CORNUCOPIA

including AGFD abstracts for the
252nd American Chemical Society National Meeting
August 21 - 25, 2016
in
PHILADELPHIA

NAVINDRA SEERAM, Program Chair

Attend AGFD oral technical sessions and posters at the Philadelphia Convention Center

Join the AGFD Awards Banquet
Tuesday, August 23, 5:30-8:30 pm at Drexel University Academic Bistro 101 N. 33rd St., 6th floor (directions below)

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Directions to Banquet from Convention Center proceed west on Arch St, then south (left) on N. 15th St, then west (right) on Market St*, over the Schuylkill River, then north (right) on S. 33rd St, continue 2 blocks to # 101. (1.9 mi. total)
*or take the Market-Frankford line west (towards 69th St) from 15th and Market, 2 stops to 34th and Market.

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 privilege and honor to serve the Division of Agricultural and Food Chemistry (AGFD) as the 2016 Chair. The 2016 AGFD program for the Spring ACS Meeting in San Diego was another successful event with great organization and attendance by many active AGFD members from around the world.

The AGFD program in San Diego included 13 symposia, 26 sessions, 210 papers, comprised of 150 oral presentations and 60 posters. Overall the meeting was another demonstration of AGFD leadership with numerous technical and networking opportunities. AGFD also supported the ACS President’s Task Force on Employment by communicating AGFD opportunities and advances in future chemistry.

Fourteen members of the AGFD Executive Committee participated in a Strategic Planning Retreat run by ACS on April 30 and May 1, 2016 in Washington, DC. The Society encourages its divisions to hold retreats periodically, and our last retreat was held in 2008. Special thanks go to Lauren Jackson for leading the organization of the meeting. A new vision statement for AGFD was established: Enhance quality of life by advocating safe, nutritious and sustainable food and agricultural supplies that meet global challenges, and a new mission statement was produced: Lead and foster a diverse community to promote and advance agricultural and food chemistry research, education, outreach, and communication. Aligning with the ACS strategic plan, three goals were developed for 2016-2021: 1) Continue and expand high quality technical offerings, 2) increase engagement of existing and new members in AGFD activities by 10% over the next 3-5 years, and 3) increase stakeholder engagement by expanding cooperative programming and other offerings with outside organizations – internal and external to ACS.

The 2016 Award for the Advancement of Application of Agricultural and Food Chemistry was won by Zen-Yu Chen of the Chinese University of Hong Kong, who is honored at an AGFD Division Award Symposium on Tuesday. Shi Feng received the Roy Teranishi Graduate Fellowship in Food Chemistry. Juhong Chen won the Withycombe-Charalambous Graduate Research Award and Elvira Sukamtoh won the Undergraduate Research Award. May Berenbaum was awarded the Sterling Hendricks Award. Congratulations to Susan Ebeler, Qingrong Huang, Peter Winterhalter, and Wallace Yokoyama for becoming the 2016 AGFD Fellow Awardees. Lauren Jackson and Kim Morehouse were named to the 2016 class of ACS Fellows.

Leading scientists developed 16 symposia for the Fall Meeting, including the Young Scientist Award, AGFD Division Award, Sterling Hendricks Memorial Lectureship, and an additional 31 sessions with 295 abstracts.

During this Fall Meeting, the Division will host an Awards Banquet at Drexel University Academic Bistro, 101 N. 33rd St., 6th floor, Philadelphia, PA 19104 at 5:30-8:30 PM. Join us for this and other AGFD events to meet people from across industry, academia, and government with diverse interests in AGFD research and outreach.

I thank the numerous volunteers who have given me so much support. I especially thank past chair, Kathryn Deibler; program chair, Navindra Seeram; and strategic planning chair, Lauren Jackson, for their invaluable leadership and assistance. Special thanks are extended to Michael Appell, Mike Morello, Alyson Mitchell, Steve Toth, Michael Qian, John Finley, Agnes Rimando, Neil Da Costa, and many others, for their volunteered contributions in making the division a success. I give special thanks to Michael Tunick who organized the Division Reception and Banquet at this Fall Meeting. Thank you all for your support of the division.

Bosoon Park    bosoon.park@ars.usda.gov
FUTURE PROGRAMS

SAN FRANCISCO  April 2-6, 2017
Chemistry of Tree Nuts  Alyson Mitchell  UC Davis  aemitchell@ucdavis.edu

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

Chemistry and Biological Activities of Phenolic Compounds from Fruits and Vegetables  G. K. Jayaprakasha Texas A&M Univ.  gkjp@tamu.edu  Bhimu Patil Texas A&M Univ.  b-patil@tamu.edu  Giuseppe Gattuso Univ. di Messina  Messina, Italy  ghattuso@unime.it

Chemistry and Biological Effects of Maple Food Products  Navindra Seeram  Univ. of Rhode Island  nseeram@uri.edu  Hang Ma  Univ. of Rhode Island  hang_ma@uri.edu

Chemistry of Korean Foods and Beverages  Choon Ho Do  National Fisheries R&D Inst.  choondo@sunchon.ac.kr  Agnes Rimando  USDA ARS  agnes.rimando@ars.usda.gov  Kwang-Geun Lee  Dongguk Univ.  kwglee@dongguk.edu

Synthetic Biology in Food and Agriculture  Joey Talbert  Iowa State  jotalber@iastate.edu  Nitin Nitin  UC Davis  nnitin@ucdavis.edu  Rashmi Tiwari  PepsiCo  rashmi.tiwari@pepsico.com

Advances in Nanotechnology for Food and Agriculture  Mike Appell  USDA ARS, Michael.Appell@ars.usda.gov  Bossoon Park  USDA ARS  bossoon.park@ars.usda.gov

General Papers and General Posters  Navindra Seeram  Univ. of Rhode Island  nseeram@uri.edu

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

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

Artisanal Foods  Mike Tunick  USDA ARS  michael.tunick@ars.usda.gov  Andrew Waterhouse  UC Davis  alwaterhouse@ucdavis.edu

Water as a Food Component  John Finley  Louisiana State Univ.  jfinle5@lsu.edu

Coffee and Cocoa Products  Michael Qian  Oregon State Univ.  michael.qian@oregonstate.edu  Michael Granvogl  Technical Univ. of Munich  michael.granvogl@tum.de

Chemistry of Cellulosic Natural Products  SeChin Chang  USDA ARS  sechin.chang@ars.usda.gov

Food Packaging Materials  John Finley  Louisiana State Univ.  jfinle5@lsu.edu  Michael Morello  PepsiCo  mike.morello@pepsico.com

Structure and Chemistry of Proteins of Food Safety and Food Manufacturing Interest  Yuzhu Zhang  USDA ARS  yuzhu.zhang@ars.usda.gov

The Bliss Point: Food Satiety and Food Mood Effects  Indika Edirisinghe  IIT  iedirisi@iit.edu  Britt Burton-Freeman  IIT  bburton@iit.edu

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

WASHINGTON DC  August 20-24, 2017
Food Additives and Packaging II  Vanee Komolprasert  FDA/CFSAN  vanee.komolprasert@fda.hhs.gov  LaShonda T. Cureton  FDA/CFSAN  lashonda.cureton@fda.hhs.gov  Diana Doell  FDA/CFSAN  diana.doell@fda.hhs.gov  Romina Shah  FDA/CFSAN  romina.shah@fda.hhs.gov

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

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Non-targeted Detection Approaches for Food Quality and Safety Assurance  Liangli (Lucy) Lu  U. Maryland  lyu5@umd.edu

Young Scientist Award Symposium  Kathryn Deibler  Pfizer  kdd3@cornell.edu  Charles Brine  Princeton  ChitoCare LLC  brinec11@verizon.net

AGFD Division Award Symposium  Navindra Seeram  Univ. of Rhode Island  nseeram@uri.edu

