance to phase separation and resulted in stable emulsions. This is likely because XG and LBG have a strong synergistic interaction that increases viscosity. XG- LBG mixtures can used to form stable emulsions, which help in development of novel structures and textures to create healthier foods.

AGFD 130 Comparison of a brewer's water analysis kit to standardized methods and implications for brewing Nick O. Flynn1,2, nflynn@wtamu.edu, David Reasoner3, Jared Read4, Paul T. Baumgardner2. (1) Chemistry and Physics, West Texas A&M Univ., Canyon (2) Advanced Biogenetics & Life Sciences, Panhandle, Texas (3) City of Amarillo Environmental Lab, Amarillo, Texas (4) Long Wooden Spoon Brewing, Amarillo, Texas There are commercial kits that are available for homebrewers to use to analyze water for making beer. This research explored how closely one of these kits matched the ion concentrations obtained by the City of Amarillo Environmental Lab using standardized methods. A secondary objective was the comparison of ion values in different water sources which can also have implications for brewing. Sources that were analyzed for these studies included tap water, boiled tap water, RO water, well water, bottled water and water from a vending machine (charge per gallon). Measured ions that were relatively close to Lab values using the kit included calcium, magnesium and chloride concentrations whereas ions that did differ included sodium and sulfate ions. The most significant implication of this comparison is that misadjusted sodium and sulfate levels can lead to undesirable bitterness in beers. Furthermore, many brewers believe that chloride : sulfate ratios are important for moderating flavor profiles in beer so it is important to be able to determine sulfate ratios accurately. In regard to water source, RO water was predictably lowest in all ions analyzed. Tap water was highest in calcium whereas boiled water was second lowest. Boiling did not affect magnesium concentration and well water contained the highest amount of magnesium. Magnesium in higher concentrations can impart bitterness to beer. Chloride concentrations were highest in boiled tap water with bottled water containing the second lowest value. Sodium and sulfate values were expectedly highest in boiled tap water thus suggesting that some ions, perhaps chloride as well, are affected by the volume reduction associated with boiling. The low concentration of ions in RO water is an important consideration for the homebrewer given the impact this has on both flavor profiles, off flavors and yeast metabolism.

AGFD 131 Survey of amino acid composition in cider apples grown in Virginia by UPLC-PDA Sihui Ma1, sihuima@vt.edu, Gregory Peck2, Amanda Stewart1. (1) Food Science and Technology, Virginia Tech, Blacksburg, Virginia (2) Horticulture, Cornell Univ. , Ithaca, NY Recent rapid growth of the cider industry calls for research on juice chemistry of cider apples, with emphasis on the impact of fruit chemistry on fermentation performance and cider quality. Amino acids are essential for yeast metabolism. Along with ammonium ions, they constitute the yeast assimilable nitrogen in apple juice. The composition and concentration of yeast assimilable nitrogen will influence both the fermentation kinetics and volatile aroma production in cider making. Twenty-one amino acids were characterized and quantified in juice of 15 cider apple cultivars grown in Virginia that have potential for use in cider making. Amino acids were identified and quantified by UPLC-PDA system with Waters AccQ●TagTM Ultra derivatization kits. The amino acid composition was significantly different cross apple cultivars. The total amino acid concentration ranged from 14 mg/L in Golden Delicious to 127 mg/L in Enterprise. Asparagine, aspartic acid, and glutamine are the principal amino acids in most apple juices. Serine, arginine, threonine, alanine, γ-amino butyric acid, proline, lysine, tyrosine, methionine, valine, isoleucine, leucine, and phenylalanine were also present in most apple juice with relatively lower concentration. The relative concentration of amino acids in cider apples is different than in Vitis vinifera wine grapes, which are rich in proline and arginine, and the impact of these differences on fermentation of apple juice by wine yeast warrants further research. These results are informative for further study on yeast metabolism and nitrogen management during fermentation in cider production.

AGFD 132 Physicochemical properties of amorphous granular starches prepared from corn, tapioca and non-waxy rice starches using high hydrostatic pressure Jong Hyun Choi, choi6167@khu.ac.kr, Mi-Ra Song, Byung-Yong Kim, Moo-Yeol Baik. Food Science and Biotechnology, Kyunghee Univ., Yong-in, Kyunggi, Korea Corn, tapioca and non-waxy rice starches were treated at 20oC for 30min under HHP (550 MPa) to prepare amorphous granular starches (AGS) and their physicochemical properties, such as water holding capacity (WHC), rapid visco analyzer (RVA) pasting properties, solubility, swelling power and apparent viscosity were investigated. All AGS (corn, tapioca and non-waxy rice starches) revealed different physicochemical properties compared to native starches. Also all AGS revealed the thicker pastes than native starches when mixed with cold water. WHC of native starches were significantly different each other and non-waxy rice starch showed the highest value followed by corn and tapioca starches, whereas WHC of all AGS showed no-significant difference. WHC of all AGS were much higher than those of native starches. It is interesting to note that solubility and swelling power of all AGS were higher at 60oC and lower at 90oC than those of native starches, respectively. This is possibly due to disintegration of crystalline region in AGS. In case of RVA pasting properties, all AGS showed distinctively different pasting pattern compared to native starches. Pre-gelatinized starch,

which has no crystalline and no granular structure, did not show pasting properties in RVA analysis because they do not have granular structure. However, all AGS showed similar pasting pattern with native starches with relatively lower peak viscosity and setback, and relatively higher pasting temperature than native starches. Preparation and physicochemical properties of AGS provides possible future application of AGS in various industries.

AGFD 133 Effects of processing and storage temperature on browning index, furosine, and HMF in aseptic cold break tomato paste during storage time Hye Won Yeom, hwyeom@yahoo.com, Joseph Conte, Rasheed Mohammed, Steve DeMuri. Campbell Soup Company, Camden, New Jersey To evaluate heat damage by process and storage temperature, a cold break tomato paste was aseptically filled into 5 liter aseptic bags at different process temperature (104 °C and 112 °C). The aseptic bags were stored at different storage temperature (21 °C and 33 °C) for 12 months of storage time. The level of Browning Index, Furosine, and HMF was monitored in the cold break tomato paste during the storage time. Higher storage temperature (33 °C) significantly increased the level of Browning Index, Furosine, and HMF in the tomato paste compared to the lower storage temperature (21 °C) during the storage time. However, there was no significant difference in the Browning Index, Furosine, and HMF analysis results between the tomato pastes processed at 104 °C and 112 °C.

AGFD 134 Effects of storage and heating on serum viscosity of hot break tomato paste Hye Won Yeom, hwyeom@yahoo.com, Andy Janosko, Marco Ramirez, Steve DeMuri. Campbell Soup Company, Camden, New Jersey, Representative samples were collected from commercially produced aseptic hot break tomato paste during 11 months of ambient storage time. Serum viscosity of the hot break tomato paste was analyzed at each sampling interval and compared to the initial serum viscosity measured at the time of manufacturing. As storage time increased, serum viscosity decreased. After 6 months of storage, 16 - 27% reduction of serum viscosity was observed in the hot break tomato paste. To evaluate the effects of the heating process on hot break paste serum viscosity, the paste samples were reconstituted with water to the same level of tomato solids as typical finished products using hot break paste. The diluted paste was heated at 95 °C for 3 min. and serum viscosity was measured. As a result of the heating process, serum viscosity was found to recover slightly closer to time of manufacture levels at up to 6% of initial values.

AGFD 135 Determination of ceftiofur and its metabolites in plasma using reverse-phase liquid chromatography Sherry Cox, scox6@utk.edu, Molly White, Kristen Gordon, Joan Bailey. Biomedical and Diagnositic Sciences, Univ. of Tennessee, Knoxville A high performance liquid chromatography procedure for the determination of ceftiofur and all its desfuroylceftiofur metabolites, in plasma has been developed and validated using reverse phase liquid chromatography. Following a derivatization method that converts ceftiofur and all desfuroylceftiofur metabolites to desfuroylceftiofur acetamide, separation was attained on a Symmetry C18 column and quantification occurred using UV detection at 265 nm. The mobile phase was a mixture of (A) 0.1% trifluroracetic acid (TFA) in water and (B) 0.1% TFA in acetonitrile. The mixture was pumped at a starting gradient of 90% A and 10% B and was adjusted to 75% A and 25% B over 25 min, and back to initial conditions over 3 min. with a flow-rate of 1.0 ml/min. The procedure produced a linear curve over the concentration range of 0.1 – 100 µg/mL with a lower limit of quantification of 100 ng/mL. Intra-assay variability ranged from 0.7 to 4.5% and inter-assay variability ranged from 3.6 to 8.8% for desfuroylceftiofur acetamide, respectively and the average recovery was 99%. This method could be useful to those investigators dealing with small sample volumes, particularly when conducting pharmacokinetics studies which require multiple sampling from the same animal.

AGFD 136 Reversed-phase high performance liquid chromatography (HPLC) studies of the sweet diterpene glycosides isolated from Stevia rebaudiana bertoni Venkata Chaturvedula, sprakash@wisdomnaturalbrands.com, Srinivasarao Meneni. Natural Products Research Group, Wisdom Natural brands, Gilbert, Arizona A series of HPLC studies were performed on sweet steviol glycosides isolated from the leaves of Stevia rebaudiana including the Joint Expert Committee on Food Additives (JECFA) compounds namely rebaudioside A, steviolbioside, stevioside, rubusoside, rebaudioside B, rebaudioside C, rebaudioside D, rebaudioside F, and dulcoside A. Using Reversed-Phase (RP) HPLC method, individual retention times and area for various ent-kaurane diterpene glycosides of S. rebaudiana have been determined at various temperatures from 20 to 79C under three different pH 2.4, 2.6, and 2.8 at various UV absorbance. HPLC results suggested that temperatures between 40 and 60C would be ideal for better separation of steviol glycosides under pH 2.4 at 200 nm.

AGFD 137 Analysis of volatile flavor components of steamed rice and identification of key odorants causing old rice smell Hatsuho Takemitsu1,3, hatsuho@ipe-jp.com, Yoshihiro Sako2, Kei Shibakusa4, Shinichi Kitamura5, Hiroshi Inui1. (1) Dept. of Clinical Nutrition, Osaka Prefecture Univ., Sakai, Osaka, Japan (2) Acesystem Co., Ltd., Izumi, Japan (3) International Polysaccharide Engineering (IPE) Inc., Sakai, Osaka 4) Fuji Foods Co., Ltd., Funahashi, Chiba, Japan (5) Graduate School of Life and Environmental Sciences, Osaka Prefecture Univ., Sakai, Osaka, Japan The volatiles of steamed rice and of the steam used to cook rice were analyzed in order to identify the undesirable odor components of old rice. Cooked rice was prepared with a newly developed superheated steam rice cooking machine shown in Fig.1. Steam during steam-processing was collected as condensation water by using a distillation column attached to the outlet of the machine. Cooked rice prepared with an ordinary pod style rice cooker was used as a reference. Volatile components were extracted from each rice sample using methyl tert-butyl ether (MTBE). To remove the nonvolatile materials, the collected suspension was distilled under reduced pressure using solvent- assisted flavor evaporation (SAFE). Volatile compounds were extracted from the condensation water by MTBE using a separatory funnel. These suspensions were concentrated and analyzed by gas chromatography-mass spectrometry (GC-MS) and gas chromatography-olfactometry (GC-O) equipped with an Agilent DB-WAX column. About 30 volatiles including aldehydes and acids were identified in cooked rice, with additional ones in the steam that were evidently lost during steam processing. From the GC-O analysis, we detected a lot of undesirable odor in the region with column temperatures ranging from 150-190 °C. This suggests that the compounds in this range might be the key odorants in cooked rice responsible for old rice smell. We are now trying to identify the compounds and confirm their existence in cooked rice, to know how these compounds affect flavor.

AGFD 138 Comparison between traditional-SERS and RCA-SERS assays for 35S promoter gene detection Burcu Guven1, burcuguven@hacettepe.edu.tr, Ismail H. Boyaci1, Ugur Tamer2, Esra Acar-Soykut3. (1) Food Engineering Dept., Hacettepe Univ., Ankara, Turkey (2) Analytical Chemistry, Gazi Univ., Ankara, Turkey (3) Food Research Center, Hacettepe Univ., Ankara, Turkey In this study, we developed the genetically modified organism detection method by using the combination of rolling circle amplification (RCA) and surface-

enhanced Raman spectroscopy (SERS) and compared the developed RCA-SERS assay with traditional-SERS assay. As part of the study, gold surfaces and gold nanorods were used to form sandwich structure. Gold nanorods were labeled with 5,5'-Dithiobis(2- Nitrobenzoic acid) (DTNB) to enhance SERS intensity. Quantification of the target concentration was performed via SERS spectra of DTNB on the nanorods. SERS spectra of target molecules were enhanced through the RCA reaction and the detection limit was found to be 6.3 fM. The sensitivity of developed RCA-SERS assay was compared with traditional SERS assay and the detection limit was found to be 0.1 pM. For the developed RCA-SERS assay, the control studies were performed using the 35S promoter of Bt-176 maize gene and nonsense sequence. It was found that the developed RCA-SERS sandwich assay method is sensitive, selective and specific for target sequences in model and real systems.

AGFD 139 Exposure estimate for semicarbazide from the use of azodicarbonamide in bread for the U.S. population Salome Bhagan1, Salome.Bhagan@fda.hhs.gov, Diana L. Doell2, Hyoung Lee1, Teresa Croce1, Susan E. Carberry3. (1) FDA, College Park, Maryland (2) FDA, Alexandria, Virginia (3) FDA, Silver Spring, Maryland Azodicarbonamide (ADA) is approved for use in the US as an aging and bleaching ingredient in cereal flour and as a dough conditioner in bread products. When used as an ingredient to make bread, ADA quickly reacts with water to form biurea, which may undergo thermal decomposition during baking to form semicarbazide. Because of concerns that have been raised regarding the potential exposure to semicarbazide from the use of ADA in bread making, the US FDA has conducted an exposure estimate for semicarbazide from the consumption of bread products that list ADA as an ingredient on the product label. FDA sampled bread products from various locations in the US and determined the presence of semicarbazide in these samples using liquid chromatograph tandem mass spectrometry (LC-MS/MS) with 2-nitrobenzaldehyde as a derivatization reagent. Bread products identified as containing semicarbazide were grouped into broad categories and matched with food codes from the combined 2009 - 2012 National Health and Nutrition Examination Survey (NHANES). NHANES contains food consumption data based on a 2-day dietary intake survey. Dietary exposure of semicarbazide was estimated for each broad category, as well as for all bread products containing semicarbazide for the US population aged 2 years or more, and for various subpopulations. The use of 2-day food consumption data to assess chronic exposure can lead to an overestimation of exposure, especially for certain types of breads that are not commonly consumed. For this reason, data collected from a 10-14 day survey are considered to be more representative of actual consumption patterns in the U.S. Therefore, exposure of semicarbazide was also estimated using 14-day food consumption data. The exposure to semicarbazide from the use of ADA in bread products will be presented.

AGFD 140 Determination of total dietary fiber in extruded food products containing grape pomace La'Quana Hordge2,1, lnhordge@aggies.ncat.edu, Jianmei Yu2. (1) Chemistry, North Carolina Agricultural and Technical State Univ., Greensboro, (2) Family and Consumer Sciences, North Carolina Agricultural and Technical State Univ., Greensboro The objective of this collaborative study was to evaluate the Total Dietary Fiber (TDF) contents in extruded food products containing different levels of grape pomace (GP), the residue of grapes after wine making, using enzymatic and gravimetric procedures. The products were formulated with yellow corn grits, GP and water. The grape pomace contents in the formulas were 5, 10 and 15%. The products without GP were used as controls. At each GP level, the mixture were extruded at moisture level of 15, 17 and 19% and at constant temperature120°C. Twelve extruded samples were ground to smaller particles, then digested with heat stable α-amylase, protease and amyloglucosidase at the optimal pH and temperature of each enzyme. Ethanol was added to precipitate the soluble dietary fiber. The residue was filtered and washed with ethanol and acetone. After drying, the residue was weighed and the ash content of the residue was determined. The TDF determination of each sample was conducted in duplicate. Results: The TDF content of the extruded product increased with increasing amount of GP almost linearly, and was affected by the moisture of formula. The TDF of extruded product was 6.6-6.8% without GP, 8.2-9.1% with 5% GP, 10.7-13.4% with 10% GP and 14.4-16.2% with 15%GP, depending on the moisture of formula. The TDF content of Coefficient of Variation (CV) values range from 0.9-6.6% for the 9 out of 12 samples, but the CV for 3 samples were in the range of 20.0-26.9%, respectively. The study suggests that GP could serve as a dietary fiber source in extruded food products.