Sterling Hendricks Memorial Lectureship  (co-sponsored by AGRO/AGFD)  Michael H. Tunick  USDA ARS  michael.tunick@ars.usda.gov  Kim Kaplan, USDA ARS  kim.kaplan@ars.usda.gov

Kenneth A. Spencer Award Symposium  (co-sponsored by AGRO/AGFD)  Eckhard Hellmuth  UMKC  hellmutc@umkc.edu

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

Advances in Flavor Analysis  Michael Qian  Oregon State Univ.  michael.qian@oregonstate.edu  Tony Shao  PepsiCo  Tony.Shao@pepsico.com

Advancing Analytical Methods in Food Forensics & Authentication  Lauren Jackson  FDA  lauren.jackson@fda.hhs.gov  Alyson Mitchell, Univ. of California Davis  aemitchell@ucdavis.edu

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

Clean Labels: Alternatives to Synthetic Ingredients  Keith Cadwallader  University of Illinois at Urbana-Champaign  cadwlldr@illinois.edu

From Fermentation to Fume Hood: The Chemistry of Wine  Gavin Sacks  Cornell Univ.  gls9@cornell.edu  Dimitra Capone, Australian Wine Research Institute  dimitra.capone@awri.com.au

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

NEW ORLEANS  March 18-22, 2018

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

Metabolomics Diet & Effects  Sourav Chakraborty  Central CT State Univ.  schakraborty@ccsu.edu

Chemistry of Sex  Alyson Mitchell  UC Davis  aemitchell@ucdavis.edu  Mike Tunick, USDA ARS  michael.tunick@ars.usda.gov  Kathryn Deibler  Pfizer  kdd3@cornell.edu  John Finley, Louisiana State Univ.  Jfinle5@lsu.edu  Gavin Sacks  Cornell Univ.  gls9@cornell.edu  Steven Toth  International Flavors and Fragrances  stephen.toth@iff.com

(C3) Culinary Competition  Gavin Sacks  Cornell Univ.  gls9@cornell.edu  Justin Miller  Hobart & William Smith Colleges  jsmiller@hws.edu  Donnie Golden  Fresno State  dgolden@csufresno.edu

Chemistry of Spirits  Mike Qian  Oregon State Univ.  michael.qian@oregonstate.edu  Michael Granvogl  Technical Univ. of Munich  michael.granvogl@tum.de  Keith Cadwallader  University of Illinois at Urbana-Champaign  cadwlldr@illinois.edu

Phosphates from the Farm to the Dead Zone  John Finley  Louisiana State University  Jfinle5@lsu.edu

International Student Symposium  Philipp Schmidberger Philipp  Technical Univ. of Munich  Schmidberger@lrz.tu-muenchen.de  Roberta Tardugno  Univ. of Modena and Reggio Emilia  roberta.tardugno@unimore.it

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In Memoriam – Marshall Phillips

Marshall Phillips, a Fellow of the ACS with over 50 years of service to the Society passed away on March 25, 2016. Marshall was born December 1, 1932, in Yankton, South Dakota and grew up on a farm in Crofton, Nebraska. After 2 years in the Army he earned his B.A. in Biology at Yankton College, his M.A. in Organic Chemistry at the Univ. of South Dakota and his Ph.D. in Biochemistry at the Univ. of Kansas. He became a research chemist as part of the USDA at the National Animal Disease Control Lab an Ames, Iowa. With his late wife Karen, he had 2 daughters, Tacy and Dori. In addition to his Fellow status, he held many ACS positions including Chair of the Agricultural and Food Chemistry Division and was awarded several distinguished service commendations. He served as Journal of Agricultural and Food Chemistry Associate Editor for over 20 years. After the death of his wife Karen, he moved to Pennsylvania and retired, taking on duties as grandfather to grandchildren, Jack and Hannah. He married Dorothy Upchurch in 1988 and was active in the Westminster Presbyterian Church of West Chester, Pennsylvania. He remained active with family and friends, with his hobbies – photography, travel, gardening, writing (example below, from Perspectives in Biology and Medicine, Spring 1973), drawing, collecting coins, seashells and oyster plates. He was an excellent cook, sharing his creations with family and friends. He loved his bulldogs, both named Winston. He had a fine wit and sense of humor; a ready conversationalist with a gracious, easy manner that was trademark Marshall. One of a kind. His friends at AGFD miss him and extend condolences to his family.

(Thx to Cynthia Mussinan for help w/this Memoriam)

Fishing

Those that fish for men,
Serve Themselves.

Those that fish for wisdom,
Serve Mankind.

Those that do not fish at all,
Serve neither themselves nor mankind – not even God.
PHILLY PHUN

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

ACROSS
1 1977 Steely Dan album
4 cool – a cucumber
6 some business leaders
10 first 3 of 26
13 historic cracked chimer
16 --- thermal or --- metric
17 wild mountain goat
18 British poet -. Housman
19 Easter ---- or Navy ----
21 ‘attention!’ or At. No. 42
22 exactly suitable
23 not he or she but --
24 country-named element
25 cheer the ----------- blue
31 glow-in-the-dark element
32 PBS science show
33 common sign on diners
34 where to find 13 across
35 excellent tennis servers
37 law school entry hurdle
39 magazine for 6 Across
41 -- 47
42 element used in 33Across
43 J. Goldblum flick The ---

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1 ‘The Greatest’ boxer
2 triangular sail
3 he’s on the US $5 bill
4 laser and lighting gas
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6 trucker radio
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8 bull ring exclamation
9 killed
10 -- & Food division
11 he’s on the US $100 bill
12 sports car by Carroll Shelby
14 former spouse
15 Himalayan bigfoot
20 Ford model starting in 1965
22 – shucks!
25 the Italian Stallion
26 first lady
27 way to mend a sock
28 Oh, mommy. ------- story!
29 NOLA, a.k.a. ‘The Big ----’
30 No pushing! One --- time!
31 second part
32 Mumbai flat bread
34 some call March 14 ‘-- Day’
AGFD DIVISION MEMBERSHIP APPLICATION

The Agricultural and Food Chemistry Division (AGFD) of the American Chemical Society (ACS) is a non-profit organization dedicated to the technical advancement of all aspects of agricultural and food chemistry. AGFD encourages technical advancement in the field by -
- organizing symposia/workshops on agricultural/food chemistry at ACS national meetings and other venues
- publishing proceedings of AGFD symposia
- publishing the Cornucopia newsletter
- 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 2700 members of AGFD. At ACS National Meetings you can meet and discuss division activities at the AGFD Information table located near the AGFD technical session rooms. Join us via the membership application form (below) or 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 (800)333-9511 in US. Payment by Visa/Master Card or AmEx.

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Be cool JOIN AGFD

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 55391
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
efreyenterprise@gmail.com
203-918-6007

Councilors - Represent Division for 3 years on ACS council.
Michael Appell (thru ’16)
michael.appell@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)
cadwildr@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 Sukan (thru ’18)
mlsukan@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@Krftfoods.com
Secretary Elizabeth Kreger
Ekreger@wildflavors.com

Functional Foods & Natural Products
Chair - Steve Talcott
stalcott@tamu.edu
Chair-Elect Mathias Sukan
mathias.sukan@pfizer.com
Vice Chair Kwang-Geun Lee,
kwlege@dongyangku.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
nitin@ucdavis.edu

Nutrition
Chair Anne Kurilich
anne.kurilich@meccain.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 Granvogel
michael.granvogel@tum.de
ELECTION OF DIVISION COUNCILORS

If you are a full member of AGFD, please vote by marking the ballot below, signing in the space provided, and printing your name legibly beneath the signature. Fold the page on the dotted lines so that the ballot is on the inside and the mailing address on the outside. Tape or a staple the open edges, affix postage and mail. Ballots must be received by November 1, 2016. After your membership is verified, the portion of the form with your signature and name will be removed prior to opening and counting the ballots. Thank you for exercising your democratic franchise.

Vote for 2 Alternate Councilors for the 2017 - 2019 term (or write in your own candidate)

[ ] Lauren Jackson
[ ] Alyson Mitchell

or write in [ ] ________________________________

and

Vote for 1 Councilor for the 2017 - 2019 term (or write in your own candidate)

[ ] Michael Appell

or write in [ ] ________________________________

------------------------------ fold down & tape -----------------------------

member signature ________________________

member printed name ____________________

------------------------------- affix stamp ----------------------------------

to Michael H. Tunick
USDA-ERRC
600 E. Mermaid Lane
Wyndmoor PA 19038
Executive Committee Meeting Minutes  
Sunday, March 13, 2016  US Grant Hotel, San Diego, CA  
*Takes place at each ACS National Meeting*

Attendees: Michael Appell, Keith Cadwallader, Kathryn Deibler, John Finley, Michael Granvogl, Lauren Jackson, Alyson Mitchell, Michael Morello, Bossoon Park, Michael Qian, Agnes Rimando, Gavin Sacks, Navindra Seeram, Tony Shao, Stephen Toth, Michael Tunick

AGFD Chair Bosoon Park called the meeting to order at 5:03 p.m. Those present introduced themselves.

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

Stephen Toth gave the Treasurer’s Report. AGFD has not yet received the $11,500 dues and $33,600 allotment from ACS. $15,000 in industry donations were received in 2015. The investments gained money in 2015 and have lost so far in 2016. The total assets for the division are $589,800. $39,780 was spent at the Boston meeting. Mike Morello pointed out ACS pays us for the attendance at the two highest-attended oral sessions for each half-day of the national meeting, and Mike Appell said that they pay us for each member attending the national meeting along with each poster presented. By programming a symposium within the meeting theme and cosponsoring it with another division, both divisions receive attendance credit if the session is among the top two in audience size.

Bosoon Park reported that the San Diego AGFD Program has 13 symposia, 26 sessions, and 210 oral and poster presentations. There are 60 posters, 22 of which are also in Sci-Mix. Gavin Sacks said that 12 students from Cal Poly, Radford, and University of the West Indies will participate in the Caribbean Cooking Competition. Mike Appell and Bosoon Park will display an AGFD poster for the Presidential Task Force on Employment and at Sci-Mix. Navindra Seeram reported that the Philadelphia meeting has 19 sessions scheduled and proposed a $30,000 budget; the motion passed. He also said that the San Francisco meeting in March 2017 (theme: Advanced Materials Technologies, Systems, and Processes) has 9 symposia scheduled so far, along with general and poster sessions. Mike Qian and Steve Toth reported that a new International Flavor and Fragrance Conference will be held in different countries, starting with Columbia in May 2017. Gary Reineccius and Fereidoon Shahidi are also behind this effort, and Mike Qian will write an Innovative Projects Grant proposal for it.

Bosoon Park reported for Joey Talbert, Biotechnology Chair, and Indika Edirisinghe, Nutrition Chair, that their Subdivisions are planning symposia. Food Safety Past Chair Lauren Jackson reported that they are targeting one symposium annually.

Mike Appell, John Finley, Mike Morello, and Agnes Rimando gave the Councilor’s Report. Mike Appell is now on the Divisional Activities Committee (DAC). The Council will be voting on two presidential candidates and recommendations for membership dues. About 30% of ACS members belong to a division. ACS wants each division to have a Strategic Planning Committee. Navindra Seeram is doing an ACS Pod Short for AGFD. Agnes Rimando is on the International Activities Committee, which put out a white paper with DAC in 2015. There are 16 international chapters, and partnership with divisions is encouraged. Three applications for chapters, two from China and one from Iraq, have been received. John Finley, who is on the Committee on Science and the Multidisciplinary Program Planning Group, said that the theme of the August 2017 meeting in Washington, DC will be Chemistry’s Impact on the Global Economy, and that the March 2018 theme for the New Orleans meeting will deal with food, energy, and water. He recommended that AGFD participate in both. He would also like us to reach out to liberal arts colleges without formal food science programs. Mike Morello is now on the Technical Programming Subcommittee of the Committee on Meetings & Expositions. They would like to get students involved, have divisional
representatives at CHED posters, and have posters describing divisions at Sci-Mix.

Mike Morello is the new Awards Committee Chair. The Award for the Advancement of Application of Agricultural and Food Chemistry has been won by Zhen-Yu Chen, Chinese University of Hong Kong. Chi-Tang Ho sent a report saying that the Teranishi Fellowship award went to Shi Feng, University of Florida. Kathryn Deibler reported that the Undergraduate Student Award and the Withycombe-Charalambous Graduate Student Award winners will be announced at the Chair’s Reception on Tuesday. (The Undergraduate winner was Elvira Sukamtoh and the Graduate winner was Juhong Chen, both from University of Massachusetts, Amherst. Jarrod Creameans from Arkansas State finished second in the Undergraduate competition). Mike Tunick reported that the Sterling Hendricks Award will go to May Berenbaum, University of Illinois, Urbana-Champaign. Mike Appell reported that the Kenneth Spencer Award was won by Agnes Rimando. A discussion about nominations for ACS Fellow Awards followed. A division can nominate up to double its number of Councilors, which entitles AGFD to 8 nominees. About 35% of nominees are selected. The division plans to nominate two people.

Cornucopia editor Carl Frey sent a report saying that we had to change printers, and we have a faster turnaround now. The last issue cost $950 to print and $471 to ship to San Diego. The number of leftover copies will be checked toward the end of the meeting to see if we are making and shipping too many.

In Hospitality/Public Relations, Bosoon Park reported that Charlie Brine and Gavin Sacks organized the reception for this meeting at the San Diego Wine and Culinary Event Center.

Membership Chair Lucy Yu said that AGFD had 2634 members as of January 31. Twenty-two of them will receive 25-year pins.

Kathryn Deibler gave the Nominations report. The slate of officers consists of Navindra Seeram, Chair, Brian Guthrie, Chair-Elect, Xuetong Fan, Vice-Chair, with Michael Tunick as Secretary and Stephen Toth as Treasurer. Mike Appell and Alyson Mitchell will again run as Councilor and Alternate Councilor, respectively. The candidate for the other Alternate Councilor position will be determined.

Bosoon Park gave the Journal report sent in by Editor-in-Chief Thomas Hofmann. There were 1172 papers published in 2015, almost 2 million article requests, and more than 73,000 citations of papers. One person left the Editorial Board and two new members were added. The Excellence in reviewing Award began in 2015, with ten awards being handed out.

Mike Appell gave a report about the Communications Committee. He and Kathryn are operating the website, Mike Tunick is handling the Facebook page, Neil DaCosta is doing the LinkedIn site, and Alyson Mitchell is sending e-mail blasts each month. She needs a two-day turnaround time for these messages.

Lauren Jackson reported that 15 people will participate in the AGFD Strategic Planning session in Washington, DC on April 30-May 1. Twelve of them had a preliminary meeting in the afternoon and several issues were discussed. An online survey of participants and a membership survey will be sent around April 4.

In New Business, Mike Morello proposed that the Executive Committee meeting be moved to Monday evening at 5 p.m., with the AGFD poster session to be held on Sunday evening from 7 to 9. The posters would allow attendees a chance to network over light refreshments. The motion was approved. He also moved to fund this reception with an estimated budget of $5000, which was also approved.

Mike Tunick pointed out that Division dues had to be set for 2017. The dues will remain the same, at $10 for ACS members and $15 for non-members.