AGFD 141 Preparation of gelatin films incorporated with tea polyphenol nanoparticles for enhancing controlled-release antioxidant properties Fei Liu1, s110102086@vip.jiangnan.edu.cn, Wallace Yokoyama2, Fang Zhong3, Yue Li3. (1) Healthy Processed Foods Research Unit, WRRC , USDA, Albany, California (2) USDA, Albany, California (3) Food Science and Technology, Jiangnan Univ., Wuxi, China Tea polyphenols (TP) were incorporated into gelatin films either alone or incorporated into nanoparticles in order to determine the physicochemical and antioxidant properties of films. The TP-containing nanoparticles were prepared by cross-linking chitosan hydrochloride (CSH) with sulfobutylether-β-cyclodextrin sodium (SBE-β-CD) at three different encapsulation efficiencies (EE, ~50%, ~80% and ~100%) of TP by adjusting the concentration of CSH. Inclusion complexes of TP and SBE-β-CD were previously prepared to effectively encapsulate TP. Composite films showed no significant difference in visual aspects, while the light barrier (250-550 nm) was improved with incorporation of TP. The stability of TP-loaded nanoparticles was maintained during film drying process from the analysis of free TP content in the redissolved film solutions. Nanoparticles appeared to be homogeneously dispersed within the gelatin matrix by microstructure analysis. TP-loaded films had ferric reducing and DPPH radical scavenging power that corresponded to the EEs Sunflower oil packaged in bags made of gelatin films embedded with nanoparticles of 80% EE showed the best oxidation inhibitory effect, followed by 100% EE, 50% EE, and free TP, over 6 weeks of storage. However, when the gelatin film was placed over the headspace and was not in contact with the oil, the free TP showed the best effect. The results indicate that sustained release of TP in the contacting surface can ensure the protective effects, which vary with free/encapsulated mass ratios, thus improving antioxidant activities instead of increasing the dosage.

AGFD 142 Rapid front end cleanup of cannabis-infused edibles using automated flash column chromatography Melissa J. Wilcox3, melissa.wilcox@grace.com, Jahan Marcu2, James P. Kababick1, Mark Jacyno4. (1) Flora Research Laboratories, Grants Pass, Oregon, US (2) Green Standard Diagnostics, Inc., Brooklyn, New York, US (3) Grace Discovery Sciences, Deerfield, Illinois Thirty-four states plus the DC have adopted medical marijuana programs and many more states are considering it for 2016. The American Herbal Pharmacopeia (AHP) recently published a Cannabis monograph, setting standards for identification, analysis, and quality control. The recommendations from AHP and other organizations are steadily being adopted, however a number of significant hurdles must be overcome to reach higher levels of product safety. New cannabis products are being developed at a rapid pace, challenging quality control chemists to quickly develop analytical methods to comply with testing requirements. Traditional extraction methods don't always work with complex food or topical matrices. Problems such as non- homogenous samples can lead to inaccurate measurements when using traditional solvent based extraction methods.

In addition, large amounts of chlorinated solvents are often needed. Flash chromatography has been employed to address these challenges by isolating cannabinoids away from interfering compounds (fat, sugar, salts, etc) present in the matrix before analysis, and ensuring a homogenious extraction process. The authors show successful application of the methodology to analysis of several cannabis-infused products: brownies, gummy candies, caramels, and lotion.

AGFD 143 Fatty acid profiles of marine fishes from Rhode Island coastal waters Mary Yurkevicius2, myurkevicius061@g.rwu.edu, Joshua Jacques1, Nancy E. Breen3, David L. Taylor4. (1) Marine Biology, Roger Williams Univ., Bristol, Rhode Island (2) Chemistry, Roger Williams Univ., Bristol, Rhode Island Marine fish are an excellent source of omega-3 fatty acids, including eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA), which provide numerous health benefits to human consumers. Further, the majority of consumed fish are of marine origin, thus underscoring the importance of research focused on this topic. In this study, fatty acids were analyzed in Rhode Island coastal fishes, including summer flounder, Paralichthys dentatus (n = 10); black sea bass, Centropristis striata (n = 10); striped bass, Morone saxatilis (n = 6); scup, Stenotomus chrysops (n = 11); winter flounder, Pseudopleuronectes americanus (n = 10); and bluefish, Pomatomus saltatrix (n = 11). Fatty acid profiles of fish muscle tissue were determined by esterification and gas chromatography. Data were categorized as mono-saturated, saturated, omega-3, and omega-6 fatty acids, and results were expressed as concentrations (mg/100 g wet weight; [FA]) and percent of total fatty acid content (%FA). Irrespective of fish species, mono-saturated fatty acids had the highest [FA] and %FA (mean [FA] = 183.5 mg/100 g; %FA = 46.2%), followed by saturated ([FA] = 146.6 mg/100 g; %FA = 32.7%), omega-3 ([FA] = 44.3 mg/100 g; %FA = 18.6%), and omega-6 fatty acids ([FA] = 7.5 mg/100 g; %FA = 2.5%). Fatty acid profiles also demonstrated significant inter-species differences. With respect to %FA, mono-saturated fatty acids were significantly higher in scup and bluefish relative to summer flounder and striped bass (SCP = 54.6%, BF = 48.8%, SF = 40.1%, SB = 39.3%). Conversely, omega-3 fatty acids were significantly higher in both flounder in comparison to black sea bass and scup (SF = 31.1%, WF = 26.3%, BSB = 12.1%, SCP = 8.3%). With respect to [FA], bluefish had significantly higher concentrations of mono-saturated and saturated fatty acids relative to summer flounder (BF = 245.4-307.4 mg/100 g, SF = 52.5-81.3 mg/100 g). Ratios of omega-6-to-omega-3 (n6:n3) fatty acids were reduced in flounder and striped bass (n6:n3 = 0.14-0.23) relative to scup, bluefish, and black sea bass (n6:n3 = 0.30-0.36); hence suggesting the former species provide greater health benefits for human consumers. Future research will examine total mercury and selenium concentrations of each fish species to further evaluate their respective health risks and benefits to human health.

AGFD 144 Synthesis and fungicidal activity study of 2-(thiophen-2-yl)pyridine derivatives Yong Xie, xieyong1@sinochem.com, Ying Xu, Yu L. Chen, Chang L. Liu. Shenyang Research inst. of Chemical Industry, Shenyang, Liaoning, China Thiophen which could be reactive group with excellent biological activity has already been widely used in pesticide molecular design. Many pesticide containing thiophen were reported in recent years, such as thifensulfuron-methyl, fluensufone and silthiofam. In order to search new highly active compound containing thiophen, 20 novel compounds of 2-(thiophen-2-yl)pyridine derivatives were designed and synthesized from the starting material of 2-acetylthiophene by the Intermediate Derivatization Methods in an attempt to obtain novel compound candidates for insect and fungi control. The structures of all compounds were confirmed by 1H NMR, 19F NMR and elemental analyses. And all compounds were bio-assayed against fungi. The preliminary assays showed that some compounds exhibited significant fungicidal activity. Some compounds could control cucumber downy mildew, rice blast, cucumber gray mold Pseudoperonospora cubenis, cucumber anthracnose and Puccinia sorghi schw at the concentration of 400 mg/L. Especially, compound 12 could excellently inhibit cucumber anthracnose at the concentration of 6.5 mg/L. This study will be useful for the design of new fungicides.

AGFD 145 Design, synthesis, and biological activities of novel carboxylic ether derivatives containing oxime Qiao Wu, Jichun Yang, Jingjing Zhang, Guan Aiying, Hongjuan Ma, Chang L. Liu, liuchangling@vip.163.com. Shenyang Research inst. of Chemical Industry, Shenyang, Liaoning, China The oxime ether compounds containing 1,2,4-triazole moiety have been widely reported as fungicides. They play an important role in the discovery and development of new agrochemicals, however, the compounds of this kind had not been published with herbicidal activity. To find new compounds with high herbicidal activity, the novel carboxylic ether derivatives containing oxime were designed and synthesized by introducing the herbicide carboxylic acid into traditional triazole compounds via the intermediate derivatization method. The structureactivity relationships of the synthesized compounds was also discussed. The structures of all target compounds prepared were confirmed by 1H NMR, IR, MS and elemental analysis. Bioassays indicated that most of the title compounds exhibited high herbicidal activity against gramineous weeds and broadleaf weeds. Some compounds displayed more than 95% control against Zinnia elegans Jacq., and Abutilon theophrasti Medic. at 150~300 g (a.i.)/hm2, and it was safe to corn at this dose. The present work demonstrates that carboxylic ether derivatives containing oxime can be used as potential lead compounds for developing novel herbicides. Further syntheses and structure optimization studies are in progress.

AGFD 146 Herbicidal properties of substituted 3-(pyridin-2-yl)benzenesulfonamide derivatives Yong Xie, xieyong1@sinochem.com, Hui w. Chi, Guan Aiying, Chang L. Liu, Hongjuan Ma. Shenyang Research inst. of Chemical Industry, Shenyang, Liaoning, China Substituted 2-phenylpyridines which could be used as intermediates for drugs and agrochemicals showed good herbicidal activity. For instance, some 2-phenylpyridine derivatives could efficiently control velvet leaf (abutilon thephrasti), redroot pigweed (amaranthus retroflexus) and morningglory (ipomoea subspecies). In our previous works, we have reported the syntheses of a series of novel substituted 3-(pyridin-2- yl)benzenesulfonamide derivatives using 2-phenylpridines as the lead compound by Intermediate Derivatization Methods in an attempt to obtain novel compound candidates for weed control, of which compound 2h gave excellent herbicidal activities against velvet leaf, youth-and-old age (Zinnia elegans jacq.), dayflower (Commelina tuberosa), bur beggarticks (Bidens tripartita linn.), cassia tora (Cassiaobtusifolia L.), purslane (Portulaca oleracea) and false daisy (Eclipta prostrata L.). The result of the herbicidal activity assay in field test demonstrated that compound 2h could effectively control dayflower and nightshade (Disambiguation) with long-lasting persistence. In order to understand the herbicidal properties of substituted 3-(pyridin-2-yl)benzenesulfonamide derivatives, several biological assays of compound 2h were finished. The results suggested that differences in activity are believed to be due to difference in suitable growth stage of weed, compound 2h could show excellent activities at 2-4 leaf stage and weaken activity at 6 leaf stage. And the mode of action experiment proved that compound 2h could be absorbed and shifted through leaves and stem of weeds.

AGFD 147 Synthesis and characterization of novel luminescent sodium carboxymethyl cellulose nanocomposites for potential safety inspection of food applications Mingming zhang1, Li qingyong2, Jun Ye1, 1792418653@qq.com, Xiong Jian2, lcjxiong@scut.edu.cn. (1) State Key Laboratory of Pulp and Paper Engineering, South China Uni. of Techn., Guangzhou Guangdong, China (2) School of Light Chemistry and Food Science, South China Uni. of Techn., Guangzhou In this paper, a green approach was described that generates nanocomposites containing terbium (Tb) reacting with sodium carboxymethyl cellulose (NaCMC) in aqueous media and under microwave irradiation (MW) at 70 digrees Celsius. The structure of resulting nanocomposites was characterized by FTIR, TEM and WAXD. The results showed that -OH, –COO and -COC groups of NaCMC were involved in interactions with Tb3+ and a particle size in the range of dozens of nanometers were well dispersed in the sodium carboxymethyl cellulose matrix. Optical properties were analyzed by UV–Vis and photoluminescence spectroscopy (PL). The results showed that ultraviolet absorption came from macromolecule ligand, which was the energy donator for Tb3+ and made it emit fluorescence. All products exhibited typical fluorescence emission spectra of Tb3+, which consist of the characteristic transitions from 5D4→7F6(489 nm) , 5D4→7F5(545 nm), 5D4→7F4(584 nm) and 5D4→7F3(619 nm), and show the narrow line emissions with the half peak width of the strongest green fluorescence of 5D4→7F5 was less than 10 nm (see Figure). In addition, the fluorescence intensity increased with increasing concentration of Tb3+. These nanocomposites could find potential applications such as biolabeling for quality and safety inspection of food and agricultural products. Acknowledgments We gratefully acknowledge the financial support provided by the National Natural Foundation of China (project 31270617).

AGFD 148 Characterization of pepsin-solubilized collagens and the hydrolysates from sea cucumber species Masataka Saito, msaito@eiyo.ac.jp. Kagawa Nutrition Univ., Saitama, Japan Collagen and the hydrolysates derived from marine resources have a wide range of applications in cosmetic and food industries. In Japan, edible sea cucumber species, Apostichopus japonicus, Stichopus naso Semper, and Cucumaria frondosa, are commercially harvested and contain high amounts of collagens. On the other hand, physicochemical properties and nutritional applications of collagen hydrolysates are dependent on peptide molecular mass distribution, with which functional and physiological attributes vary considerably. The aim of this work is to determine the structure and property of the major collagen in sea cucumber and to estimate peptide molecular mass distribution in the hydrolysate. The pepsin-solubilized collagens were successfully purified from the body walls of three sea cucumber species by a method involving disaggregation with a reductant, alkali treatment and limited pepsin digestion of collagen fibers. The SDS-PAGE containing Urea and anion exchange chromatography showed that the major component of pepsin-solubilized collagen consisted of two different α chains which formed (α1)2α2 heterotrimers, but not (α1)3 homotrimers. The hydrolysates by a protease had a molecular mass distribution of 0.2- 1.5kDa and were rich in a few amino acids such as glutamic acid when compared with other collagens. These results suggest that the sea cucumber collagen containing heterotrimers has a variation of the amino acid sequence and the hydrolysates may have suitable properties for use as food materials.

AGFD 149 Red shortening: Characterization and utilization in formulating novel functional biscuits Hany Abou Gharbia, samehmawad@gmail.com, Mohamed M. Youssef, Mohamed Abd-El-Aal, Nesma Nabil. Food Science, Alexandria Univ., Egypt Functional biscuits were manufactured by replacing white shortening (WSh) with red shortening (RSh) by about 80%. White shortening was found to be comparable to RSh in terms of moisture content, refractive index, iodine value, saponification value and unsaponifiable matter. On the other hand, WSh was different from RSh in cloud point, color, slip melting point, acid and anisidine values as well as free fatty acids. The fatty acid composition of WSh and RSh was different. The total saturated fatty acids in WSh and RSh was 57.4 and 50.8%, respectively, whereas, the total unsaturated fatty acids for WSh and RSh amounted for 42.4 and 49.0%, respectively. It was obvious that RSh possessed higher content of antioxidants than WSh, the total α-tocopherol and tocotriends were 654 and 530 ppm, respectively. Moreover RSh contains 645 ppm of carotenes as compared to only 2 ppm present in WSh. In conclusion, biscuit samples formulated in the present study could be stored up to 10 months at room temperature without any significant deterioration in terms of oxidative stability, peroxide a nsidine and acid values.

AGFD 150 Presence of Protostrongylus stilesi in Rocky Mountain goats and the effects of infestation Christa Dunlap, ruffianracer014@yahoo.com. Colorado State Univ.-Pueblo The lungworm, Protostrongylus stilesi, is a nematode that burrows into the lungs of large animals, particularly ungulates, thus creating an ideal habitat for the pneumonia- causing bacteria, Pasteurella haemolytica. Effects of Protostrongylus stilesi have been accounted for in bighorn sheep herds throughout much of North America, but their presence in Rocky Mountain goats has yet to be tested. In order to investigate the effects of lungworms on the mountain goats, DNA extractions from fecal matter were executed. Polymerase chain reaction and gel electrophoresis was then performed on the isolated DNA. It was hypothesized that Rocky Mountain goat herds, in Colorado, currently contain heavy lungworm parasite loads given their immense similarities to bighorn sheep, thus leading to herd declination. Although a few aspects regarding the results are still being conducted, the findings reveal that the goat fecal samples taken from various Colorado locations including, Mount Evans, Cottonwood Pass, and Lake Deluge do contain DNA associated with an unidentified, non-goat source. Specific primers tailored for Protostrongylus stilesi were utilized in order to investigate if the DNA belongs to lungworms. Prominent DNA bands were revealed after polymerase chain reactions and gel electrophoresis was conducted on the lungworm specific concoction. In order to ensure the DNA bands belong to Protostrongylus stilesi the DNA was extracted from the gel, purified, and sent off for sequencing. In the event that there is affirmative confirmation of lungworm infestation in the Rocky Mountain goat herds mentioned, de-worming protocols will be implemented in association with the Colorado Division of Wildlife.

AGFD 151 Polyphenol-aluminum complex formation: Implications for aluminum tolerance in plants Ann E. Hagerman1, Liangliang Zhang1,2, zhangl23@miamioh.edu. (1) Miami Univ, Oxford, Ohio (2) inst. of Chemical Industry of Forest Products, Nanjing, Jiangsu, China It has recently been proposed that high molecular weight polyphenols (PP) may plan an important role in aluminum detoxification in certain aluminum resistant plants such as Eucalyptus. Although interactions between small phenolics and metals are well characterized, less is known about high molecular weight (MW) polyphenol-metal interactions. In this paper, we examined the interaction between purified polyphenols pentagalloyl glucose (PGG), oenothein B (OeB) and methyl gallate (MeG) and Al(III) by using spectrophotometric titration and Job's method to determine the apparent affinity constants. We did the study at two pH values, pH 4 and pH 6, representing the pH range of acidic, Al-toxic soils. We used molecular modeling (Gaussian) to evaluate structures and spectral features of methyl gallate-Al complexes. We found that PGG (MW 940) forms an Al2PP complex with LogK 11.94±0.09 at pH 6 and an AlPP complex with LogK 2.61±0.70 at pH 4. OeB formed AlPP complexes at both pH values with lower apparent binding constants than those of PGG. The low molecular weight monomer of these hydrolyzable tannins, methyl gallate, formed AlPP complexes at both pH values with lower apparent affinity constants of

LogK 5.87±0.02 at pH 6 and 3.69±0.08 at pH 4. We examined the solubility of complexes formed at physiological concentrations of polyphenol and metal, and found that at intermediate metal:polyphenol ratios both OeB and PGG formed insoluble complexes, but when either metal or polyphenol was in excess the complexes remained soluble. MeG did not form insoluble complexes at any metal:polyphenol ratio tested. All three of these gallate-derived polyphenols are effective metal chelating agents. Either OeB or PGG could detoxify Al by forming insoluble complexes that either prevent Al uptake (exclusion) or trap Al in the vacuole (tolerance). We propose that OeB is a more effective Al-detoxifying agent because of its water solubility, compared to the very nonpolar and water insoluble PGG. Potential roles of polyphenols in metal uptake and utilization by plants need to be explored in living systems as well as by chemical analysis.