The meeting adjourned at 7:30 p.m. Submitted by Michael Tunick, AGFD Secretary
The 2016 Award for the Advancement of Application of Agricultural and Food Chemistry will be presented to Zen-Yu Chen of the Chinese University of Hong Kong at the AGFD Award Banquet on Tuesday. Shi Feng received the Roy Teranishi Graduate Fellowship in Food Chemistry. Juhong Chen won the Withycombe Charalambs Graduate Research Award and Elvira Sukamtoh won the Undergraduate Research Award. May Berenbaum won the Sterling Hendricks Award. Susan Ebeler, Qingsrong Huang, Peter Winterhalter, and Wallace Yokoyama become 2016 AGFD Fellows. Lauren Jackson and Kim Morehouse were named to the 2016 class of ACS Fellows. Congratulations to all.

**AWARD NEWS**

**Schedule of AGFD Technical Sessions**

**SUNDAY MORNING**  August 21  Pennsylvania Convention Center Room 110A  Section A

**Recent Advances in Functional Biopolymers**

Y. Ito, L. S. Liu, **Organizers, Presiding**

8:00 Introductory Remarks.
8:05 1. Protein engineering using bioorthogonal and combinatorial chemistry. Y. Ito
9:35 Intermission.
11:20 7. Establishing a working intestinal microbiota community in multi-phase structure from biopolymers. L.S. Liu, J. Firmman, P.M. Tomasula
11:50 Concluding Remarks.

**General Papers**

Pennsylvania Convention Center Room 110B  Section B
N. P. Seeram, **Organizer, Presiding** W. Liu, H. Ma, **Presiding**
8:00 Introductory Remarks.
8:05 8. Triterpenoids from the Chinese hawthorn (Crataegus cuneata) fruits: Extraction, structure, quantification, and bioactivity. T. Yuan
8:30 9. Withdrawn.
8:55 10. Alkanal suppression of the enzyme tyrosinase. A. Murray, H. Satooka, K. Shimizu, W. Chavasiri, I. Kubo
9:45 Intermission.
11:15 15. Inhibitory effects of a phenylacetaldehyde-flavonoid adduct, 6-(3-phenylethynyl)naringenin, on human colon cancer cells. Y. Zhao, M. Wang
11:40 Concluding Remarks.

**SUNDAY AFTERNOON**  August 21  Pennsylvania Convention Center Room 110A  Section A

**Flavor Stability: Chemical Changes in Flavor Molecules, Flavor-Food Matrix Interactions, Flavor Encapsulation**

R. J. McGregor, M. C. Qian, **Organizers, Presiding**
1:00 Introductory Remarks.
1:30 17. Withdrawn
1:55 18. Assuring accuracy in the quantitation of the unstable odorant 2-acetyl-1-pyrroline in aromatic rice. K.R. Cadwallader, Y. Yin, B. Hausch, F. Chen
2:20 19. Odor active compounds and their chiral compositions in Bluecrop and Elliot blueberry. D. Zhang, Y.L. Qian, M.C. Qian
2:45 Intermission.
3:00 20. Changes in key orange juice aroma compounds during chilled storage of NFC juice. P.H. Schieberle, V. Mall, I. Sellami
4:15 Concluding Remarks.

**Journal of Agricultural & Food Chemistry Best Paper Award & Young Scientist Award Symposium**

Pennsylvania Convention Center Room 110B  Section B
N. P. Seeram, **Organizer & Keibler, Organizer, Presiding**
1:00 Introductory Remarks.
1:05 23. Identification of bioactive components in wheat bran: An example of team science. S. Sang
1:45 Intermission.
2:00 24. Characterization of oligomeric anthocyanins and proanthocyanidins from red grape pomace by mass spectrometry (MALDI-TOF and ORBITRAP ESI-MS). E. Salas
2:30 25. Development of specific dietary biomarkers to better
capture whole grain wheat exposure and beneficial health effects. Y. Zhu
3:00 26. Integrating traditional disciplines to develop novel technologies to address agricultural and environmental issues. R. Li
3:30 Concluding Remarks. Advances in Residues Analysis of Bee Relevant Matrices: Analytical Methods & Sampling Techniques Sponsored by AGRO, Cosponsored by AGFD and ENVR
Extraction Efficiency-Bridgeing between Metabolism Studies & Residue Analytical Methods
Sponsored by AGRO, Cosponsored by AGFD and ENVR Glyphosate: Current Status & Future Prospects
Sponsored by AGRO, Cosponsored by AGFD and ENVR

SUNDAY EVENING 5:00 - 7:00PM August 21
Pennsylvania Convention Ctr Terrace Ballroom  Section A General Posters
N. P. Seeram, Organizer
27. Structural and functional studies of ice nucleation protein and its applications in food industry. L. Zhang
30. Enhanced anti-inflammatory efficacy of Calebin-A encapsulated in modified starch. L. Perera, M. Pan, Y. Ting
31. Role of novel multi-starter on the generation of volatile compounds in buckwheat (Fagopyrum scullentum) soksungjang according to fermentation period. M. Park, H. Choi, Y. Kim, I. Cho
33. Comparison of mineral contents in vegetables (white cucumber, red paprika, water parsley and kohlrabi) undergoing different cooking methods. J. Hwang, D. Seo, S. Kim, E. Park, H. Kim, S. Lee, M. Yang
34. Edible packaging: improved strength and thermal stability of casein films with citric pectin. L. Aburto, L. Bonnaillie, P.M. Tomasula
35. Determination of structural amino acid contents in bamboo shoot, tomato and corn undergoing different cooking methods using automated amino acid analyzer. D. Seo, W. Yoon, H. Lee, J. Hwang, M. Yang
36. Aroma composition of kale (Brassica oleracea L. Var.) tea. I. Cho, J. Oh
37. Heat-stabilized rice bran metabolome reveals biochemical contents and metabolic pathways with medicinal properties. I. Zarei, E.P. Ryan
41. Understanding sodium diffusion in turkey breast meat. J.K. Pandya, A. Kinchla
42. Development of lecithin emulsion gels system: Influence of formulation parameters on physicochemical properties and digestion kinetics. W. Huang, Y. Ting
43. In vitro release, anti-proliferative and antimicrobial activity of carnosic acid nanoemulsion. H. Zheng, Q. Huang
44. Stability of beta-carotene and alpha-tocopherol in cooked Moringa oleifera leaves, By HPLC-UV. A. Vasilatis
45. Physical characterization of mushrooms as taco filling extender. K. Wong, A. Kinchla
46. Total polyphenol antioxidants in the US diet. J.A. Vinson
47. Effects and molecular mechanisms of soy foods or soy isoflavones in prostate cancer prevention. C. Jang, C. Wu
49. Nondestructive analysis of vitamin C content in dietary supplement tablets by using terahertz time-domain spectroscopy. J. Kang, K. Kwak, H. Chun
50. Fabrication of oil-in-water nanoemulsions by dual-channel microfluidization using natural emulsifiers: saponins, phospholipids, proteins, and polysaccharides. L. Bai, D. McClements
52. High throughput analysis of caffeine in beverages using 2.3 μm analytical reversed phase chromatography column with dual functionality for use both in HPLC and UHPLC. A. Chakrabarti, C. Benner
54. Investigation of the lymphatic transport of solid-lipid curcumin particles (Longvida®) in comparison to curcumin extract in rats. T. Eidenberger, N. Kheradia, S. Cropper
55. Chemical composition and anti-hyperglycaemic effects of triterpenoids enriched Eugenia jambolana Lam. berry extracts. Y. Li, J. Xu, C. Yuan, H. Ma, T. Liu, F. Liu, N.P. Seeram, L. Han, X. Huang, L. Liu
56. In vitro anti-neuroinflammatory effects of urolithins, ellagitannin-gut microbial metabolites. N. DaSilva, P.P. Nahar, H. Ma, A. Slitt, N.P. Seeram
57. Inhibitory effects on the formation of advanced glycation endproducts by hydroponically grown Moringa oleifera. S. Johnson, W. Liu, H. Ma, S.M. Meschwart, J. Chace, N.P. Seeram
58. Natural anthraquinones inhibited protein glycation and amino acids side chain modification by protecting protein structures. W. Liu, H. Ma, J.A. Dain, N.P. Seeram
60. Bioactive glucitol-core containing gallotannins and other phytochemicals from silver maple (Acer saccharinum) leaves. A.J. Bin Muhsinah, H. Ma, T. Yuan, N.P. Seeram
61. Comparison of acidic collagen extraction methods of collagen from channel catfish skin. Y. Tan, S. Chang
63. Tyrosine nano-emulsion stability for supplementation of Army rations. K.R. Conca, K.R. Kenso
65. Expression and characterization of a thermostable endo-
1,5-α-arabinanase (TS-ABN) in *Pichia pastoris* for biocatalytic solubilization of bioactive feruloylated arabino-oligosaccharides from sugar beet pulp. N. Zhang, J. Xu, B.J. Savary
66. Biochemical investigation into the functional properties of *Delonix regia*, *Cassia fistula* and *Bignonia capreolata* extracts. A. Goldson-Barnaby, R. Williams
68. Simultaneous determination of unregistered pesticides in Korea for agricultural products using LC-MS/MS. S. Lee, J. Hwang, M. Kang, M. Chang, Y.D. Lee, J. Kim, G. Lee
69. Quantitative analysis of allergens in peanut varieties from USDA Core Collection and other resources and assessment of food processing effects on peanut allergens. S. Meng, S.K. Chang, L. Jiang, J. Li, N. Puppala, S. Chung
70. Development of carbonyl compounds in kombucha using HPAE-PAD. B. Huang, J. Hu, J. Rohrer
71. Quantitative analysis of allergens in peanut varieties from USDA Core Collection and other resources and assessment of food processing effects on peanut allergens. S. Meng, S.K. Chang, L. Jiang, J. Li, N. Puppala, S. Chung
73. Application of volatile quantification using isotopically labeled internal standards for SPME analysis of a grape mapping internal standards for SPME analysis of a grape mapping. A. Guan, L. Ban
75. Molecular modeling of plant ripening receptors and their interactions with ethylene and ripening inhibitors. J. Gold, E. Rosa, R.S. Kelly
76. Design, synthesis, and structure-activity relationships of novel substituted piperazines derivatives. Y. Xie, C. Liu, Y. Xu, A. Guan, L. Ban
77. Assessment of dietary exposure to emulsifiers of regulatory interest for the United States population. R. Kolanos, R. Shah, M. DíNovi, A. Mattia, K. Kaneko
78. Tyrosol-based liposomal behavior: size, zeta-potential, TEM, QCM-D and fluorescence analysis. K. Evans, D.L. Compton
79. Cellulose-bodipy nanohybrids for single oxygen production. P. Chauhan, N. Yan
80. Development of an absorbent to reduce pesticide residue in ginseng. S. Byung Kon, J. Kim
81. Solid phase mesh enhanced sorption from headspace (SPMESH) coupled to DART-MS/MS for high throughput quantification of trace-level odor-active volatiles. J.A. Jastrzembiski, G.L. Sacks
82. Aromatic esters of volatile propanoic acid and their effect on the sensory properties of apple juice. M. Li, L. Li, B. Chai, J. Yang, Y. Song, C. Liu
83. Design, synthesis and biological activity of novel substituted diamides derivatives containing thiophene ring. M. Li, L. Li, B. Chai, J. Yang, Y. Song, C. Liu
84. Changes of polyphenolic compounds level in artichoke (*Cynara scolymus* L.) grown in Korea during cultivation. K. Hwang, D. Son, C. Kim, K. Seong, J. Moon
85. Changes of organic acids level in coffee during roasting. K. Hwang, J. Moon
86. Self-assembling behavior of food globular proteins and applications in stabilizing Pickering emulsions. W. Jin, Y. Jiang, B. Li, Q. Huang
88. 5-hydroxtryptophan, cyanoglycoside, and flavonoid content of 10 *Grifola simplicifolia* populations. D. Giurleo, R. Juliana, L. Hwang, J. Asante-Darcey, Q. Wu, J. Simon
89. Development of a slow releasing hydrogen sulfide donor. B.J. Savary, D. Huang, J. Rohrer
90. Biochemical investigation into the functional properties of *Rosa galactosyloligosaccharide (GOS)*. L. Jiang, J. Li, N. Puppala, S. Chung
91. Simultaneous determination of unregistered pesticides in Korea for agricultural products using LC-MS/MS. S. Lee, J. Hwang, M. Kang, M. Chang, Y.D. Lee, J. Kim, G. Lee
92. Identification and quantification of phenolic acids and flavonoids in three phenolic-rich legume varieties as affected by thermal treatments. Y. Zhang, S.K. Chang
93. Comparative study of phenolic substances in astringent and non-astringent persimmon fruits during development and ripening. S. Kumari, S.K. Chang, Y. Zhang, Y. Zheng
94. Design, synthesis and biological activity of thienopyrimidine derivatives. F. Yang, C. Liu, A. Guan, Z. Yao, Z. Li, Y. Song
95. Design, synthesis and fungicidal evaluation of novel substituted arylxy pyridine compounds containing pyrimidinamine moiety. A. Guan, X. Sun, J. Yang, Y. Xie, J. Zhou, C. Liu
96. Design, synthesis, and biological activity of novel N-substituted piperazines derivatives. Y. Xie, C. Liu, Y. Xu, A. Guan, L. Ban
100. Peptidolytic activity of three probiotic lactic acid bacteria for possible use as sourdough starters. H. Hernandez-Sanchez, M. Nava-Romero
103. Peptidolytic activity of three probiotic lactic acid bacteria for possible use as sourdough starters. H. Hernandez-Sanchez, M. Nava-Romero
105. Withdrawn
106. Relationship between structural characteristics and digestibility of debranched starch. G. Liu, Y. Hong, Z. Gu, Y. Jiang
109. Alginic conjugated keratin for wound dressing materials. R. Wang
110. Triacylglycerol compositions of sunflower, corn and soybean oils examined with supercritical CO2 ultra-
performance convergence chromatography combined with quadrupole time-of-flight mass spectrometry. B. Gao, Y. Luo, W. Lu, L.L. Yu

111. Evaluation of hydrogen peroxide scavenging activity of phenolic acids by employing optical nanoprobe sensors based on gold nanoshells. W. Qian

112. Growth inhibition of bladder cancer cells is greater with quercetin-3-glucoside than with quercetin or quercetin-3-rutinoside. M.A. Lea, A. Tandon, C. desBordes


114. Synthesis and development of a new selective ryanodine receptor activator insecticide. W. Lee

115. Fluorescence fingerprinting of antioxidants in sorghum and sugarcane. S.M. Uchimiya

116. Starch modified by wet-milling process to stabilize Pickering emulsions. X. Lu, Q. Huang

117. Chromatography method for determination of penicillin used for dairy production. A. Miranda, M. de Moura, D. da Silva

118. ELISA detection of soy proteins in traditionally brewed soy sauce samples obtained during manufacture and commercial soy sauce products. P. Kande, M. Bakke, B. Bedford, J. Hammerstone, L. Jackson

MONDAY MORNING  August 22  Pennsylvania Convention Center Room 110A  Section A

Challenges in Flavor Chemistry Associated with Developing Healthy Foods & Beverages

K. Tandon, Organizer  V. M. Acquarone, R. Elias, J. A. Grover, Organizers, Presiding

8:00 Introductory Remarks.

8:05 119. Taste biology and its application to new ingredient discovery. S. Gravina

8:35 120. How sweet works and what it means for non-caloric sweeteners. R. Margolskee


9:35 Intermission.

10:00 122. Stevia innovation: Improved leaf extracts from advanced understanding of taste. J.C. Fry


Chemistry Behind Health Effects of Grains

Pennsylvania Convention Center Room 110B  Section B

R. Landberg, S. Sang, Organizers, Presiding

8:00 Introductory Remarks.