AGFD 152 Natural soil benign bacterium with an insecticidal activity Savannah Stark, sstark.f12@warren-wilson.edu. Warren Wilson College, Swannanoa, North Carolina The rhizobacteria Pseudomonas chlororaphis (EA105), isolated from a California strain of rice, has previously demonstrated antibacterial activity and antifungal activity against rice blast disease. Because this disease is responsible for destroying enough crops to feed 6 million people, EA105 is a candidate in agriculture as a useful biocontrol agent, which could potentially increase global food security. With the additional antibacterial activity, more research is needed to fully characterize and understand the pseudomonad before the bacteria is applied and used on rice crops. This study investigates the insecticidal activity of a benign EA105 using Galleria mellonella as a model host for determining pathogenicity. EA105 and a non-pathogenic Bacillus subtilis (UD1022) were cultured overnight, serial diluted, and injected into healthy larvae. The larvae mortality was then monitored for 6 days, and the results were analyzed using the Kaplan-Meier survival estimate. The trend in survival suggests that both EA105 and UD1022 exhibit insecticidal activity in G. mellonella, although EA105 resulted in a greater lethality. Therefore, this study contributes to the known characterization of EA105 while adding to the potential benefits of using the rhizobacteria as a biocontrol agent on rice crops.

AGFD 153 Chemical and supramolecular structural modifications in lignin during acid catalyzed ionic liquid pretreatment: A case study of Arundo donax linn Tingting You, youtingting0928@gmail.com, Liming Zhang, Feng Xu, xfx315@163.com. Coll of Material Sci Tech, Beijing Forestry Univ, Beijing, China Solid acid enhanced ionic liquid (IL) pretreatment is a recyclable, environmentally benign and cost effective novel method for boosting the yield of sugars from lignocellulosic biomass. To unravel the chemical and supramolecular structural changes of lignin after pretreatment, IL-acid lignin (ILAL) and subsequent residual cellulolytic enzyme lignin (RCEL) were isolated from Arundo donax Linn. The structural features were compared with the corresponding milled wood lignin (MWL). Results indicated that the pretreatment caused loss of β-O-4′, β-β', β-1' linkages and formation of condensed structures in lignin. A preferential breakdown of G-type lignin was observed, evidenced by increased S/G ratio revealed by 2D HSQC NMR analysis. It was determined that the depolymerisation of β-O-4′ linkage, lignin re-condensation, and cleavage of ferulate- lignin ether linkages were took place. Moreover, a simulation module was first developed to define the morphological changes in lignin. MWL appeared as tree branch like aggregates, consisting of oblate ellipsoid-shaped monomers with different sizes. After the pretreatment, the supramolecular organization was completely destroyed and transformed into monodisperse monomers with some collapse present on monomer surfaces. These modifications contributed to reduction in molecular weight and lower maximum decomposition temperature of ILAL relative to MWL. The results presented will contribute to better understanding of native recalcitrant and facilitate the design of more effective deconstruction strategies for biorefineries.

AGFD 154 Seed-specific phosphate allocation with coordinated expression of genes involved in phosphate transport function during wheat grain development Vishnu K. Shukla, shukla@nabi.res.in, Mandeep Kaur, Sipla Aggarwal, Kaushal Bhati, Shivani Sharma, Shrikant Mantri, Ajay Pandey. Agriculture Biotechnology, National Agri-food Biotechnology inst., Mohali, Punjab, India Under P-limiting environments, plant exploits selective high- and low-affinity phosphate transporters (PHTs) to enhance their ability of Pi uptake into roots, translocation to shoots and re-mobilization into developing sink tissues. Cereal grains accumulate high amount of P during seed development either as free Pi or bound P (~80% is phytic acid). Although, seed is a major 'sink' for P utilization, not many reports addressing the importance of the P homeostasis and phytic acid accumulation in seeds. This warrants detailed investigations on P homeostasis and Pi transport functions in developing seed tissues. Therefore, the current study aims to identify seed-specific wheat (Triticum aestivum) PHTs and evaluate their importance during wheat grain development. Genome wide survey, EST analysis and phylogeny revealed 23 putative TaPHTs in wheat, mainly distributed into four sub-families including PHT1 (1.1-1.13), PHT2 (2.1), PHT3 (3.1-3.6), PHT4 (4.1-4.6). Genomic coordinates was ascertained for all identified TaPHTs and their location on the chromosomes was also confirmed. Real-time PCR analysis revealed differential expression response of certain TaPHTs under P-starvation in roots and shoots tissues. The Pi concentration gradient between the seed tissues (principally aluerone, endosperm, embryo and pericarp) was correlated with seed tissue-specific preferential expression of few TaPHTs. Further, high expression of specific TaPHTs in low phytic acid (lpa) mutant Triticum monococcum in comparison to wild type showed their possible involvement in phytic acid sythesis. The results obtained in this study will help in deciphering the role of wheat PHTs in developing seeds and will contribute towards the environmental-friendly agricultural production through effective P utilization.

AGFD 155 Detection of pesticides in edible oil using LC-MS analysis Subhra Bhattacharya, subhra.bhattacharya@thermofisher.com. Thermofisher Scientific, Fair Lawn, NJ Detection of pesticides in food ingredients is a challenge. Edible oils are one of the essential food ingredients used to prepare many types of food. Detection of pesticide residues was carried out in six different oils purchased from supermarket, including canola oil, corn oil, olive oil, extra-virgin olive oil, vegetable oil and peanut oil. Sample preparation was performed using high purity acetonitrile followed by easy clean-up with QUECHERS (Quick, Easy, Cheap, Effective, Rugged, Safe) method. Sample extractions with acetonitrile only followed by the clean-up step showed much cleaner sample peaks in LC-MS. Extraction of pesticides in the presence of sodium acetate and water showed a peak of acetic acid in the chromatogram which masked other peaks of relatively lower amounts of pesticide. From LC-MS analysis, a few pesticides were detected in olive oil, extra virgin olive oil, canola oil and corn oil. No pesticides were detected in vegetable oil or peanut oil in either method described above. Our comparative study shows variation in the amount and type of pesticide residues in these oil substances in positive and negative mode of ionization. The pesticides detected are mainly chlorinated species. To our knowledge, this is the first comparative study to assess pesticide residues in edible oils by LC-MS analysis.

AGFD 156 Heated headspace solid phase microextraction of marijuana for chemical testing Anastasia Brown1, amb139@shsu.edu, James Sweet2, Chi C. Yu1. (1) Dept. of Forensic Science, Sam Houston State Univ., Huntsville, Texas (2) US Customs and Border

Protection, Houston, Texas There are over 60 cannabinoids found in marijuana (dried Cannabis). Among these cannabinoids, Δ9-tetrahydrocannabinol (THC) has been known as the primary psychoactive cannabinoid. Other important cannabinoids for medical purposes in states with legalized marijuana include cannabidiol (CBD) and cannabinol (CBN). Most analytical methods for the extraction of cannabinoids from marijuana samples include destructive solvent extractions, which destroy and consume marijuana samples. Therefore, increase the cost associated with each analysis of marijuana. Multiple testing of marijuana sample for the purpose of quality control is somehow discouraged. In our research, we adopt heated headspace solid phase microextraction (HS-SPME) for headspace extraction of cannabinoids in marijuana samples to eliminate such limitations and leave the marijuana sample intact after extraction and chemical analysis. In this presentation, an automated heated HS-SPME extraction process developed for the extraction of cannabinoids from marijuana samples will be described. Cannabinoid standard reference materials and actual marijuana plant materials were used during the optimization of extraction conditions. During extraction method development, standard reference materials were placed in a vial and the solvent was evaporated under gentle air stream before HS-SPME. Marijuana plant material was ground and sieved before being weighed out into sample vials for HS-SPME. Unlike liquid extraction methods, the HS-SPME method only required the sample to be sealed in the sample vial. No solvent is needed during the extraction process. The optimized extraction temperature for cannabinoids was found to be 150°C, and the optimal extraction time was found to be 5 minutes. Under the optimal condition, the HS-SPME was capable of extracting THC, CBD, CBN from the headspace of 10 mg marijuana in a 20 mL vial. After HS-SPME extraction, the original marijuana remained intact with only little discoloration. We believe this HS-SPME extraction process for cannabinoid testing with almost no consumption of valuable marijuana products can encourage more marijuana testing for the purpose of quality control.

AGFD 157 Nutritional value and total phenolics of tortillas obtained by extrusion cooking of red pigmented creole maize Ada k. Milan1, keilamilan@hotmail.com, Cuauhtemoc Reyes-Moreno2, Jorge Milan Carrillo2. (1) Centro de Biotecnologia, Tecnologico de Monterrey, Nuevo Leon, Mexico (2) Programa Regional de Posgrado en Biotecnología, Universidad Autonoma de Sinaloa, Culiacan , Sinaloa, Mexico Mexico had the highest diversity in genetic resources of Maize (Zea mays L.) in the world with 61 genotypes of creole maize. There are several types of pigmented genotypes with colors such as purple, blue, yellow, red, black and white. Nowadays, pigmented maize has received increased attention from a nutraceutial perspective because its potential health benefit. Extrusion cooking is a continuous process that can make dough suitable for tortillas with similar characteristics as counterparts produced with traditional processes. The main advantage of this process is the null generation of wastewater (nejayote). The aim of this study was to evaluate the effect of extrusion cooking process on nutritional value and total phenolics of tortillas prepared with four genotypes of red creole maize from Sinaloa, Mexico. The red maize tortilla had a good puffing, sensorial acceptation. The red maize tortilla presented a protein content of 7.56- 8.23%, fat 3.48-3.8 % and carbohydrates of 86.42-86.99 % among genotypes. The genotype RM495 showed the highest lost in protein content 1.55 % ($p<0.0001$) and fat 4.92% ($p<0.0001$) in the process into tortilla. In contrast genotype RM241 showed lowest lost in protein (0.49 %) and fat (0.71%). The extrusion cooking significant affected the total phenolic content in red maize tortilla decreasing 25-35% ($p<0.05$) compared to raw maize. The results suggest that the pigmented grains of maize races studied may hold promise for the development of grain-based functional foods regarding nutritional value as genetic resource in breeding programs.

AGFD 158 Evaluating Raman spectroscopic data by using principal component analysis to determine the freshness of fish samples Havva Tumay Temiz1, tumaytemiz89@gmail.com, Hasan Murat Velioglu2, Ismail H. Boyaci1. (1) Food Engineering, Hacettepe Univ., Ankara, Turkey (2) Namik Kemal Univ., Tekirdag, Turkey Low content of saturated fats and cholesterol and high content of polyunsaturated fatty acids (PUFA) makes fish an indispensable element of a healthy diet. On the other hand, its high moisture content and weak muscle tissue does not allow the long-term storage. Freezing is the most commonly applied preservation method used for extending the shelf life of fish. Improper practices of freezing and thawing, results with undesirable textural and functional changes, which mostly cannot be realized by consumers. Enzymatic and chemical changes as well as dielectric properties of fish samples were monitored in many studies in order to differentiate fresh and frozen-thawed fish samples. Fourier-transform infrared spectroscopy, impedance spectroscopy and near infrared spectroscopy are frequently used novel technologies with the advantages like rapidness and on-site usability. As one of the vibrational methods, which gives structural information and requires no sample preparation Raman spectroscopy is used in the present study in order to differentiate fresh and frozen-thawed fish samples. Unlike the reported studies, relatively short freezing (24h) and thawing (12h) periods were used in the present study. By using the advantage of its high sensitivity, very little changes in the lipid structure, which occurred during the very short storage periods, were monitored using Raman spectroscopy. Collected Raman data was analyzed by using Principal Component Analysis (PCA). Developed PCA models allowed us to obtain a successful differentiation between fresh, once frozen-thawed and twice frozen-thawed fish samples. Gas chromatography (GC) was used as reference method and fatty acid composition of fish samples were determined by GC analysis. A correlation was established between GC and Raman spectroscopy in terms of changes in the lipid structure.

AGFD 159 Fatty acid composition as a tool for screening industrial applications of vegetable oils Bryan R. Moser, Bryan.Moser@ars.usda.gov. USDA ARS NCAUR, Peoria, Illinois Fatty acid (FA) composition influences applications and properties of bio-based industrial products and fuels produced from vegetable oils. For instance, saturated FAs have high oxidative stability but poor low temperature properties whereas polyunsaturated FAs exhibit the opposite behavior. Monounsaturated FAs strike an acceptable balance between oxidative stability and cold flow properties. As a consequence, FA composition often dictates what industrial applications a vegetable oil is best suited for, either with or without chemical modification. For example, paints, varnishes and detergents are prepared by chemically modifying vegetable oils enriched in polyunsaturated FAs whereas those enriched in saturated FAs find applications in soaps, cosmetics and detergents. Biodiesel, lubricants and plasticizers are prepared from vegetable oils containing a high percentage of monounsaturated FAs. This paper surveys the FA composition of numerous vegetable oils, including common commodity lipids as well as several alternative feedstocks not currently in commercial production, and summarizes what applications each is best suited for. A selection matrix based on FA composition is proposed that aids in the determination of potential applications of vegetable oils.

AGFD 160 Dolabella-3,7,18-triene:The main constituent of Nymphaea lotus essential oil Daniela M. Navarro1, dmafn@ufpe.br, Maud Pottier2, Bheatriz N. Albuquerque1, Artur C. Maia3, Fernando Hallwass1, Armando Navarro-Vazques1. (1) Fundamental Chemistry Dept., Federal Univ. of Pernambuco, Recife Pernambuco, Brazil (2) Institut Universitaire et Technologique, Université Paris-Est Créteil Val-de-Marne, Paris, Créteil, France (3) Programa de Pós-graduação em Biotecnologia, Universidade Católica Dom Bosco, Campo Grande, Mato

Grosso, Brazil The essential oil from N. lotus flowers is tradionally used against eye inflamation, jaundice, liver spots, palpitations, rheumatism, toothaches, sciatica, sprains, tuberculosis and vomiting. Regardless of their obvious potential in various health-related applications, there is no evident record of the chemical composition of the essential oils of Nymphaea spp. in the literature, nor any mention of their biological activity against pathogens or insect vectors of infectious diseases. In the current study, we obtained the essential oil from flowers of Nymphaea lotus through hydrodestillation, identified its constituents and tested their larvicidal activity against Aedes aegypti, the main vector of dengue, zika and chinkungunya fever. The GC-MS analysis showed the presence of 21 compounds, of which only 12 were tentively identified (92.47% of the relative total amount). It is comprised of 52.94% diterpenes, 20.89% fatty acids, 10.56% linear hydrocarbons, 7.86% of ketones and 0.22% monoterpenes (Table 1). The major constituent of the essential oil was identified by RMN analysis as dolabella-3,7,18- triene, a diterpene identified for the first time as a floral scent compound in Cyperus alopecuroides. Previous studies dealing with the characterization of floral volatile organic compounds isolated in scent samples of N. lotus have either probably misidentified it as an isomer (cembrene; Ervik & Knudsen 2003) or refrained from further identification atempts. The essential oil yield from dehydrated flowers of N. lotus was 0.063% (80.58 mg).

AGFD 161 Molecularly imprinted polymers with desorption electrospray ionization mass spectrometry for high throughput analysis of neonicotinoids pesticides in water and food Christina S. Bottaro, cbottaro@mun.ca, Jeremy Gauthier, Stefana Egli. Chemistry, Memorial Univ. of Newfoundland, St. John's, Canada Neonicotinoid pesticides are often viewed as less toxic than other classes of pesticides, and so have seen widespread adoption for the insecticidal treatment of food crops. Given their solubility, they have even been added to irrigation water to facilitate easy and targeted application. Nevertheless, these pesticides also persist in the environment and have been implicated in the collapse of honey bee colonies and declines in insect- eating bird populations. While there is evidence for these associations, more extensive environmental monitoring campaigns are needed to better assess their occurrence and fate, particularly at locations farther removed from application sites. Currently, the neonicotinoids are routinely analyzed by solid phase extraction with high performance liquid chromatography-mass spectrometry (SPE-HPLC-MS). Though analytical advances (e.g. ultra-HPLC) have increased throughput for analyses, SPE is usually needed to concentrate the target compounds and minimize matrix interferences. SPE can be time-consuming and use substantial amounts of solvent. To increase the throughput of analysis in water and liquid matrices, we have fabricated thin-film molecularly imprinted polymers (MIPs) for selective analyte uptake of analytes in situ or in a controlled environment. In the film format, the analytes bound in the MIPs can be analyzed directly by desorption electrospray ionization (DESI)-MS. MIPs rely on a simple mode of molecular recognition that occurs in cavities formed through polymerization of functional monomer(s) and crosslinker(s) in the presence of the template (usually the target analyte). For an optimal MIP system, several aspects of polymer fabrication and composition must be considered, including: choice of template and functional monomer, ratio of polymer components, nature and amount of the porogen, etc. The sensitivity of DESI-MS, like electrospray ionization, also depends on a careful selection of conditions, but with geometric parameters also playing key roles. Results of the optimization efforts for the neonicotinoid MIPs, and data from method development studies with DESI-MS will be presented. Suitability for the analysis of neonicotinoids in water will also be discussed.

AGFD 162 Chemical compositions of essential oils of Psidium guajava and Syzygium sp. and their in vitro antivirus activities Nornisah Mohamed1, nornisah@usm.my, Ashraf Ahmad A. Abdalsalam1, Hasnah Osman2, Ezatul Ezleen E. Kamarulzaman1, Habibah Wahab1. (1) School of Pharmaceutical Sciences, Universiti Sains Malaysia, George Town (2) School of Chemical Sciences, Universiti Sains Malaysia, George Town, Penang Plants have been used as a source of traditional medicines for thousands of years. Due to these traditional uses, the chemical compositions of essential oils of Psidium guajava ans six Syzygium sp. were examined and evaluated for in vitro H1N1 and dengue inhibition activities. The essential oils from the leaves were extracted using hydrodistillation method and amalyzed by head-space gas chromatography-mass spectrometry. The extracted essential oils were then subjected to in vitro H1N1 neuraminidase inhibition activity by using MUNANA assay, The dengue activity was evaluated by using DEN-2 NS2B-NS3 protease assay. Monoterpenes were found in all the leaves studied ranging from 7.63% in S. grandes to 77.24% in S. samarangense. The sesquiterpenes were found the lowest in S.cumini (6.23%) and the highest in S. malaccense cultivated jambu susu (69.94%). The H1N1 neuraminidase inhibition activity was observed in three plants namely S. jambos, S. malaccense cultivated jambu susu and jambu bol with 0.8%, 14.4% anf 16.8%, respectively at 250 ug/mL samples. Essential oils of five Syzygium sp. inhibited the protease activity at 250 ug/mL with the highest inhibition of 54.1% by S. cumini. In conclusions, the essential oils from Syzygium sp. could be useful as a potential source of dengue protease inhibitors.

AGFD 163 Detecting delta-9-tetrahydrocannabinol (Δ9-THC) and delta-8- tetrahydrocannabinol (Δ8-THC) by UV-HPLC Ken Tseng1, ken@nacalaiusa.com, Toshi Ono1, Tsunehisa Hirose2, Kazuhiro Kimata2. (1) Nacalai USA, San Diego, California (2) Nacalai Tesque, Kyoto, Japan Of the roughly 60 cannabinoids, delta-9-tetrahydrocannabinol (Δ9-THC) is the primary psychoactive molecule found in cannabis plants. Delta-8-tetrahydrocannabinol (Δ8- THC) is an isobaric isomer of Δ9-THC that differs by the position of a double bond. It has lower psychoactive potency, more chemically stable, and potentially better medicinal properties than Δ9-THC. Cannabinol (CBN) is used to monitor the freshness of the sample since Δ9-THC easily oxidizes to CBN. Cannabidiol (CBD) has no psychoactive activity but it has many potent medicinal properties. These four cannabinoids, CBD, CBN, Δ9-THC, and Δ8-THC were analyzed by core- shell HPLC columns. The C18 core-shell column produced co-eluting peak of Δ9-THC and Δ8-THC. The peak shapes in this column were fronting under the MS-friendly experimental condition. Cosmocore Cholester is a core-shell HPLC column that has similar hydrophobicity as C18. The rigid cholesterol functional group provides it with higher steric selectivity to resolve Δ9-THC and Δ8-THC peaks. The peak shapes were symmetrical using MS- compatible solvents as the mobile phase. Other cannabinoids and metabolites are also successfully separated and identified to the baseline level.

AGFD 164 Nutritional variation and antioxidant properties of wild fruits revealed through a fluorescence-based method Susan Smith1, sbssbi@rit.edu, Franly Ulerio Nunez2, Morgan Bida2, Todd E. Pagano2. (1) Thomas H. Gosnell School of Life Sciences, Rochester Inst. of Technology, New York (2) Dept. of Science and Mathematics, Rochester Inst. of Technology, New York Fluorescent properties of several species of wild fruits commonly found in New York State were investigated and used to generate a unique fingerprinting tool for characterizing and comparing nutrients of antioxidant importance in the fruit. Analyzed fruits included both native and introduced species to the area that can be considered relevant as food sources for wildlife. Traditional bench-based assays were performed on aqueous extracts of freeze-dried fruit pulp, including those for total phenol content, total anthocyanins, and antioxidant capacity, in addition to other

macronutrient analyses. Multidimensional fluorescence spectroscopy with chemometric analysis was used to characterize the fluorophoric properties of the fruits using Parallel Factor Analysis (PARAFAC). It was shown that each fruit had a distinct spectral profile and the resulting PARAFAC scores correlated with biochemical components that contribute to antioxidant properties, particularly polyphenols that are catechins-like in nature. Anthocyanins also contributed to the antioxidant profiles of the samples, though likely represent a smaller portion of the antioxidant profile than the cathechins. Further, PARAFAC scores were used to group the fruits by taxonomic families. The fluorescence-based technique shows promise as a more specified tool for the characterization of fruit quality over traditional assay methods. The method could be broadly applicable for assessing food quality among locations and growing seasons for wildlife.

AGFD 165 Using dietary preferences of wildlife to discover bioactive polyphenols in plants Debbie Conner1, deborah.conner@yotes.collegeofidaho.edu, Hana Hoang1, Marcella Fremgen3, Jennifer S. Forbey4, Carolyn Dadabay2. (1) Chemistry, College of Idaho, Caldwell (2) Chemistry Dept., The College of Idaho, Caldwell (3) Bird Conservancy of the Rockies , Montrose, Colorado (4) Biological Sciences, Boise State Univ., Idaho The extensive sagebrush ecosystems of the western US provide a model of complex interactions at the chemical level between plants, herbivores, and pests. A better understanding of these chemical interactions could provide insight for development of natural products for use in combatting pests and diseases in humans and in the agricultural industry. For example, Greater sage-grouse (Centrocercus urophasianus), an endangered species candidate, feeds mainly on sagebrush, which in turn produces a diversity of chemical compounds to deter herbivores and pests. Despite lower crude protein in three-tip sagebrush (Artemisia tripartia) than Wyoming big sagebrush (Artemisia tridenta ssp. wyomingensis),sage-grouse consumed both species. We hypothesized that polyphenol content may explain dietary selection between and within each species. We found that Wyoming sagebrush had significantly higher total polyphenol levels than three-tip sagebrush. In some cases, total polyphenol levels in the same sagebrush species differed between foliage selected or avoided by grouse. High performance liquid chromatography (HPLC) was optimized to compare types and levels of individual polyphenols between and within species. HPLC-fractionated polyphenols were also used to screen for bioactive properties that could be exploited to combat pests and diseases in humans and in the agricultural industry.

AGFD 166 Antimicrobial activity of extracts from seaweeds of northeast Brazil Patricia C. Bezerra-Silva1, patriciacristin@gmail.com, Bheatriz N. Albuquerque3, Bruno S. Santos5, Thiago N. Reis4, Patrícia M. Paiva5, Marcia V. Silva5, Daniela M. Navarro2. (1) Dept. of Fundamental Chemistry, Federal Univ. of Pernambuco, Recife, Brazil (2) Fundamental Chemistry Dept., Federal Univ. of Pernambuco, Recife, Brazil (4) Dept. of Oceanography, Federal Univ. of Pernambuco, Recife, Brazil (5) Dept. of Biochemistry, Federal Univ. of Pernambuco, Recife, Brazil Natural products have been a source of bioactive compounds and is directly or indirectly responsible for about 40% of all drugs available in modern therapy. Due to its diverse environment, macroalgae have the potential to biosynthesize a variety of bioactive molecules. Taking this into consideration, the aim of this study was to investigate the biological activities of extracts from 25 species of macroalgae of Pernambuco state coast, including species of green, brown and red. The macroalgae were collected, identified, dried and extracted with dichloro methane/methanol 2: 1, with yields ranging from 0.2 to 16.8%. The extracts were then subjected to antimicrobial testing against three species of gram-positive (Bacillus subtilis, Enterococcus faecalis, Staphylococcus aureus) and three species of gram- negative (Escherichia coli, Klebsiella pneumoniae, Pseudomonas aeruginosa) bacteria. The extracts promoted inhibition of growth of bacteria, particularly of gram-negative bacteria with the species of brown algae Sargassum cymosum showing the best results (MIC = 1.56, 1.56 and 0.78 for the bacteria E. coli, K. pneumoniae and P. aeruginosa, respectively). The extracts also showed bactericidal activity for Gram-positive bacteria with the species of red seaweed Hydropuntia caudata presenting the best results (MBC = 6.25 and 3.13 for B. subtilis and S. aureus, respectively). Our results suggest that antimicrobial compounds can be found in species of seaweeds.

AGFD 167 In situ analysis of interrelation between topochemistry and cellulose accessibility in poplar cell walls Xia Zhou2, xiazhou0818@126.com, Feng Xu1, Dayong Ding1. (1) Coll of Material Sci Tech, Beijing Forestry Univ, China (2) Coll of Material Sci Tech, Beijing Forestry Univ, China Plants have evolved the inherent recalcitrance with chemical and structural complexity of their cell walls to resist deconstruction by pathogens. Although considerable progress has been made in understanding the basic organization and functions of plant cell wall components, due to the highly complex and dynamic nature of the plant cell wall, the variation in ultrastructural topochemistry and the establishment of its relationship with biomass conversion remain poorly understood. The plant cell wall is a layered construction composed mainly of cellulose microfibrils embedded in an amorphous matrix of hemicelluloses and lignin, thus both hemicelluloses and lignin have been considered to act as barrier elements during biomass deconstruction. Due to the higher spatial resolution (<1nm) and specificity when combined with chemical staining and immunolabeling approaches, transmission electron microscopy (TEM) was employed to investigate the interrelation between cell wall topochemistry and cellulose accessibility. A comparative study was conducted to determine which component contributes to the major barrier in cellulase attack by localization of cellulase on both transverse and tangential wood sections after successive removal of hemicelluloses and lignin respectively. Highest cellulose accessibility and enzymatic hydrolysis efficiency were realized on sections with moderate hemicelluloses removal, suggesting that the increase of cellulose accessibility primarily occurs when exposing cellulose surface by getting rid of the hemicelluloses coating on it. The results not only contribute to improving the efficiency of biomass conversion, but will also help us to understand the assembly of the plant cell wall. Keywords: Plant cell wall, Topochemistry, Immunolabeling, Cellulose accessibility

AGFD 168 Bioassay-guided isolation of secondary metabolite inhibitors of Xylella fastidiosa produced by endophytic fungi Morgan Papineau1, morganpapineau0215@pointloma.edu, Lindsey D'Elia1, Philippe E. Rolshausen2, Caroline Roper2, Katherine N. Maloney1. (1) Chemistry, Point Loma Nazarene Univ., La Jolla, California (2) Dept. of Plant Pathology and Microbiology, Univ. of California, Riverside Pierce's Disease in grapevines is an economically devastating infection caused by the bacterium Xylella fastidiosa (Xf). In previous studies, our lab identified radicinin, an Xf- inhibitory natural product of Cochliobolus sp. isolated from grapevines resistant to Pierce's Disease. We have isolated seven additional strains of endophytic fungi from grapevines that inhibit the growth of Xf in vitro, belonging to Geomyces, Eurotium, Cryptococcus and Ulocladium. We hypothesize that these strains of fungi also produce secondary metabolites that inhibit the growth of Xf, thereby protecting the winegrapes from Pierce's Disease. We report the results of bioassay-guided isolation of active compounds produced by these strains of fungi.

AGFD 169 Chemistry and mass spectral characterization of methylglyoxal adducts formed with metformin, aminoguanidine and okra seed extract: Relevance to diabetic complications Bishambar Dayal1, dayalb77@gmail.com, Rajeshri Gohil3, rajeshrig@gmail.com, Patrick O'Connor2, oconnojp@njms.rutgers.edu, Michael A. Lea4. (1) Medicine, Rutgers Univ. New Jersey Med. Sch. Princeton Jct (2) Microbiology, biochemistry and Molecular Genetics, Rutgers Univ., New Jersey Med. Sch., Newark (3) Medicine, Biochemistry and Molecular Biology, Rutgers Univ., New Jersey Medical School, Newark (4) Microbiology, Biochemistry and Mol. Genetics, Rutgers Univ. New Jersey Medical School, Newark Accumulation of advanced glycation end products (AGEs) in diabetes leads to progressive neurodegeneration and development of end-stage renal disease. In chronic hyperglycemia enormous amounts of reactive oxygen species (ROS) are generated and highly reactive molecules such as methylglyoxal (MGO), glyoxal (GO) and 3- deoxyglucosone (3-DG) formed from glucose in the cells cause microvascular and macrovascular complications in diabetes. They affect secretion of insulin from pancreatic β-cells as well. Recently we studied binding and modification of proteins (HAS-MGO, BSA-MGO, RNAs-MGO) and reported the efficacy of Okra Seed phytochemicals in inhibiting AGEs. Inhibitory effects of OSE were comparable with the well-established antidiabetic drugs, metformin and aminoguanidine as revealed by AGEs-associated absorbance changes, SDS-gels and fluorescence emission profiles. Unusual changes in the absorbance of AGEs and fluorescence data of modified proteins tempted us to study in detail the mass spectral characteristics of MGO-Metformin, MGO-Aminoguanidine and OSE-MGO adducts followed by UV-visible NanoDrop spectrometry and analytical TLC. ESI-MS: MGO-Met Adduct showed M/Z 184 (100%) [Triazepinone], its condensation product M/Z 202, its dehydration product M/Z 184 as triazepinone. Higher mass range peaks provided M/Z 256 (40%) , M/Z 274 (22%) (the peak (274-18) =256. This signifies the addition of another mole of MGO to triazepinone. Peak at M/Z 114 (is attributed to loss of carbon monoxide (CO) from the triazepinone molecule. ESI-MS: [MGO-Aminoguanidine(AG) Adduct] M/Z 111 (100%), M/Z 129 (15%) and (129-H2O)= 111. Similarly reaction of MGO (1.4 equivalent) with OSE was performed with the Phosphate buffer at PH 7.2 analyzed and reaction monitored via UV-visible NanoDrop Spectrometry and TLC. The typical fragmentation mass spectral data of different metabolites generated in these studies show that the further reaction of MGO with triazepinone (M/Z 256) is a mechanism for the excretion of toxic metabolites methylglyoxal and glyoxal which get excreted in urine of diabetic patients suffering from end-stage renal disease. The reaction of these adducts with N-acetyl cysteine, a powerful antioxidant will be discussed.

AGFD 170 LC/MS metabolomic profiling of an amber ale fermented with four different yeast strains Chrisi A. Hughey1, hugheyca@jmu.edu, Kearney M. Foss1, Karen Fortmann2. (1) Dept. of Chemistry & Biochemistry, James Madison Univ., Harrisonburg, Virginia (2) White Labs, San Diego, California Metabolomic profiling of beer by LC/MS has largely focused on the hops used or compositional changes that occur during storage. Here we profiled metabolomic differences in an amber ale that was fermented by White Labs with four different yeast strains. A 20-barrel batch of the ale was equally divided and fermented with Bedford British ale yeast, Dusseldorf alt yeast, Tennessee whiskey yeast and Abbey ale yeast. The yeasts imparted distinctly different flavor profiles that ranged from fruity to spicy, as determined by a sensory panel. Within two days post-fermentation, samples were received by JMU, sonicated, filtered and stored at -80 °C. Both positive and negative ion ESI q-TOF MS was used for metabolomic profiling. Principle component analysis (where P1 and P2 accounted for ~55% of the variance) revealed that the Tennessee whiskey yeast was least similar to the other strains in P1. The other three strains clustered together in P1 but were separated in P2. ANOVA with a Tukey post-hoc test was then used to identify up- and down-regulated ($p<0.05$) molecular features (MFs, unique mass and retention time) across samples. These features were then searched against the Metlin database. Efforts moving forward will focus on more putative identification of differentially expressed MFs using MS/MS, spectral library searches and Agilent's Mass Profiler Professional Pathway Analysis for Saccharomyces cerevisiae in order to better understand the role of yeast on a beer's metabolome.