8:05 124. Dietary fibers and associated phytochemicals in cereals. K. Bach Knudsen

8:35 125. Alkylresorcinols as dietary biomarkers of whole grain wheat and rye intake. R. Landberg

9:00 126. Biomarkers of whole grain wheat intake identified by targeted and non-targeted metabonomic approaches. Y. Zhu, W. Sha, P. Wang, S. Sang

9:25 127. Non-targeted metabolite profiling for characterization of bioactive compounds in cereals and their metabolic effects in different models. K. Hanhineva


10:15 Intermission.

10:30 129. Rice-bran phytochemical extracts inhibit invasion and intracellular replication of Salmonella typhimurium in mouse and porcine intestinal epithelial cell. E.P. Ryan


Flavor Stability: Chemical Changes in Flavor Molecules, Flavor-Food Matrix Interactions, Flavor Encapsulation

Pennsylvania Convention Center Room 111A  Section C

R. J. Mcgorrin, M. C. Qian, Organizers, Presiding

8:00 Introductory Remarks.

8:05 133. Chemical stability of citral. Y. Wang, C. Ho

8:30 134. Stability of the curry leaf aroma impact compound 1-phenylethanethiol during traditional processing and use in the kitchen. M. Steinhaus

8:55 135. Flavor and off-flavor in canned tuna fish. F. He, Y.L. Qian, M.C. Qian

9:20 136. Unraveling the off-flavor formation of native cold-pressed rapeseed oil using the molecular sensory science concept. M. Granvogl, K. Matheis

9:45 Intermission.

10:00 137. NMR approaches to studying wine oxidation: Pathways of acetaldehyde. A.L. Waterhouse, A. Peterson


10:50 139. Stability of smoke taint during the aging of smoke-affected wine. L. van der Hulst, R. Ristic, K. Wilkinson

11:15 Concluding Remarks

Glyphosate: Current Status & Future Prospects

Sponsored by AGRO, Cosponsored by AGFD and ENVR

Synthetic Biology & Genetically Modified Organisms Evolution or Revolution? Policy Challenges & Opportunities in the Biotechnology Golden Age

Sponsored by ENVR, Cosponsored by AGFD, AGRO, CEI, COMSCI

MONDAY AFTERNOON  August 22  Pennsylvania Convention Center Room 110A  Section A

Challenges in Flavor Chemistry Associated with Developing Healthy Foods & Beverages

K. Tandon, Organizer  V. M. Acquarone, R. Elias, J. A. Grover, Organizers, Presiding

1:00 Introductory Remarks.

1:05 141. Cellular and molecular mechanisms of salty taste: Implications for developing strategies to combat NaCl overconsumption. B. Lewandowski

1:35 142. Aroma compounds to rescue the taste of healthy foods and beverages. T. Thomas Danguin, C. Salles, E. Guichard

2:05 143. Mechanisms of bitterness generation in whole wheat foods. Q. Bin, D.G. Peterson

2:35 Intermission.

3:00 144. Effect of pressure and heat treatment on volatile profile in Chinese bayberry juice analysed by GC-MS during storage. S. Lin, Y. Yu, Y. Lin, S. Zhu

3:30 145. Reducing astringency in persimmons through...
4:00 145. Mitigation strategies for toxicologically relevant styrene during the production of wheat beer. M. Granvogl, D. Langos, P.H. Schieberle
4:30 Concluding Remarks.

Chemistry Behind Health Effects of Grains
Pennsylvania Convention Center Room 110B  Section B
R. Landberg, S. Sang, Organizers, Presiding
1:00 Introductory Remarks.
1:05 146. Phytochemicals in wheat bran for colon cancer prevention. S. Sang, Y. Zhu, J. Fu
1:30 147. Whole grain polyphenols in colon health: Positive interaction of complementary sorghum-legume flavonoids. J. Awika, S. Agah, L. Yang, S. Talcott, C. Allred
1:55 148. Phytochemicals in quinoa grains and their antioxidant and anti-inflammatory effects. R. Tsao, T. Yao, R. Liu
2:45 Intermission.
3:00 150. Health-promoting lipids in corn kernels and corn oils. R. Moreau
3:25 151. Phytosterols and sterol conjugates in cereal grains. L. Nystroem
3:50 152. Genetic and environmental impacts bioactive components in cereals. P.R. Shewry
4:15 153. Polyphenols in breakfast cereals and snacks: important contribution to beneficial health effects of whole grain consumption. J. Goodman, J.A. Vinson, S. Wang

Flavor Stability: Chemical Changes in Flavor Molecules,
Flavor-Food Matrix Interactions, Flavor Encapsulation
Pennsylvania Convention Center Room 111A  Section C
R. J. McGorrin, M. C. Qian, Organizers, Presiding
1:00 Introductory Remarks.
1:05 154. Differences in the non-volatile composition of younger and older Armagnac and Cognac brandies and bourbon and Scotch whiskies using UHPLC/QTOF-MS. T.S. Collins
1:30 155. Lichenysin, a novel nonvolatile compound in Chinese distilled spirits reduced the headspace concentration of phenolic off-flavors via hydrogen-bond interaction. S. Chen, Y. Xu, R. Zhang, Q. Wu
1:55 156. Research on the aroma characteristics and impacts of the nonvolatile matrix composition on the aroma release of Vidal icewine based on sensomics. K. Tang, Y. Xu
2:45 Concluding Remarks.

Glyphosate: Current Status & Future Prospects
Sponsored by AGRO, Cosponsored by AGFD and ENVR
Undergraduate Research Posters Agricultural & Food Chemistry  Spons: CHED, Cospons: AGFD, SOCED
Pollinators: Agrichemicals, Behavior & Disease
Sponsored by AGRO, Cosponsored by AGFD, ENVR, TOXI
Synthetic Biology & Genetically Modified Organisms The Debate: What Role Should We Play in the Biotechnology Era?
Sponsored by ENVR, Cosponsored by AGFD, AGRO, CEI and COMSCI

MONDAY EVENING  August 22  8:00-10:00PM
Pennsylvania Convention Center Halls D/E

TUESDAY MORNING  August 23  Pennsylvania Convention Center Room 111B  Section A
Kenneth A. Spencer Award for Outstanding Achievement in Agricultural & Food Chemistry
Food Components for Cardiovascular & Brain Health
Cospons: AGRO
E. Hellmuth, A. M. Rimando, Organizers M. Appell, Presiding
8:00 Introductory Remarks.
8:10 158. Pterostilbene in blueberries and PPAR activation. A.M. Rimando
8:40 159. Physiological effects of pterostilbene and blueberries in animal models of obesity. W.H. Yokoyama, D. Shao, H. Kim, A.M. Rimando
9:10 160. Berry bioactives: the health benefits of color. B. Burton-Freeman
9:40 Intermission.
10:25 162. Phytochemicals against oxidative stress and inflammatory responses in microglial cells. G. Sun
10:55 163. Quest for indirect modulators of the endocannabinoid system from natural products. A. El-Allfy, E.A. Abourashed

Chemistry, Safety & Technology of GMO Foods
Cosponsored by AGRO, CEI, COMSCI, ENVR  Pennsylvania Convention Center Room 113B  Section B
J. W. Finley, L. Jackson, J. N. Seiber, Organizers, Presiding
8:00 Introductory Remarks.
8:05 164. Traditional plant breeding vs molecular plant breeding. W. Parrott
8:35 165. Biotechnology innovations and solutions for sustainable agriculture. D.J. Williams
9:35 Intermission.
9:50 167. Challenges for the production and acceptance on transgenic wheat. P.R. Shewry
Section B
10:20 168. How basic research can lead to development of improved cereal crops: But where are they? P.G. Lemieux

AGFD Division Award Symposium in honor of Dr. Zhen-Yu Chen
Pennsylvania Convention Center Room 110A  Section C
B. Park, Organizer, Presiding
8:00 Introductory Remarks.
8:05 169. Prebiotic-like properties of feruloylated arabinoxylan-oligosaccharides generated from rice bran arabinoxylan. S. Lee, T. Pham, B.J. Savary, M. Chen
8:30 170. Transition metal-mediated oxidation reactions of sulfidic compounds in wine. G.Y. Kreitman, J.C.
8:45 Concluding Remarks.