AGFD 171 Antimicrobial spectrum and toxicology of a natural food grade additive obtained from avocado seed Adriana Pacheco2, adrianap@itesm.mx, Ricardo C. Chávez2, Dariana G. Rodriguez- Sanchez3, Raul Villarreal-Lara2, Maria I. Garcia-Cruz2, Carmen Hernandez-Brenes1. (1) Technologico de Monterrey, Mexico (2) Biotechnology, Tecnologico de Monterrey, Nuevo Leon, Mexico (3) Instituto de Innovación y Transferencia de Tecnologia, Colinas de San Jeronimo, Mexico Avocado fruit contains a family of lipid derivatives (acetogenins) known to exhibit antimicrobial activity. Acetogenin enriched extracts, obtained at laboratory scale by centrifuge partition chromatography (CPC), possess antimicrobial activity against Clostridium sporogenes vegetative cell growth and endospore germination. The objectives of this study were to characterize a food grade acetogenin enriched extract (Avosafe), obtained from avocado seed, by its chemical profile, antimicrobial spectrum, and toxicology. Lyophilized seed extracts were enriched in acetogenins by CPC. Active fractions were then pooled and extraction solvents removed to obtain the food grade extract. Analytical standards were purified by preparative chromatography and acetogenin quantification was performed by HPLC-MS and HPLC-PDA. Avosafe was tested against important food pathogens (eight Gram-positive bacteria, two Gram- negative bacteria, and two yeasts) by the disc diffusion test and determination in liquid culture of minimum inhibitory (MIC) and bactericidal concentrations (MBC). Preliminary toxicology on Avosafe was determined by the Ames mutagenicity assay and acute oral toxicity to rats (fixed dose method). For all tests Avosafe was formulated in propylene glycol. Avosafe was enriched in a total of seven main acetogenins (71.3% w/w); persenone A and AcO-avocadene were the most abundant (20.4 and 21.9% w/w, respectively), which showed larger inhibition zones (2-4 times) than commercial food preservatives (NisaplinÒ and MineratÒ). Of the tested microorganisms, Avosafe showed antimicrobial activity only towards Gram-positive bacteria (Listeria monocytogenes), and particularly sporulated bacteria (C. sporogenes, C. perfringens, Bacillus subtilis, and Alicyclobacillus acidocaldarius). MIC values ranged from 3.9–15.6 ug mL-1. Avosafe was non-mutagenic and the acute median lethal oral dose (LD50) to rats was determined at >2 000 mg kg-1 with no signs of abnormalities in organs and tissues. Results strengthened the potential of avocado acetogenins as natural antimicrobial food additives.

AGFD 172 Functional role of fiber in the diet: Prebiotics, metabolic benefits and beyond Carolyn Slupsky, cslupsky@ucdavis.edu. Dept. of Nutrition, Univ. of California, Davis Although increasing consumption of dietary fiber and mixed whole-grain products is widely recommended for maintaining a healthy body weight, little is known about the relationship between different types of fiber and background diet. Two well-known functional foods: resistant starch and nopal (an edible cactus, containing primarily pectin) have been shown to have promising health benefits on reducing circulating glucose levels, improving insulin resistance, and reducing body fat in the context of a western-style diet. The complexity of the interaction between fiber and the microbiome, evaluated through both sequencing and fecal metabolomics, reveals that the type of fiber consumed drives both the bacterial community profile and its metabolic activities. Moreover

other components of food, such as polyphenols, also exert positive health benefits. There is a need for considerable research to understand how the components of food act synergistically to create positive metabolic health benefits. Future integrative research that addresses the underlying mechanisms will help expand the understanding of functional foods in health promotion.

AGFD 173 Effects of indigestible polysaccharides on obesity related metabolic diseases and inflammation Yukari Egashira, egashira@faculty.chiba-u.jp. Laboratory of Food and Nutrition, Chiba Univ., Japan Some indigestible polysaccharides or oligosaccharides have been reported to yield a variety of health promoting activity such as anti-obesity effects, and blood glucose-, cholesterol-, triacylglycerol (TG) -lowering effects in both animal models and humans. Moreover, some indigestible polysaccharides also affect immunological system. However, we have limited understanding of how these materials regulate molecular events at the gene level and energy metabolism as well as inflammatory events. To clarify the mechanism, we demonstrated whether the intake of indigestible polysaccharide activates energy consumption in the tissue using DNA microarrays. Psyllium fiber composed a highly branched arabinoxylan has cholesterol- and TG -lowering effects in many studies. The results from our study showed that Acadm, Acadl, Hadb, Hadbb, Acsl1, Lpl, Cd36, Cpt1b and Cact gene expression in the skeletal muscle were significantly elevated in the high-fat diet+ psyllium group compared with high-fat diet group. These genes encode key enzymes and transporters involved in fatty acid oxidation and lipid transport. The results from our study suggest that dietary psyllium enhance the transfer of excess fatty acid from the liver to the skeletal muscle and promote lipid consumption in the skeletal muscle. Psyllium contributes to the consumption of lipid in the muscle and this phenomenon is partly attributable to ameliorates lipid metabolism and obesity. We also investigated the effects of long-term intake of wheat bran hemicellulose arabinoxylan (WBH) and guar gum on blood glucose, lipid levels, and abdominal fat accumulation in high-fat-fed mice. Plasma total cholesterol, abdominal fat accumulation and leptin mRNA of epididymal fat were significantly lower in the WBH group compared with high-fat diet control group. Blood glucose level was significantly lower in the guar gum group compared with high-fat diet control group. We reported that partially hydrolyzed arabinoxylan from rice bran (MGN-3) significantly suppressed D-galactosamine-induced inflammation. We showed that this protective mechanism is mediated in part by suppress of interleukin-18 and by inhibition of NFκB, and JNK phosphorylation expression. These indigestible polysaccharides or oligosaccharides may have beneficial effects on high-fat diet lifestyle and its related disease.

AGFD 174 Anti-obesity properties of mushroom polysaccharides: A review Mendel Friedman, mendel.friedman@ars.usda.gov. Healthy Processed Foods, USDA, Western Regional Research Center, Moraga, California Mushrooms are widely consumed for their nutritional and health benefits. To stimulate broader interest in the reported health-promoting properties of bioactive mushroom polysaccharides, this presentation will survey the chemistry (isolation and structural characterization) and reported antiobesity properties and associated antioxidative, anti- inflammatory, and imunostimulating activities. The following examples demonstrate the potential value of structurally different polysaccharides from several mushroom sources to alleviate obesity, an aspect that merits further study in humans. (a) The dietary supplement ReishiMax containing polysaccharides extracted from the medicinal mushroom Ganoderma lucidum can control growth and glucose uptake in 3T3-L1 adipocyte (fat) cells. (b) A water extract of Ganoderma lucidum reduced body weight, inflammation, and insulin resistance in mice fed a high-fat diet by modulating the composition of the gut microflora. (c) Pleurotus eryngii mushroom heteropolysaccharides inhibited insulin resistance, oxidative stress, and live dysfunction in mice fed a high-fructose diet. (d) Three polysaccharides from Pleurotus tuber-regium mushrooms exhibited antihyperglycemic properties and attenuated oxidative stress in diabetic rats on a high fat diet; and (e) Dietary supplementation of a mouse diet with chitosan derived from mushrooms decreased feed efficiency, fat mass and fat deposition in the liver and the muscle of obese mice. Possible mechanisms of the beneficial properties will be discussed.

AGFD 175 Polysaccharide structure and physiological effect: Glycemic and non-glycemic carbohydrates Madhuvanti Kale1, madhuvanti.kale@ars.usda.gov, Bruce Hamaker2. (1) USDA-ARS Western Regional Research Center, Albany, California (2) Whistler Center for Carbohydrate Research, Purdue Univ., West Lafeyette, Indiana The structure of polysaccharides is a fundamental factor determining their fate in the body. Advances in analytical techniques over the past few years have made it possible to relate very specific aspects of polysaccharide structure, such as monosaccharide composition and glycosidic linkage profiles, with their utilization in the body. This talk will summarize some of the established relationships between structure of polysaccharides, both glycemic and non-glycemic, and their utilization by small intestinal enzymes or gut microbiota. For glycemic carbohydrates such as starch, the role of structure in determining rates and patterns of utilization by digestive enzymes will be emphasized. In particular, the utilization of various types of starches by small intestinal mucosal α- glucosidases will be discussed. In the context of dietary fiber, much knowledge has been gained in the recent past by focusing on gut microbial utilization of fermentable dietary fibers, such as arabinoxylans and pectins. To offer a perspective on gut microbial utilization of various polysaccharide structures, the role of structural complexity of arabinoxylans in their differential utilization by gut bacteria will be discussed as an example. Finally, an overall perspective on understanding polysaccharide structure and its physiological effects in the context of obesity and metabolic disorders will be offered, highlighting the direction of current research in building a thorough body of knowledge on the effects and importance of glycemic and non-glycemic polysaccharides in the health and nutrition.

AGFD 176 Yeast β-glucan down-regulates blood glucose level in obesity/type 2 diabetes Xiaojuan Xu, xuxj@whu.edu.cn, Yan Cao, Lina Zhang. Wuhan Univ., China Yeast glucan is a well-known bioactive β-glucan, but it often has different formulations including branched, linear, water-soluble and water-insoluble β-glucans, leading to various experiment data and imperfect mechanism. In this study, we isolated a pure linear β-(1→3) Baker's yeast glucan (BYGlc), and reported that BYGlc raised glucose uptake in vitro and down-regulated blood glucose and body weight of obese/type 2 diabetic (T2D) mice. It was found that more than 50% FITC-labled BYGlc was directly excreted through the feces, and a small amount of BYGlc was adhered on the intestine epithelium, taken up into the blood circulatory system, and then mainly distributed in liver and spleen. It is interesting that BYGlc in gastrointestinal tract significantly suppressed the expression of sodium-glucose transporter-1 (SGLT-1) on the surface of intestin mucosa to slow down glucose uptake from intestine into blood. Additionally, BYGlc effectively decreased the high level of Firmicutes induced by high-fat diet and increased the proportion of Akkermansia, the top candidate to decrease body weight and improve glucose homeostasis. In liver of T2D mice, BYGlc promoted glycogen synthesis and inhibited lipid accumulation through IRS/Akt pathway. BYGlc also improved the inflammation symptoms indicated by supressing the TNF-a, IL-6 and macrophage infiltration in adipose tissue induced by high-fat diet. Taken together, oral administration of BYGlc has comprehensive benificial effect on gut microbiome, metabolism, inflammation in obese/T2D model, and has a promising application as a drug or food component for preventing or treating obesity/T2D patients.

AGFD 177 Digestibility and health benefits of native and modified resistant starch Jay-Lin Jane2, jjane@iastate.edu, Yongfeng Ai2, Michael Reed2, Hongxin Jiang2, Jovin Hasjim2, Diane Birt1. (1) Iowa State Univ., Ames (2) Food Science and HumanNutrition, Iowa State Univ., Ames High-amylose maize starch (HAMS, a Type-2 resistant starch, RS-2), stearic acid complexed HAMS (SA-HAMS, RS-5), and chemically modified HAMS using octenyl- succinic anhydride (OS-HAMS, RS-4) were used to feed rats for nine weeks, and normal-maize starch (NMS) was used as a control. Results showed that NMS was 99.9% digested and utilized by rats, and no detectable starch granules were found in the feces; whereas there was 1.7%, 2.7%, and 20.2% starch not being utilized and found in the feces for HAMS, SA-HAMS, and OS-HAMS, respectively, after nine-week feeding. As the feeding studies progressed for nine weeks, unutilized starch decreased from 4.9% (week 1) to 1.7% (week 9) for HAMS, from 16.1% to 4.7% for SA-HAMS, and varied between 22.5%, 31.1% and 20.2% for OS-HAMS. The results showed that the digestion of the native HAMS and physically modified SA-HAMS complex by rats increased as the feeding progressed, whereas the chemically modified starch, OS- HAMS, did not show an increase in digestion. The pH of cecal content of rats was 7.5, 5.3, 5.6, and 5.8 for NMS, HAMS, SA-HAMS, and OS-HAMS group, respectively, indicating some variation in the fermentation of different resistant starches but little fermentation for the NMS. The average weight of cecal content was 1.05, 3.55, 3.78, and 4.25 g/rat (dry basis), respectively. With the different levels of digestion and utilization of starch in the feed and similar intakes of feed by the rats, body weights of the rats, however, were similar. Populations of microbiota phyla present in the colon of rats differed with the different starches in the feed.

AGFD 178 New strategy for the biocontrol of Fusarium verticillioides in corn based on endophytic bacterial-fungal interactions Charles W. Bacon1, charles.bacon@ars.usda.gov, Dorothy M. Hinton1, Trevor Mitchell2. (1) Toxicology & Mycotoxin Research Unit, USDA, Athens, Georgia (2) Toxicology & Mycoroxin Research Unit, USDA, ARS, Athens, Georgia Bacterial endophytes are being used as biocontrol organisms for the control of plant pathogens such as the corn fungal endophyte Fusarium verticillioides and its production of the fumonisin mycotoxins. It is our hypothesis that factors by which plant endophyte communities are regulated involve host-produced compounds that modify behavior of endophytic microbes, often reducing growth rates and suppressing pathogenic behaviors. These behavior-modifying compounds are proposed to include phenolic acids, quorum-quenching and -inhibiting compounds, and perhaps other secondary metabolites that are toxic and recorded as mycotoxins. There is a plethora of substances and structures peculiars to endophytes that inhabit plants that are interactive in protecting and regulating the success of endophytes. Biofilms are important indicator extracellular polymeric compounds produced by bacteria that are useful for developmental phases including motility, swarming, signaling processes, and for hydrophobic nutrient utilization, all of which are important attributes for biocontrol bacteria. As a start for the test of our hypothesis, an endophytic biocontrol bacterium, Bacillus mojavensis, was used as the model organism for the biocontrol used in corn for fumonisin reduction. A bank of biosensor bacteria were used to screen fungal, plant and bacteria for quorum sensing or inhibiting signals. Laser ablation electrospray ionization (LAESI) MS technology is a modern method that allows the in situ cell imaging of tissues, resulting in a noninvasive measure and chemical analyses of microbes and hosts parasitic interactions to test for such interactions. LAESI MS was use to determine biofilm production relative to specific biosurfactants, other metabolites for antagonisms to the maize pathogen F. verticillioides and its fumonisin mycotoxins. Results are presented and characterized according to the reaction of the producing organisms, fungus or bacterium, and an interaction to the plant that should lead to information useful for field-testing of bacteria and their requirement for success in reducing the ubiquitous presence of F. verticillioides in corn.

AGFD 179 Bioplastic formulation of beneficial microbes to control agricultural pests Hamed K. Abbas, Hamed.Abbas@ars.usda.gov. BCPRU, USDA-ARS, Stoneville, Mississippi Biocontrol agents are used to control various agricultural pests including fungi, insects, weeds, and bacteria. The efficacy of these beneficial microbes depends on their delivery systems. Because of difficulties in maintaining viability during storage and field application, improved methods are required to enhance their effectiveness. Novel biodegradable formulations comprising biocontrol microorganisms impregnating a starch-based bioplastic are effective for delivering biocontrol microorganisms and bioactive compounds to soil, plants and seeds. Granules of bioplastic containing Aspergillus flavus are sprinkled on soil to reduce aflatoxin in maize. Coating seed with bioplastic containing Trichoderma helps to establish seedlings and prevent root rot. On tomatoes, impatiens and annual bluegrass Trichoderma formulated in bioplastic granules reduces damping off, a fungal disease, by 85%. Application of a sprayable liquid formulation of bioplastic containing Beauveria bassiana significantly reduced damage caused by the European corn borer in maize and the tarnished plant bug in cotton. Applying bioplastic formulated with spores of a non-toxigenic A. flavus isolate resulted in a 97% reduction of aflatoxin contamination of maize. The bioplastic dispersion formulation is effective in delivering crystals of Bacillus thuringiensis endotoxins to European Corn Borer larvae, causing 72% mortality". These results suggest that bioplastic formulations have the potential for effective delivery of several biocontrol agents.