General Papers
Pennsylvania Convention Center Room 110B  Section D
N. P. Seeram, Organizer, Presiding  W. Liu, H. Ma, Presiding
8:00 Introductory Remarks.
8:55 173. Solid/oil/water emulsions as novel approaches of encapsulating probiotic bacteria. Y. Zhang, Q. Zhong
9:20 Intermission.
10:00 175. Microencapsulation of tributyrin to improve sensory qualities and intestinal delivery. Y. Lee, W. Kuo
10:50 Concluding Remarks.

USDA-ARS Sterling B. Hendricks Memorial Lectureship: Symposium in honor of May Berenbaum
Cosponsored by AGRO Pennsylvania Convention Center Room 110B Section D
K. Kaplan, M. H. Tunick, Organizers, Presiding
11:00 Introductory Remarks.
11:05 177. How to eat a plant: phytochemical detoxification in bees vs. butterflies. M.R. Berenbaum
11:55 Concluding Remarks.

Agrochemicals & Pollinators: Current Science & Risk Assessment Approaches
Sponsored by AGRO,
Cosponsored by AGFD, ENVR and TOXI
Cannabis & Agrochemicals: Analytical, Environmental & Regulatory Challenges
Sponsored by AGRO,
Cosponsored by AGFD

TUESDAY AFTERNOON AUGUST 23 Pennsylvania Convention Center Room 111B Section A
Kenneth A. Spencer Award for Outstanding Achievement in Agricultural & Food Chemistry
Anticancer Food Components: Functional Food Polymers, Food Flavor & Odor Chemistry & Processing-Induced Food Toxicants Cosponsored: AGRO E. Hellmuth, A.M. Rimando, Organizers M. Appell, Presiding
1:00 Introductory Remarks.
1:05 178. Dietary pterostilbene is a novel chemopreventive and therapeutic agent in prostate cancer: Preclinical studies. A. Levenson
1:35 179. Topical pterostilbene prevents UV-B-mediated skin damage. R. Dellinger
2:05 180. Health benefits of natural tocopherol mixtures. N. Suh
2:35 Intermission.
2:50 181. Chemistry, safety and caloric value of partially hydrolyzed guar gum. J.W. Finley
3:20 182. Fifty years of smelling sulfur: From the chemistry of garlic to the molecular basis for olfaction. E. Block
4:20 184. Chemical mechanisms for 3-MCPD ester formation. L.L. Yu

Chemistry, Safety & Technology of GMO Foods
Cosponsored by AGRO, CEI, COMSCI and ENVR
Pennsylvania Convention Center Room 113B Section B
J. W. Finley, L. Jackson, J. N. Seiber, Organizers, Presiding
1:00 185. GMO crops may contribute to decline of monarch butterfly populations. J.N. Seiber
1:30 186. Impressive progress, opportunities, and obstacles in the use of genetically engineered trees. S.H. Strauss
2:00 187. Progress on transgenic approaches to solving citrus greening disease. M. Dutt, J.W. Grosser
2:30 Intermission.
3:15 189. Transgenic and gene edited animals for use in agriculture: Where are we now? J.D. Murray
4:15 Concluding Remarks.

International Student Symposium Nanoparticles & Delivery Systems
Pennsylvania Convention Center Room 110A Section C
P. Schmidberger, R. Tardugno, Organizers, Presiding
1:00 Introductory Remarks.
1:05 191. Supramolecular design of coordination bonding architecture on zein nanoparticles for pH-responsible drug delivery and the cellular uptake mechanism. H. Liang
1:30 192. Preparation, characterization, in vitro lipolysis and cell study on antioxidant and anti-inflammatory activities of carnosic acid nanoemulsion. H. Zheng, Q. Huang
Section C
1:55 193. Evaluation of postharvest washing on Ag NPs removal from spinach leaves. Z. Zhang, L. He
2:20 Intermission.
2:40 194. Influence of food matrix on the fate of titanium dioxide (TiO2) nanoparticles in gastrointestinal tract. X. Cao, H. Xiao, D. McClements
3:30 196. Assemblies, properties and food applications of kafirin nanoparticles based Pickering emulsions. J. Xiao, Q. Huang
3:55 197. Real-time and in situ monitoring of pesticide penetration in edible leaves by surface-enhanced Raman scattering mapping. T. Yang, L. He
4:20 Concluding Remarks.

General Papers
Pennsylvania Convention Center Room 110B Section D
N. P. Seeram, Organizer, Presiding W. Liu, H. Ma, Presiding
1:00 Introductory Remarks.
1:30 199. Effects of brewing conditions and re-infusion on the antioxidant activity of twenty-four varietal green teas. E.M. Sharpe, F. Hua, S. Schuckers, S. Andreescu, R. Bradley
1:55 200. Comparative study of performance of regular pyrolysis oil and TGRP oil for catalytic cracking with HZSM-5. Y. Choi, Y. Elkasabi, P. Tarves, C.A. Mullen, A. Boateng
2:20 201. Novel promising biocomposite derived from calcined...
eggshells for mitigating soil antibiotic resistance bacteria/gene dissemination and accumulation in bell pepper. Y. Mao, S. Mingming, X. Li, A. Schwab, X. Jiang
2:45 Intermission.
3:00 202. Stability of anthocyanin pigments in purple wheat bran and powder isolates. E.M. Abdelaal, P. Hul
3:50 204. Analysis of changes in anthocyanin and volatile compounds of Fuji apple under different sizes and storage conditions. H. Jang, M. Jeong
4:15 205. Measuring color in turbid beer and wort samples. R. Barth
4:40 206. Investigation of monoterpene enantiomers in Pinot gris wine and sensory perception of these compounds on matrix interactions. M. Song, E. Tomasoni
5:05 Concluding Remarks.

Agrochemicals & Pollinators: Current Science & Risk Assessment Approaches  Sponsored by AGRO, Cosponsored by AGFD, ENVR and TOXI
Cannabis & Agrochemicals: Analytical, Environmental & Regulatory Challenges  Sponsored by AGRO, Cosponsored by AGFD
Glyphosate: Current Status & Future Prospects  Sponsored by AGRO, Cosponsored by AGFD and ENVR

WEDNESDAY MORNING August 24 Pennsylvania Convention Center Room 110A Section A
Natural & Bio-Based Antimicrobials for Food Applications
X. Fan, H. L. Ngo, C. Wu, Organizers, Presiding
8:00 Introductory Remarks.
8:05 207. Safer salads and grilled meats: Clean and green approaches. S. Ravishankar
8:30 208. Organic acids as food antimicrobials. J. Gurtler
8:55 209. Natural and value-added antimicrobials for pathogen control. B. Brehm-Stecher
9:45 Intermission.
10:05 211. Improve microbial food safety of fresh fruits and vegetables with aqueous and vaporous essential oils. X. Fan, C. Wu
10:30 212. Berry pomace extracts in enhancing microbial food safety. D. Biswas

Chemistry, Safety & Technology of GMO Foods
Cospons: AGRO, CEI, COMSCI and ENVR  Pennsylvania Convention Center Room 111B  Section B
J. W. Finley, L. Jackson, J. N. Seiber, Organizers, Presiding
8:00 Introductory Remarks.
9:35 Intermission.
10:50 219. It is about safety. V.C. Knauf

International Student Symposium  Bioactive Compounds
Pennsylvania Convention Center Room 111A Section C
P. Schmidtberger, R. Tardugno, Organizers, Presiding
8:00 Introductory Remarks.
8:05 220. Synergism between sulforaphane and luteolin in anti-inflammation. K. Rakariyatham, X. Wu, H. Xiao
8:30 221. 3-MCPD 1-palmitate induced tubular cell apoptosis via JNK/P53 pathways. G.Huang, M.Liu, W.Lu, X.Sun, L.L.Yu
8:55 222. Functional analyses on antioxidant and anti-inflammatory effects of polyphenols extracted from a Chinese bitter tea (ilex latifolia thunb). T. Zhang
9:20 Intermission.
9:40 223. Role of cell walls in controlling the release and bioaccessibility of polyphenols from raw compared to processed apples. D. Liu, M.J. Gidley, P. Lopez-Sanchez
10:05 224. Redox active antioxidants increase chemical stability and biological function of curcumin. W. Wang
10:30 225. Enhancing bioavailability of lipophilic nutraceuticals in natural food: Excipient emulsion design. R. Zhang, D. McClements
10:55 Concluding Remarks.