AGFD 180 Reduction of fumonisin toxicity by extrusion and nixtamalization (alkaline cooking) Kenneth Voss3, ken.voss@ars.usda.gov, Dojin Ryu4, Lauren Jackson1, Ronald T. Riley2, Janee Gelineau-van Waes5. (1) Inst. for Food Safety and Health, US FDA, Bedford Park, Illinois (2) Toxicology and Mycotoxin Research Unit, USDA-ARS (retired), Athens, Georgia (3) Toxicology & Mycotoxin Research Unit, USDA Agricultural Research Service, Athens, Georgia (4) School of Food Science, Univ. of Idaho, Moscow (5) Dept. of Pharmacology, Creighton Univ., Omaha, Nebraska Fumonisins are found in corn. The most common, fumonisin FB1 (FB1) is toxic to animals, disrupts sphingolipid metabolism, and is a suspected risk factor for neural tube defects (NTDs; serious birth defect) and cancer in humans that consume contaminated corn as a diet staple. FB1 levels in foods and animal feeds should therefore be reduced as much as possible. Quantification of FB1 in uncooked and cooked grits or corn combined with rodent bioassays utilizing FB1-specific toxicological endpoints were done to evaluate the effectiveness of extrusion and nixtamalization for reducing FB1 concentrations and toxicity. (A) Extrusion reduced (64-72%) FB1 concentrations in 2 batches of grits initially containing low (10 ppm) or high (50 ppm) amounts of FB1. Reductions improved to 89-94% when 10% glucose was added before cooking. No (low dose batch) or markedly reduced (high dose batch) kidney pathology and sphingolipid effects were found when extruded, glucose supplemented grits were fed (50% w/w in the diet) to rats for up to 8 weeks. Extrusion without glucose was less effective but none the less reduced toxicity. (B) Alkaline cooking whole kernel FB-contaminated corn (3 batches; initial FB1 concentrations of 1.8 – 4.2 ppm) reduced FB1 concentrations by about 90%. Kidney pathology and sphingolipid effects were absent (2 batches: FB1 diet concentrations about 0.1 ppm) or significantly reduced (1 batch; FB1 diet concentration 0.4 ppm) in rats fed the alkaline cooked corn. (C) Hydrolyzed FB1 (HFB1) is formed from FB1 during nixtamalization. Unlike FB1 (10

mg/kg body weight = 14 µmol/kg), doses up to 20 mg/kg (= 49 µmol/kg) body weight HFB1 did not cause NTDs when test using the LM/Bc mouse bioassay. Furthermore, FB1 caused liver pathology and significantly disrupted sphingolipid metabolism whereas only slight sphingolipid effects and no pathology were found in mice given HFB1. Together, these findings show that extrusion, especially with glucose supplementation, and nixtamalization effectively reduce the toxicity of FB1 contaminated corn.

AGFD 181 Mycotoxin deactivation strategies – past, presence and future Gerd Schatzmayr, gerd.schatzmayr@biomin.net. BIOMIN Research Center, Tulln, Austria The most frequently used approach to deactivate mycotoxins in animal feeds is the application of adsorbents which bind toxins and reduce the absorption in the gastrointestinal tract. However, the drawback of this method is that only a group of bentonite clays with a high smectite content work against aflatoxins and ergot alkaloids, but have limitations against other relevant mycotoxins. Microorganisms or their enzymes with the capability to detoxify mycotoxins by degradation or biotransformation can be used to overcome the limitations of binding agents. Such microorganisms can be found in the environment where they prevent any significant accumulation of fungal toxins by utilizing them as carbon- or energy source. Our objective is to isolate microorganisms or their enzymes which catabolize mycotoxins and apply those as additives in food and feed. One of these microorganisms designated as BBSH 797 originates from the rumen of a cow and was identified as genus novus of family Coriobacteriacae. This bacterium is capable of detoxifying trichothecenes by reduction of their epoxide rings. We also isolated several microorganisms for catabolizing and detoxifying fumonisins. For several reasons none of these strains was useful as a direct fed microbial type of mycotoxin detoxifying additive. Therefore we explored the catabolic pathway of fumonisin degradation and identified the key gene of detoxification, which was a carboxylesterase. Then we cloned and expressed this gene in a yeast strain, purified the enzyme and tested it in swine for its gastrointestinal detoxification capacity. Based on various parameters like sphinganine/sphingosine biomarker and expression of immune genes we could confirm that this enzyme works in the gastrointestinal environment. Recently the European Food Safety Authority (EFSA) provided a positive opinion on BBSH797 and the carboxylesterase to the European Commission based on efficacy- and safety data.

AGFD 182 Molecular approaches for enhancing host resistance against Aspergillus flavus infection and aflatoxin contamination in corn and cottonseed Deepak Bhatnagar, deepak.bhatnagar@ars.usda.gov, Robert Brown, K. Rajasekaran, Jeffrey Cary, Matthew Gilbert. USDA, SRRC, New Orleans, Louisiana Aflatoxin contamination in crops such as corn, cottonseed, peanut, and tree nuts caused by Aspergillus flavus is a worldwide food safety problem because aflatoxins are potent carcinogens. In developing countries this contamination results in enormous economic losses because regulatory guidelines prevent sale of contaminated crops. Even though the biological control strategy has been effective in significant reductions in aflatoxin contamination, utilizing resistant germplasm against A. flavus growth and aflatoxin contamination is the most practical solution for pre-harvest control. Research efforts in our lab have, therefore, focused on elucidation of the complex, multi-genic resistance mechanisms in corn identified in resistant genotypes resulting from breeding programs. The molecular basis of seed based resistance is being examined through transcriptomic analysis of the corn-A. flavus interaction allowing identification of genes and networks correlated with resistance for use in marker assisted breeding. RNA interference technology is also being utilized to not only determine the roles and contribution of selected corn genes to overall resistance; but also to target genes critical to A. flavus growth and toxin production to enhance resistance. Efforts are also underway to overexpress resistance genes identified from various transcriptome analyses of the A. flavus-cottonseed interaction to achieve enhanced resistance. Genomics and transcriptomics of A. flavus has provided significant insights into molecular aspects of the response of the fungus as it invades the crop and produces aflatoxins. All this research is allowing the development of effective and stable strategies for producing safe food and feed, free of aflatoxins.

AGFD 183 Tools to determine the identity, occurrence and toxicity of conjugated mycotoxins Veronika Nagl1, veronika.nagl@biomin.net, Gerhard Adam3, Rainer Schuhmacher2, Rudolf Krska2, Franz Berthiller2. (1) BIOMIN Research Center, Tulln, Austria (2) Dept. IFA-Tulln, Univ. of Natural Resources and Life Sciences, Vienna, Tulln, Austria (3) Dept. of Applied Genetics and Cell Biology, Univ. of Natural Resources and Life Sciences, Vienna, Tulln, Austria Mycotoxins are secondary metabolites of molds, toxic to humans and animals at low concentrations. After the infection of crop plants, mycotoxins can be modified by plant enzymes and often conjugated to more polar substances, such as sugars or amino acids. The formed metabolites are partly stored in the vacuole in soluble form or further metabolized and bound to macromolecules. As these conjugated mycotoxins are usually not detected during routine food analysis, they are also called “masked mycotoxins”. While having a low intrinsic toxicity, masked mycotoxins might be reactivated during mammalian metabolism. In particular, the polar groups could be cleaved from the molecule, liberating the native mycotoxins. The tremendous pace in the development of modern analytical equipment – first and foremost liquid chromatography coupled to mass spectrometry (LC/MS) - has enabled the discovery of many conjugated mycotoxins during the last couple of years. While there are still plenty of shortcomings to overcome, the mycotoxin community has made some great advances lately. Both targeted and non-targeted LC/MS based methods have been developed to detect novel plant metabolites of mycotoxins. Analytical standards for numerable of those compounds have been isolated or synthesized and enable quantitative determination in food and feed samples. The ultimate question, whether conjugated mycotoxins are a health concern, needs to be answered for each individual compound. Therefore, in vitro as well as in vivo studies on the toxicological relevance of masked mycotoxins are crucial. In lack of such data, the Panel on Contaminants in the Food Chain (CONTAM) of the European Food Safety Authority (EFSA) recently adopted a pragmatic approach in risk assessment by rendering the toxicity of those compounds equal to those of the native toxins. The currently best studied masked mycotoxin is deoxynivalenol-3-glucoside, for which both in vitro and toxicokinetic studies in rats and pigs have been performed lately. Concluding, the compound shows low bioavailability, but is effectively cleaved to deoxynivalenol in the intestine of the studied animals

AGFD 184 Making synthetic starch (amylose and amylopectin) from nonfood biomass Yi-heng Percival Zhang, ypzhang@vt.edu. Biological Systems Eng, Virginia Tech, Blacksburg The global food system is experiencing profound changes as a result of anthropegenic pressures. Increasing population to 9 billion and food consumption per capita means that the global food demand could increase by 70% by 2050. Food security is placing unprecedented demands on agriculture and natural resources, such as water, land, fertilizers, and fossil fuels. The World Health Organization (WHO) and Food and Agricultural Organization (FAO) recommend population nutrient intake goals for preventing diet-related chronic diseases in terms of caloric uptake: total carbohydrate (55-75%), total fat (15-30%), and protein (10-15%), where free sugars (i.e., monosaccharides and disaccharides) in the diet accounts for less than 10% of carbohydrate intake. A properly balanced diet is important to lower health risks, such as obesity, type 2 diabetes, cardiovascular diseases, hypertension, cancer and so on. In

this talk, I will talk about our recent efforts for low-cost transformation of synthetic starch from cellulose. Different from microbial fermentation, we propose that the use of in vitro synthetic enzymatic biosystem (ivSB) implements complicated biological reaction via the in vitro assembly of numerous standardized and exchangeable enzymes or their complexes and/or (biomimetic) cofactors. Compared to microbial fermentation, ivSB features numerous manufacturing advantages, such as high product yield, fast reaction rate, easy product separation, easy access and control for open systems, and so on. To convert cellulose to starch, we developed simultaneous enzymatic biotransformation and microbial fermentation for converting cellulose to starch and ethanol at the same time without sugar loss. To decrease the production cost of synthetic starch, we develop a simple way to selectively remove beta-glucosidase from commercial cellulase mixture, display a synthetic enzyme complex on the surface of yeast to increase microbial cellulose utilization rates, and convert amylose to branched amylopectin by using a branching enzyme. We will have enough new food source to support at least 20 billion persons on earth in the future.

AGFD 185 Effect of sulfite on the reactivity of exogenous acetaldehyde with wine flavonoids Marlena K. Sheridan, mks241@psu.edu, Ryan Elias. Food Science, Penn State Univ., State College Acetaldehyde is known to play an important role in reactions of flavonoids (e.g., catechins, condensed tannins) that improve the mouthfeel and color stability of red wines. However, previous studies have assumed that bridging by acetaldehyde is -6 prevented when it is bound to sulfite (1-hydroxyethanesulfonate Kd (pH 3) = 1.5 x 10). The aim of this study was to demonstrate the reaction of exogenous acetaldehyde in the presence of sulfite in real and model wine systems. Reactions were followed directly by monitoring flavonoid concentrations and indirectly by characterizing protein interactions and color stability. Studies in a model wine system containing catechin revealed that exogenous acetaldehyde reacts with catechin even in the presence of sulfite equimolar to acetaldehyde. In systems containing catechin or grape seed tannins as well as malvidin-3-glucoside, equimolar additions of sulfite and acetaldehyde led to improvements in several color stability parameters. Sodium 1-hydroxyethanesulfonate was then synthesized from acetaldehyde and sodium metabisulfite and studied in similar model systems. When this sulfonate was added, catechin was again consumed, thus confirming the reactivity of acetaldehyde from its bound form. The effect of exogenous acetaldehyde and sodium 1-hydroxyethanesulfonate were then examined in wine as a treatment immediately after alcoholic fermentation of a Cabernet Franc wine. The effects on wine tannins were characterized to determine the efficacy of free and bound acetaldehyde. The results of this work indicate that acetaldehyde bound in wine or added in its bound form contributes to beneficial tannin modifications.

AGFD 186 Dietary flavonoid luteolin chemosensitizes ovarian cancer cells by inhibiting FAK- mediated epithelial-to-mesenchymal transition Vermont P. Dia, vdia@utk.edu, Philipus Pangloli. Food Science and Technology, The Univ. of Tennessee, Knoxville Ovarian cancer is the deadliest form of gynecological cancer and the fifth leading cause of cancer-related death in women in the US. One of the major impediments in the treatment of ovarian cancer is the eventual development of resistance to both platinum and taxane-based chemotherapies. The objective was to evaluate if luteolin (5,7,3',4'-tetrahydroxyflavone),a flavonoid present in fruits and vegetables with many reported biological activities, can chemosensitize paclitaxel-resistant ovarian cancer cells and determine the mechanism of action involved in the chemosensitization effect. Ovarian cancer cells A27801AP and its paclitaxel –resistant variants PTX10 and PTX22 were used in the study. Cytotoxicity assay confirmed the resistance of two cell lines to paclitaxel with median effective dose values (ED50) of 53.3 and 21.1 μM for PTX10 and PTX22, respectively compared to parent A27801AP with ED50 of 0.16 μM. Luteolin caused a dose-dependent reduction in the proliferation of OVCA cells with ED50 values of 46.3, 38.1 and 45.6 μM against A27801AP, PTX10 and PTX22 cells, respectively indicating that luteolin is more potent in paclitaxel resistant cells. Luteolin at 31.25 μM modified the expression of proteins in PTX10 ovarian cancer cells associated with epithelial-to-mesenchymal transition by significantly increasing the expression of epithelial marker E-cadherin by 1.8-fold and decreasing the expression of mesenchymal marker vimentin by 2.6-fold ($P < 0.05$). The associated mechanism is through reduction of phosphorylation of focal adhesion kinase and extracellular signal-regulated kinase by 1.7- and 2.1-fold, respectively ($P < 0.05$). In addition, treatment of PTX10 OVCA cells with a noncytotoxic dose of luteolin at 10 μM reduced its proliferation by 23.9% ($P < 0.05$) and sensitized PTX10 cells from 12.1 to 20.7% when treated with paclitaxel from 5 to 20 μM. Our data showed that luteolin plays a role in ovarian cancer chemosensitization by modifying signaling molecules associated with epithelial-to- mesenchymal transition.

AGFD 187 Effect of cooking on saponins content in pigmented chickpea Ada k. Milan, keilamilan@hotmail.com, Janet Gutierrez-Uribe, Sergio Serna-Saldivar. Centro de Biotecnologia, Tecnologico de Monterrey, Nuevo Leon, Mexico Chickpea is an important legume crop and a good source of dietary saponins. Saponins are a group of secondary metabolites with a structure constituting of steroid or triterpenoid aglycones and sugar moieties with multiple health promoting effects. The objective of this study were analyzed the saponins concentration in 80% methanolic extracts of ten raw and cooked pigmented chickpeas cultivars (cv). The chickpeas studied had green (1 cv), black (3 cv), red (3 cv), brown (1 cv) and cream (2 cv) colored seed coat. The saponins were identified by their corresponding mass spectra obtained by HPLC-IT-MS and quantified by HPLC-ELSD using soyasaponin I as external standard. In the raw chickpea 3 predominant saponins were found. The content of soyasaponin βg (m/z 1068), soyasaponin Bb (m/z 942) and lablab saponin I (m/z 1084) ranged 1581-261 μg/g, 224-56 μg/g and 172-44 μg/g, respectively. The cooking process caused minor lost of total saponins content and an increase in soyasaponin I content by converted of βg to I. These chickpeas cultivars are a potential source of saponins for promoting health effects

AGFD 188 Hydrophobically-modified nanoporous silica aerogel: Novel food-contact surface inhibiting adhesion of gram-negative and gram-positive bacteria Jun Kyun Oh1, junkyun09@tamu.edu, Luis Cisneros-Zevallos3, Mustafa Akbulut2. (1) Materials Science and Engineering, Texas A&M Univ., College Station (2) Chemical Engineering, Texas A&M Univ., College Station (3) Horticultural Sciences, Texas A&M Univ., College Station In the context of food safety, contamination of food-contact surfaces with pathogenic bacteria is a global concern. This work investigates the potential of "hydrophobically- modified nanoporous silica aerogel" (HNSA) as a bacterial anti-adhesive food-contact surface. The bacterial anti-adhesive efficacies of HNSA, hydrophilic nonporous silica, and hydrophobic nonporous silica were evaluated via dip-inoculation with Salmonella Typhimurium LT2, Listeria innocua, Escherichia coli O157:H7, and Staphylococcus aureus at the final concentration ranging from 8.7 to 9.1 log CFU/mL. Bacterial attachment to these surfaces were enumerated by conventional plating as well as direct counting via scanning electron microscopy. Compared with hydrophilic nonporous silica, hydrophobic nonporous silica and HNSA led to a reduced number of S. Typhimurium LT2 by 1.2 ± 0.1 log units (93.23% ± 0.91%) and by 3.1 ± 0.1 log units (99.93% ± 0.01%), respectively ($p < 0.05$). The log reductions in the number of L. innocua were 1.3 ± 0.0 (94.82% ± 0.21%) and 3.0 ± 0.0 (99.91% ± 0.01%) for hydrophobic nonporous silica and HNSA, respectively ($p < 0.05$). Also, the attachment of E. coli O157:H7 and S. aureus on HNSA was found to be significantly lower than that on hydrophilic/hydrophobic nonporous silica ($p < 0.05$):

99.91% (E. coli O157:H7) and 99.93% (S. aureus) reduction in comparison to hydrophilic nonporous silica and 82.95% (E. coli O157:H7) and 84.90% (S. aureus) reduction in comparison to hydrophobic nonporous silica. Additional bacterial proliferation studies revealed that bacterial anti- adhesive properties, not antibacterial effects, were responsible for the observed reductions. Overall, bacterial anti-adhesive properties as well as other distinctive properties such as superior thermal insulation, ultra-lightweight, large surface area, and biocompatibility make HNSA an attractive candidate as a novel food-contact surface.

AGFD 189 Bioavailability of cranberry flavonol glycosides and flavan-3-ols in healthy female adults Yifei Wang2, yifei@scarletmail.rutgers.edu, Ted Wilson3, Ajay P. Singh2, Nicholi Vorsa1. (1) Rutgers Univ, Chatsworth, New Jersey (2) Rutgers Univ., New Brunswick, New Jersey (3) Winona State Univ., Minnesota American cranberry (Vaccinium macrocarpon) contains various secondary plant metabolites including flavonoids with potential health benefit implications. Urinary excretion of cranberry flavonoids, in particular flavonol glycosides and flavan-3-ols was analyzed by UHPLC-ESI-MS/MS in health female adults at 90, 225, 360 minutes following cranberry juice ingestion. Flavan-3-ol monomers nor dimers were not detected among all subjects. The parent flavonol glycosides, myricetin-3-arabinoside, myricetin- 3-galactoside, quercetin-3-galactoside, quercetin-3-arabinoside and quercetin-3- rhamnoside were detected in urine. Most flavonols reached highest excretion levels at 1.5-2.5 hr post ingestion except quercetin-3-arabinoside (4.0 hr). High inter-individual variability was observed indicating gastric-intestinal variability for intestinal transporter, enzyme or microbiota activity. Quercetin-3-galactoside, as the most abundant cranberry flavonol (1.8 mg total ingested), exhibited the highest peak excretion levels (average: 1.3 ng/mg creatinine). Despite having lower juice concentrations, myricetin-3- arabinoside and quercetin-3-rhamnoside showed higher urinary excretion levels than myricetin-3-galactoside and quercetin-3-arabinoside respectively, suggesting the influence of sugar moiety on flavonol absorbance efficiency.

AGFD 190 Inhibitory effect of Gynostemma pentaphylla saponin on adipogenesis of 3T3-L1 cells through modulating Wnt/β-catenin pathway and cell cycle in mitotic clonal expansion Jie Liu1, liujiefantasy@163.com, Puyu Yang1, Haiming Shi1, Xiangjun Sun1, Liangli L. Yu1,2. (1) Shanghai Jiao Tong Univ., Shanghai, China (2) Univ of Maryland, College Park Gynostemma pentaphylla has been consumed as a popular functional tea worldwide. Its saponins were responsible for several beneficial effects including anti-obesity, however the underlying mechanisms and active components remain unclear. In this study, a novel saponin (JS) was isolated from tetraploid and characterized for its chemical structure. JS was aslo investigated for its inhibitory effect on adipocyte differentiation and the potential molecular mechanisms using 3T3-L1 murine pre-adipocytes. JS treatment down-regulated the expression of peroxisome proliferator-activated receptor g (PPARγ) and CCAAT/enhancer-binding protein a (C/EBPα) at both mRNA and protein levels. Detailed analysis proved that the inhibition was primarily limited to the early stage of adipocyte differentiation, where JS decreased the DNA-binding activity of C/EBPβ by blocking its phosphorylation. Furthermore, JS treatment increased expression of β-catenin and inhibited glycogen synthase kinase 3β activity modulating Wnt/β-catenin pathway. The anti-adipogenic effects of JS were significantly attenuated in β-catenin siRNA-transfected cells compared with the control.

AGFD 191 Development of graphene based room temperature gas sensors for agricultural applications Hyejin Park, hpark22@gmail.com. Materials Eng, Auburn Univ., Auburn, Alabama Recognition of food quality has been paid attention for several years to provide human with safe and healthy life. Among diverse characterization methods, non-destructive approaches have been employed such as optical analysis, surface-enhanced Raman spectroscopy, and bio-sensors1,2. These methods are primarily focused on detection of bacteria or cells to determine food contamination. However, these detection systems have challenges for rapid monitoring or continuous monitoring of food quality. Recently, development of electronic nose (e-nose) is suggested as a recognition system for agriculture product3. Detection of ethanol (C2H5OH), ammonia (NH3) and acetone ((CH3)2CO) gases is reported to be related to the conditions of food and agricultural product4,5. When considering food environment, room temperature gas detection is advantageous for quality inspection. Graphene based materials have been already demonstrated as an excellent material for room temperature gas detections6 but development of various kinds of graphene based composites can be necessary for e- nose system for realizing multiple sensing materials in a sensor prototype.

AGFD 192 Bioactive pectic oligosaccharides and obesity Arland T. Hotchkiss, arland.hotchkiss@ars.usda.gov. Errc, USDA ARS, Wyndmoor, Pennsylvania For 13 years, evidence has accumulated for the prebiotic properties of pectic oligosaccharides (POS). The original data was based on fluorescence in situ hybridization using 16s rRNA probes of fecal fermentations supplemented with oligosaccharides but we now have animal data that supports the bifidogenic activity of pectic oligosaccharides. Structure function studies have demonstrated that the arabino- and galacto-oligosaccharide pectin side chains are responsible for prebiotic properties in mixed batch fecal fermentations as well as the specific pectic domains responsible for blocking the adhesion and invasion of food-borne pathogens, antagonizing galectin-3 mediated tumor cell metastasis, reducing colon cancer cell proliferation, inducing colon cancer cell apoptosis and immunomodulatory activity. In human fecal fermentations, pectic oligosaccharides shifted the Firmicutes:Bacteriodetes ratio which has been observed in obese compared to non-obese humans and mice. Based on synbiotic growth and short chain fatty acid production under stressed conditions as well as other bioactive properties, pectic oligosaccharides could play a role in correcting dysbiosis associated with several chronic diseases. Therefore, POS may be very important in how the gut microbiome impacts our health and controls obesity.

AGFD 193 Prevention of metabolic diseases by HPMC, a non-fermentable fiber Maciej Turowski1, mturowski@dow.com, Wallace H. Yokoyama2. (1) Analytical Technology Center, Dow Chemical Co., Midland, Michigan (2) USDA ARS WRRL Berkeley, California Hydroxypropyl methylcellulose (HPMC) prevents increases in plasma cholesterol and triglycerides, body weight and liver weight gain, liver fat, abdominal fat and other characteristics associated with metabolic diseases in animal models fed high fat, hypercholesterolemic diets. Like other viscous polysaccharides such as beta-glucan and psyllium, high viscosity HPMC is more bioactive than low viscosity HPMC. Unlike cereal beta-glucans that promote the same health benefits, HPMC is not hydrolyzed by mammalian digestive enzymes nor fermented by gut bacteria. In several studies HPMC at 5% of diets containing 20% fat hamsters fed for 3 weeks lowered LDL cholesterol by 50%. HPMC feeding also decreased insulin resistance as determined by the euglycemic hyperinsulinemic clamp method. Liver cells show decreased fat vacuoles in HPMC fed animals compared to control. Addition of HPMC to common fast foods such as pizza and hamburger also resulted in reduction of metabolic syndrome characteristics. Bile acids, neutral sterols, and lipids increased in feces of animals fed HPMC. The expression of genes related to fat, cholesterol and bile acid metabolism in liver were also associated with HPMC intake.

AGFD 194 Impact of processing on physicochemical properties and nutritional function of dietary fibers: Balancing consumer taste and tangible health effects Nicolas Bordenave, Nicolas.Bordenave@pepsico.com. Nutrition Category R&D, PepsiCo , Leicester, United Kingdom As part of a healthy lifestyle and diet, consumption of soluble fibres such as oats β- glucans or citrus pectins can play a role in reducing the risk of obesity-related metabolic diseases (attenuation of glycaemic response to meals, satiating effects, production of anti-inflammatory short chain fatty acids through colonic fermentation, etc.). Nevertheless, dietary fibers are often embedded in complex food matrices that limit their potential efficacy and their impact on sensory properties of food products is often not acceptable for consumers. Here, we'll address some strategies to effectively enable preventive nutrition through the delivery of efficacious dietary fibers in palatable food products. Examples taken form the processing of oats and of orange fruits will be discussed, showing that contrary to widespread belief, processing of food ingredients can help maximize their health benefits and consumer acceptability. Nevertheless, these approaches raise new regulatory questions, so new analytical and regulatory challenges will also be discussed.

AGFD 195 Characteristics of EGCG loaded modified starch during digestion Yue Li, 53242326@qq.com, Fang Wang, Fang Zhong. Dept. of Food Science and Technology, Jiangnan Univ., Wuxi, China EGCG is widely used as a natural antioxidant in food, healthcare and cosmetics products. It has also been proved to slow down digestion rate of starches. In this study, the physically modified cassava starch with high water/oil adsorption capability was used to prepare starch-EGCG complex. The loading capacity of EGCG in the starch is about 100mg/g. The digestion properties of this EGCG loaded modified starch and the structure changes of the starch during digestion were studied by SEM, HPSEC-RI- MALLS and ion chromatogram. It indicated that EGCG greatly inhibited the enzymatic hydrolysis of starch during digestion. The resistant starch content of the modified starch was about 80% compared to that of 30% for the native cassava starch. Few starch granules were broken down after 120mins digestion compare to that of the native starch. The concentration of released glucose was 30.4, 58.4 and 79.3 mmol/L, respectively for the native starch after 20mins, 60mins and 120mins digestion, while the released glucose decreased to 14.9, 29.2 and 36.5 mmol/L, respectively for the modified starch. The digestion rate of the modified starch was around 22% during 120mins digestion. There was no significant change of the average molecular weight of the modified starch after 120mins digestion, but for the native starch it decreased from 1.2×107 Da to 1.4 ×106 Da. Analysis of amylopectin chain length distribution showed that EGCG slowed the digestion of starch mainly through restraining the hydrolysis of medium-length chains.

AGFD 196 Bioactive polysaccharides and gut microbiome Wallace H. Yokoyama2, wally@pw.usda.gov, Maciej Turowski1. (1) Analytical Technology Center, Dow Chemical Company, Midland, Michigan (2) USDA Ars Western Reg Rsrch Lab, Berkeley, California Many polysaccharides have shown the ability to reduce plasma cholesterol or postprandial glycemia. Viscosity in the small intestine seems to be required to slow glucose uptake. Cereal mixed linkage beta-glucans, psyllium, glucomannans, and other polysaccharides also seem to require higher molecular weight and viscosity to lower plasma cholesterol since oligosaccharides with the same chemistry are not bioactive. The production of short chain fatty acids by fermentation of these polysaccharides by gut microbes has been proposed as a mechanism for cholesterol lowering since SCFA reduce cholesterol synthesis in in vitro and in vivo. Bile acids, neutral sterols and other lipids are excreted through feces at higher levels by viscous polysaccharide feeding. Bile acid and cholesterol homeostasis requires increased cholesterol synthesis by the liver and uptake of cholesterol-rich LDL from the blood. Inflammation resulting from the passage of bacterial cell wall fragments from gram negative bacteria is thought to be the root cause of inflammation and associated metabolic diseases. HPMC, a nonfermentable, viscous polysaccharide and cholestyramine resin, a nonfermentable cationic polystyrene divinylenzene polymer, also have similar bioactive properties to fermentable polysaccharides. Recently, HPMC was shown to reduce weight gain and alter the pattern of bacteria families in mice on high fat diets.

AGFD 197 Immunochemical methods for rapid screening of (multi)mycotoxins Sarah De Saeger1, sarah.desaeger@ugent.be, Natalia Beloglazova1, Irina Y. Goryacheva2. (1) Lab of Food Analysis, Ghent Univ., Belgium (2) Chemistry Faculty, Dept. of General and Inorganic Chemistry, Saratov State Univ., Russian Federation Mycotoxin analytical methods include rapid screening and confirmation techniques in food and feed matrices. Furthermore, mycotoxin exposure can be determined both indirectly (based on the combination of chemical analysis of foodstuffs and food consumption data) as directly by the determination of exposure biomarkers, mycotoxin biotransformation products, in biological fluids, such as urine or blood. Nowadays the amount of publications covering rapid and sensitive on-site tests suitable for non-laboratory simultaneous determination of several analytes in various matrices is constantly rising. Development of both quantitative (ELISA, FLISA, immunosensors) and qualitative (lateral flow, membrane-based flow-through, column test) systems for (multi)mycotoxin detection is one of the fast-growing trends. Developments of various recognition elements as well as novel sensitive labels are currently ongoing in order to design a reliable and rapid test-system. Natural receptors such as antibodies are most widely used, but also their synthetic analogues and engineered elements can be employed. Working with complicated matrices or designing of a regenerable test-system can only be realized through the use of stable molecularly imprinted polymers (MIPs) or synthetic peptides. Whereas scFv and scAb fragments or aptamers cannot stand an aggressive environment, they provide high specificity, which is important for analysis of structurally-related compounds. Different labels can be used in immunochemical methods depending on the sample matrix, starting from enzymes (as the most sensitive label) to colloidal gold (widely used for rapid screening of biological fluids). Colloidal semiconductor nanocrystals or quantum dots (QDs) have emerged as a new class of fluorescent labels for biomedical diagnostics, molecular imaging and chemical analysis. The unique optical properties of QDs enable the simultaneous detection of multiple analytes on one single spot provided their conjugates are labeled with QDs which are fluorescent in different parts of the spectrum. Different strategies can be employed for QDs hydrophilization (such as encapsulation with amphiphilic polymer, silica and liposomes) performing different functionalities on the surface and therefore ensuring different conjugation techniques to synthesize QD-labeled immunoreagents. This presentation will give an insight into current trends and innovations in immunochemical methods for (multi)mycotoxin rapid screening.

AGFD 198 Application of nanobodies, sensors and other immunochemical techniques for the analysis of mycotoxins and other small molecules Candace S. Bever, crspier@ucdavis.edu, Shirley J. Gee, Bruce D. Hammock. Entomology & Nematology, Univ. of California Davis To protect human health and assure a safe food supply, monitoring food for contaminants is essential. In particular, mycotoxins are widely found and associated with known toxic effects. Changes in agricultural practices and implementation of global food monitoring regulations have resulted in decreased contamination. Nevertheless, mycotoxins and especially aflatoxin, continue to be a significant

problem. A number of commercially available immunoassays are widely used for monitoring because they are accurate, easy to use, rapid and low cost. We have been exploring the use of single domain heavy chain antibodies (VHH) as an alternative to the classic polyclonal or monoclonal antibodies used in commercial kits. These are a unique antibody found in camelids and sharks. The binding domain is smaller and less complex than in conventional antibodies making it more amenable to cloning techniques. The engineered antibodies, known as VHHs, have affinities to their antigens that are similar to the corresponding IgG. The VHHs have additional advantages such as thermal stability, stability toward chaotropic agents, improved water solubility and ease of genetic manipulation. These characteristics have made VHH a viable agent in clinical diagnostics and therapeutics. However, there have been few reports of the development of VHH for small molecules, in particular food contaminants. We have developed alpaca-derived VHH for mycotoxins, pesticides and flame retardants. Stringent panning strategies have led to selection of VHH that had similar sensitivity and cross reactivity patterns to the existing polyclonal and monoclonal antibody assays. The versatility of the VHH has been demonstrated by their use in classical ELISA as well as in a microfluidic biosensor driven by a smart phone and an impedance biosensor. We also demonstrated the ease of genetic manipulation by fusing the VHH to an enzyme resulting in a faster, simpler, one-step assay. Recombinant VHHs have proven to be an excellent alternative to existing antibody technology and should prove valuable for the next generation of mycotoxin immunoassay.

AGFD 199 Waveguide optical immunosensors for the simultaneous detection of melamine and aflatoxin M1 and kinetic analysis
Hongli Guo, hollymasten@163.com, Xiaohong Zhou, Hanchang Shi. School of Environment, Division of Water Environment, Beijing, China Mycotoxins and industrials chemical now commonly exist in milk such as aflatoxin M1 and melamine caused the potential health risks. Due to the widespread occurrence of melamine and aflatoxin M1in milk products, great efforts have been made to develop rapid, sensitive, on site and low-cost methods. The study presents an indirect competitive immunoassay through the multiplex planar waveguide fluorescence immunosensor for sensitive and simultaneous detection and quantification of aflatoxin M1 and melamine, also analysis the kinetic between the high-affinity antibody/antigen interactions by applying the principle of total internal reflect fluorescent. The chip immobilized by BSA-Mel was reusable and highly resistive to non-specific binding of proteins. The regeneration of the sensor allows more than 100 assay cycles within 20 minutes for each assay cycle. As a result, the kinetic rate constants (ka and kd) and affinity (KD) could be determined for each antibody interaction under identical conditions. Thus, it was confirmed that the application of waveguide optical immunosensors for protein interaction analysis is a promising and high throughput tool to obtain data around the binding behavior between antibodies and antigens.

AGFD 200 Development and evaluation of multi-mycotoxin analysis in foods by liquid chromatography-mass spectrometry (LC-MS/MS and LC-HRMS)
Kai Zhang1, kai.zhang@fda.hhs.gov, Jon W. Wong1, Chia-ding Liao2, Alexander J. Krynitsky1, Mary Trucksess1. (1) HFS-706, FDA/CFSAN, College Park, Maryland (2) Taiwan FDA, Taipei, Taiwan The US FDA has established regulatory limits (i.e., action, guidance, or advisory levels) for mycotoxins such as aflatoxins, deoxynivalenol, fumonisins and patulin in foods to ensure food safety. The FDA laboratories have been routinely screening for these mycotoxins in a variety of foods. The current mycotoxin methods (e.g, AOAC Official Methods) are only suited for the analysis of single or single class of mycotoxin using LC-UV/fluorescence technologies and additional confirmation is required for violative findings. As co-contamination of multiple mycotoxins in foods poses a serious threat to human health, the agency needs to monitor occurrence of mycotoxins in food products in a more time-efficient manner and prevent adulterated products from reaching consumers. With the advent of modern liquid chromatography and mass spectrometry (LC-MS) technologies, we have conducted a series of method development and validation studies to assess the performance of LC-MS/MS and LC-HRMS technologies and different sample preparation procedures including immunoaffinity column clean-up, dilute-and-shoot, staple isotope dilutions in food matrices such as cereals, nuts, dried fruits, rice, corn, wheat flour, milk, juices, and baby foods. The resulting multi-mycotoxin methods can identify and quantitate mycotoxins in different matrices using a single sample preparation procedure and LC-MS analysis, therefore improving the mycotoxin screening efficiency of the FDA laboratories in terms of identification, quantitation and sample throughput and enabling the agency to efficiently identify foods and feeds that may warrant regulatory actions.

AGFD 201 FDA regulatory program for mycotoxins in food
Henry Kim1,2, henry.kim@fda.hhs.gov. (1) FDA, College Park, Maryland, US (2) Center for Food Safety and Applied Nutrition, College Park, Maryland The US FDA (the agency) is the scientific regulatory agency responsible for the protection of human health with regards to foods in interstate commerce. FDA accomplishes this mission by enforcing applicable provisions of the Federal Food, Drug, and Cosmetic Act that provides the agency with the authority for regulating poisonous or deleterious substances, such as mycotoxins, in foods and to prohibit the entry of such foods into interstate commerce. For regulatory control of mycotoxins in foods, FDA monitors susceptible commodities for various mycotoxins, conducts science-based risk analysis, establishes regulatory limits, takes appropriate enforcement actions when warranted, and provides guidance to the food industry. FDA also works with other Federal and state agencies on food safety issues related to mycotoxins, and participates in the Codex Alimentarius Commission, which implements the Joint Food and Agriculture Organization/World Health Organization Food Standards Programme to protect the consumer and promote fair practices in food trade.

AGFD 202 Regulation of mycotoxins in Canada
Elizabeth Elliot, Luc Pelletier, Genevieve Bondy, bondygenevieve5@gmail.com. Food Directorate, Health Canada, Ottawa, Ontario The Food Directorate of Health Canada is the federal department that is primarily responsible for the regulation of mycotoxins in foods sold in Canada. It establishes policies and standards, and provides advice and information on the safety and nutritional value of food; it also administers the provisions of the Food and Drugs Act and Food and Drugs Regulations that relate to public health, safety and nutrition. The Food Directorate conducts toxicological research, generates food residue data, and assesses the human health risks associated with dietary exposure to mycotoxins in Canada. The Canadian Food Inspection Agency conducts regular surveillance of a variety of mycotoxins in the Canadian food supply and is responsible for enforcing the standards established by the Food Directorate. Such enforcement actions may involve recalling products from the Canadian marketplace, if deemed necessary based on the results of the Food Directorate's health risk assessment. The Canadian Grain Commission (CGC) is responsible for establishing and maintaining quality standards for Canadian grain through the administration of the Canada Grain Act and Regulations. The CGC also conducts research relating to the occurrence and analysis of fungi and associated mycotoxins in raw and processed grain and assesses Canadian grain for compliance with mycotoxin standards, both domestic and international. Health Canada uses a risk analysis framework consistent with that employed by other international regulatory organisations and is also an active participant in international risk assessment

and standard setting processes for mycotoxins in foods, in particular those of the Joint FAO/WHO Expert Committee on Food Additives (JECFA) and the Codex Alimentarius Commission.

AGFD 203 withdrawn

AGFD 204 Synthesis of 1,2,4,5-tetraoxanes derived from naphtaleneacetic acid with potential herbicide activity Thiago d. Silva1, silvatm@ufmg.br, Isabel Antolinez1, Almodevar Silva1, Luiz Barbosa1, John Boukouvalas2. (1) Chemistry, UFMG, Belo Horizonte, Minas Gerais, Brazil (2) Dept of Chemistry, Univ Laval, Quebec, Canada Nowadays, with the development of herbicide resistance by weeds the search for compounds with novel mechanisms of action has been more studied. In this context, natural compounds as a research model are a very useful strategy. Compounds with endoperoxides bonds in their structure are among the most studied. In this class of compounds, ozonides exhibit potent herbicidal activity. Furthermore, our research group discovered that tetraoxanes have also potent herbicide activity. The synthesis of this type of compound shows some problems. Therefore, the first aim of this project was to develop a low cost experimental process, reliable and reproducible, to allow the synthesis of 1,1-dihydroperoxides from the cyclohexanone and then convert this compound in symmetric (3) and asymmetric (4) tetraoxanes. Finally we aimed to synthesize a derivative of naphthaleneacetic acid containing this tetraoxane function to potentialize the herbicidal activity. Five catalysts were used in different concentrations: HCl, SnCl2, ZnCl2, ZnCl2-HCl, BF3.Et2O. The use of 10 mol% of BF3.Et2O resulted in obtaining dihydroperoxides in a higher yield, 77%. In the next step, the dihydroperoxide was used to obtain both the symmetrical (3) and asymmetrical (4) tetraoxanes. The same catalysts were used. The synthesis of symmetric tetraoxane (3) showed a higher yield using 100 mol% of ZnCl2- HCl (30%) and the synthesis of asymmetric tetraoxane (4) showed better yields using 50 mol% of H2SO4 (47%). By holding these results we tried to synthesize naphthaleneacetic acid derivate containing the tetraoxane function. In the final of this synthesis the compound 9 was obtained with a yield of 36%. The results of the herbicidal activity of compound 9 and some synthetic intermediates will be presented.

AGFD 205 Effect of organic matter on phosphorus recovery in dairy waste Amy Silchuk1, apsilchuk@ucdavis.edu, Sanjai J. Parikh2, Kate M. Scow2, Sungpyo Kim3. (1) UC Davis, Fair Oaks 2) Dept Land Air Water Resources, Univ. of California, Davis (3) Environmental Eng., Korea Univ., Sejong Phosphorus is one of the most important components of fertilizer and is a limiting resource for agriculture. Although high concentrations of phosphorus are found in dairy waste, the majority is not recovered. One potential way to recycle phosphorus from dairy waste is through the formation of solid struvite, which contains an equivalents amount of ammonium, magnesium and phosphorus and can be used as a valuable slow release fertilizer. However, a number of studies have shown that forming struvite from dairy waste is inefficient because of calcium competition during formation, high- suspended solid concentrations, and high ionic strength of the manure. Although several inhibitory effects of inorganic substance to struvite crystallization have been documented, few studies have been conducted to show that biomolecules, like cellulose and xylan, interferes with struvite crystallization. Cellulose and xylan are the most abundant organic matter in dairy waste and their interaction with the inorganic ions could result in poor struvite precipitation. Therefore, the objective of this study is to estimate the inhibitory effect of cellulose and xylan on struvite precipitation as a function of organic matter concentrations, pH, and Mg to P ratio. Preliminary results show that cellulose and xylan have different effects on the formation of struvite. For instance, the removal amount of NH4+ from the liquid phase was reduced by xylan concentration but not cellulose concentration. In contrast, an opposite trend occurred for the removal of P with cellulose and xylan when Mg was not sufficiently supplied. Characterization of the struvite and cellulose or xylan interactions by comparing the amount and size of crystalized struvite is ongoing.

AGFD 206 Understanding flavor in California almonds Suthawan C haroenprasert2, Guangwei Huang3, Philip Wylie1, Alyson E. Mitchell2, aemitchell@ucdavis.edu. (1) Agilent Technologies, Wilmington, DE (2) Food Science Technology, UC Davis (3) Almond Board of California, Modesto Raw almond flavor is a complex quality that includes both bitterness perception and aroma. Almonds are characterized into three taste phenotypes: non-bitter (sweet), semi- bitter (marzipan) and bitter. Bitterness is related to the inherent content of amygdalin (a cyanogenic glycoside) and the enzymatic hydrolysis rates of b-glycosidase; which hydrolyzes amygdalin into hydrogen cyanide and benzaldehyde. Benzaldehyde has a strong characteristic almond aroma and is the primary component of artificial almond aroma. To date, little is known about varietal differences in amygdalin, benzaldehyde and other aroma compounds in almonds. To address this, 14 key varieties of California almonds obtained from 3 different growing regions were evaluated. A UHPLC ESI- MS/MS method was developed to measure amygdalin. Initial studies indicate that amygdalin levels are relatively low in commercial varieties of California non-bitter almonds (2.16-157.44 mg/kg) as compared to bitter almonds (33,006.60-53,998.30 mg/kg). Volatile composition was measured (>30 compounds) using head space solid phase micro extraction (HS-SPME) GC/MS. PCA analysis demonstrates significant varietal differences with benzaldehyde predominating.

AGFD 207 Towards understanding induced resistance of ash (Fraxinus spp.) against emerald ash borer using proteomics and metabolomics Sourav Chakraborty1, scjob2008@gmail.com, Stephen O. Opiyo2, Amy L. Hill3, Don Cipollini4, Daniel A. Herms5, Pierluigi Bonello3. (1) Dept. of Chemistry and Biochemistry, Central Connecticut State Univ., New Britain (2) Molecular Cellular Imaging Center, The Ohio State Univ., Columbus (3) Plant Pathology, The Ohio State Univ., Columbus (4) Biological Sciences, Wright State Univ., Dayton, Ohio (5) Entomology, The Ohio State Univ., Wooster As sessile organisms, the survival of trees depends on their ability to defend themselves against attacks from insects and pathogens. Induced resistance in trees is triggered post-attack and is mostly associated with accumulation of phenolic compounds and/or defensive proteins. The invasive wood-boring beetle emerald ash borer (Agrilus planipennis Fairmaire) has killed millions of ash trees in the US and Canada and is a major threat to ash populations of North America. However, an Asian species, Manchurian ash (Fraxinus mandschurica Ruprecht) is resistant to this beetle by virtue of their coevolutionary history. In order to understand the molecular mechanisms of induced resistance of Manchurian ash, we performed a series of studies using comparative metabolomic and proteomic approaches. Phenolic metabolites extracted in methanol were quantitated using a combination of liquid chromatography – photodiodearray detection and tandem mass spectrometry (LC-PDA-MS/MS). Proteins were precipitated, cleaned and subjected to difference gel electrophoresis (2D-DIGE) for quantitation. In-gel digestion was performed using enzyme trypsin and the resultant peptides were identified via homologue-based search against green plant database (Viridiplantae) using MASCOT search engine. A total of 1,900 proteins were putatively identified from LC-MS/MS. Following elicitation by natural insect attack, a stringent data reduction

strategy was employed to create a more targeted protein pool. Principal component analysis and partial least square discriminant analysis identified one key metabolomic biomarker and fourteen proteins of interest.

AGFD 208 Formation of 3-MCPD fatty acid esters from monostearin and thermal decomposition of 3-MCPD mono-fatty acid ester
Yue Zhao2, zhaoyue1992@sjtu.edu.cn, Yaqiong Zhang2, Zhongfei Zhang2, Boyan Gao2,1, Haiming Shi2, Liangli L. Yu1. (1) Dept. of Nutrition and Food Science, Univ. of Maryland, College Park (2) inst. of Food and Nutraceutical Science, Shanghai Jiao Tong Univ., Shanghai, China 3-MCPD esters are a group of food processing induced toxicants. Formation of 3-MCPD esters was investigated using monostearin under a high temperature and low moisture condition. Electron spin resonance (ESR), quadrupole-time of flight (Q-TOF) MS and MS/MS were performed to examine the hypothesis of a free radical mediated formation mechanism. Different metallic chloride, including KCl, CaCl2, NaCl, MgCl2, AlCl3, CuCl2, MnCl2, SnCl2, ZnCl2 and FeCl3, were selected as chlorine donors to evaluate the effects of different cations on 3-MCPD esters and glycidyl ester formation at 120°C and 240°C using UPLC-Q-TOF MS measurements. Our results indicated iron(III) could catalyze the formation of 3-MCPD mono- and di-ester from MSG. In addition, selected factors were evaluated for their effects on thermal decomposition of 3-MCPD mono-esters. The results of this study may be used in reducing the level of 3-MCPD esters in vegetable oil and related food products.

AGFD 209 Tuning mechanical, barrier and thermal properties of poly(lactic acid) using polymorphic cellulose nanocrystals
Prodyut Dhar1, prodyut@iitg.ac.in, Debashish Tarafdar2,1, Amit Kumar2,1, Vimal Katiyar1. (1) Chemical Engineering, Indian Inst. of Technology Guwahati, Assam (2) Chemical Engineering, Indian Inst. of Technology Guwahati, Assam This paper reports the fabrication of three different cellulose nanocrystals (CNCs) polymorphs through alkali treatment followed by acid hydrolysis of raw bamboo pulp. The effect of cellulose polymorphism on the morphology, crystal structure, functionality and thermal stability of fabricated CNCs (namely CNC I, CNC II and CNC:I→II i.e. CNC II from cellulose I) were studied. Morphological studies showed that CNC polymorphs had needle, ribbon and rice-grain like dimensions with aspect ratio of~33, ~25 and ~6 for CNC I, CNC II and CNC:I→II respectively. Thermal property studies showed that onset degradation temperature of CNC polymorphs varied drastically by 176, 226 and 191C for CNC I, CNC II and CNC:I→II respectively. Therefore, the effect of three CNC polymorphs on reinforcement efficiency of poly(lactic acid) matrix and its influence on structural-property relationship of fabricated nanocomposites were evaluated. CNC polymorphs differ significantly in their reinforcement capability and ability to form percolated network which depends on morphology, aspect ratio and the degree of hydrogen bonding interaction (FH-CO) values between the PLA matrix with different CNC polymorphs. At 2 wt.% CNC loading, PLA/CNC polymorph nanocomposites showed significantly altered young's modulus of ~0.6GPa , ~1.1GPa and 0.9GPa for CNC I, CNCII & CNC: I→II, respectively. This is probably due to high hydroxyl functionality of CNC II and its ability to form entangled hydrogen bonded network with the PLA matrix, leads to improvement in both mechanical and barrier properties. Mechanical modelling with Halpin Kardos, Cox–Krenchel and Ouali models also showed good agreement between theoretical and experimental modulus, albeit at higher aspect ratio. The onset degradation temperature also showed significant variation of 310, 330 and 280C for the PLA/CNC I,CNC II and CNC:I→II nanocomposites respectively. The fiber entangled network in CNC II, also helped in improving the oxygen and water vapor barrier properties of PLA/CNC nanocomposites by ~80 and ~51% respectively. The activation energy for permeation were calculated from Arrhenius equation, which shows order of CNC II > CNC: I→II > CNC I . Therefore, this study provides an insight towards selecting appropriate CNC polymorphs and its tuning during industrial scale processing of CNC reinforced biopolymer nanocomposites for high performance applications

AGFD 210 When in silico meets in vitro: Molecular basis of function of an anion-permeable efflux transporter from barley (Hordeum vulgare L.)
Abhishek Singh1, asingh7@ncsu.edu, Yagnesh Nagarajan3, Maria Hrmova3, Yaroslava G. Yingling2. (1) North Carolina State Univ, Raleigh (2) Materials Science and Engineering, North Carolina State Univ., Raleigh (3) Univ. of Adelaide, Glen Osmond, South Australia High concentrations of boric acid in soils adversely affect cereal crop production worldwide. Solution to such problem lies in developing variants of transport proteins that can improve plant tolerance to high soil boric acid. However, the underlying molecular mechanisms of such transport proteins are largely unknown. This research work addresses such mechanisms using first computational model for a barley efflux transport protein HvBot1, which we corroborated by biochemical, biophysical and electrophysiology measurements. The challenges in computational modeling typically include predictions of a tertiary structure in the absence of prior experimental information, obtainable by X-ray crystallography, electron microscopy or NMR spectroscopy. After in silico refinement of a wild type tertiary structure, we performed structural mutations to study relative ion permeation dynamics. We correlated ion residence time inside the protein to its transport capability and established the effect of mutations on the mobility of ions, and how this affected resident ion hydration states. A profile of biologically relevant ion channels inside protein was also calculated. The need for such multi-scale modeling is to provide molecular insights and solutions to develop genetically superior cereal crops that will ensure sustainable food production in diverse soil environments. Based on our findings, we suggest that HvBot1 be designated as a channel-like Na+-dependent anion transporter with a high affinity for borate anions.

AGFD CORNUCOPIA

CORNUCOPIA

Schedule of AGFD Technical, Business, Planning, and Social Activities

Sun 12:00-1:00pm	Special Committee	US Grant Hotel Palm Court
Sun 5:00-8:00pm	Executive Committee	US Grant Hotel Palm Court
Mon 12:00-1:00pm	Future Programs	US Grant Hotel Crystal Ballroom
Mon 8:00-10:00pm	Sci-Mix	Convention Center Halls D/E
Tues 11:30 am	Business Meeting	US Grant Hotel Crystal Ballroom
Tues 12:40pm	AGFD Poster Session	Convention Center Halls B/C
Tues 2:00-4:30pm	Caribbean Cooking Competition	San Diego Wine & Culinary Center
Tues 6:00-8:00pm	AGFD Chair's Reception	San Diego Wine & Culinary Center