General Papers
Pennsylvania Convention Center Room 110B  Section D
N. P. Seeram, Organizer, Presiding W. Liu, H. Ma, Presiding
8:00 Introductory Remarks.
8:05 226. Impact of harvest time and switchgrass cultivar on conversion to sugars and pyrolysis oils using biochemical and thermochemical routes. M. Serapiglia, C.A. Mullen, A. Boateng, B.S. Dien, M. Casler
8:55 228. Effect of cluster sunlight exposure on rotundone concentration in Noiret grapes and wine. L.J. Homich, R.J. Elias, M. Centinari, J. Vanden Heuvel
9:45 Intermission.
10:00 230. Restoring herbicide control in multiple herbicide resistant black grass (Alopecurus myosuroides). M.C. Schwarz, P.G. Steel, E. Pohl, G. Mitchell
10:25 231. Withdrawn
11:40 Concluding Remarks.
Who Should Regulate Pesticides in Our Food?
Sponsored by AGRO, Cosponsored by AGFD and ETHC

WEDNESDAY AFTERNOON  August 24  Pennsylvania Convention Center Room 110A  Section A

Natural & Bio-Based Antimicrobials for Food Applications  X. Fan, H. L. Ngo, C. Wu, Organizers, Presiding
1:00 234. Anti-liesterial activity of hops beta acids on ready-to-eat meat products. C. Shen
1:50 236. Use of plant-based antimicrobials for enhanced pressure destruction of pathogens in juices. A. Mendonca
2:15 237. Use of natural antimicrobials with combined non-thermal treatments to control Listeria monocytogenes and Clostridium sporogenes in food systems. M. Lacroix
2:40 Intermission.
2:55 238. Modeling the impact of the natural antimicrobial citral and high pressure processing on the survival of Escherichia coli O157:H7 and uropathogenic E. coli in ground beef. S. Chien, S. Sheen, C. Sommers, L. Sheen
3:20 239. Development of delivery systems for essential oils and applications for foods and biofilm removal. L. McLandsborough
3:45 240. Novel uses of lauric arginate for food preservation: Physical and antimicrobial properties. Q. Ma, Q. Zhong
4:10 241. Methods to deliver natural antimicrobials to food. T. Jin

Chemistry, Safety & Technology of GMO Foods  Cosponsored by AGRO, CEI, COMSCI and ENVR
Pennsylvania Convention Center  Room 111B  Section B
J. N. Seiber, Organizer J. W. Finley, L. Jackson, Organizers, Presiding
1:00 242. Unintended effects associated with GM crops are both expected and low risk. R. Herman, W. Parrott
1:30 243. Assessing the risks of resistance evolution for transgenic crops for insect control: Capitalizing on successes and learning from mistakes. B. Siegfried
2:00 244. FDA’s safety evaluation of foods from genetically engineered plants. R.I. Merker
2:30 Intermission.
2:45 245. Intellectual property issues of GMO food crops. A. Coates
3:15 246. Communication of GMO issues to non-technical audiences. J. Finley
3:45 Concluding Remarks.

International Student Symposium Analytical Approaches  Pennsylvania Convention Center Room 111A  Section C
P. Schmidberger, R. Tardugno, Organizers, Presiding
1:00 Introductory Remarks.
1:05 247. Filter based approach to rapid and sensitive SERS detection of ferbam in environmental water. S. Gao, L. He
2:20 Intermission.
3:30 252. Extraction and isolation of stypoldione from stypopodium zonale. M.R. Denny
3:55 Concluding Remarks

High-Resolution Mass Spectroscopy Techniques for Identification & Quantification of Phytochemical Metabolites  Pennsylvania Convention Center Room 110B  Section D
Y. Kim, M. Sukan, S. Talcott, Organizers L. Howard, Organizer, Presiding
1:00 Introductory Remarks.
1:05 253. Scope and limitations of HPLC-HRESI/MS for the analysis of anthocyanins from tropical fruits. C. Osorio Roa
1:30 254. Target oriented synthesis and mass spectral characterization of curcumin-phenformin adduct: Potential insights into the role of this conjugate as anti-diabetic and anti-cancer agent. B. Dayal, D.N. Shah, S. Patel, A. Mehta, M.A. Lea
1:55 255. Analysis of urinary and fecal metabolites of tea polyphenol EGCG in mice by LC-MS/MS. S. Zhang, S. Sang
2:20 256. Qualitative and quantitative analysis of antioxidant and quinone reductase-inducing phytochemicals present in a Maqui berry (Aristotelia chilensis) botanical dietary supplement. C. Naman, J. Li, Y. Deng, W. Keller, A. Kinghorn
2:45 Intermission.
3:25 258. Accuracy of HPLC-MS methods used to assess the absorption, metabolism and excretion of bioactive (poly)phenols: Implications for nutritional and biomedical research. J. Ottaviani
3:50 259. Absorption, distribution, metabolism and excretion of orange juice flavonones in humans. A. Crozier, G. Pereira-Caro
4:15 260. Elucidating metabolic signatures of phytochemical consumption. C. Kay
4:40 Concluding Remarks

Who Should Regulate Pesticides in Our Food?  Sponsored by AGRO, Cosponsored by AGFD and ETHC

THURSDAY MORNING  August 25  Pennsylvania Convention Center Room 110A  Section A

International Student Symposium Application of Natural Ingredients  P. Schmidberger, R. Tardugno, Organizers, Presiding
8:00 Introductory Remarks.
8:05 261. Development of food-grade filled hydrogels for oral delivery of lipophilic active ingredients: pH-triggered release. Z. Zhang
8:30 262. Legume proteins as alternative emulsifiers to encapsulate omega-3 oils. C.E. Gumus, D.J. McClements
9:20 Intermission.
9:40 264. Stabilization of pickering emulsions by polysaccharide-polypeptide nanocomplexes. Y. Jiang, Q. Huang
10:05 265. Ultrasonic treatment of regenerated a-chitin with tunable capacity for stabilization of oil in water emulsion. Y. Wang
10:30 266. Phytochemical composition of essential oils and in vitro screening of the antimicrobial activity on oral pathogenic bacteria. R. Tardugno, R. Iseppi, E. Franceschini, F. Pellati, G. Bruzzi, M. Bondi, S. Benvenuti
10:55 Concluding Remarks.

Natural & Bio-Based Antimicrobials for Food Applications
Pennsylvania Convention Center Room 111A Section B
X. Fan, H. L. Ngo, C. Wu, Organizers, Presiding
8:00 276. Lactalbumin and chitosan graft copolymers for nutraceuticals encapsulation. 9. Jiang, M. Guo, L. Fan
8:50 269. Thiamine dilauryl sulfate (TDS) and organic acid combined treatment to secure microbial safety of selected products. H. Park, H. Feng
9:10 Intermission.
9:30 270. Characterization of LAB bacteriocins with the potential for food safety and functional food applications. J. Renye, G. A. Somkuti
10:45 273. Evaluation of toxicity and endocrine disruption potential of the natural antimicrobials or biobased antimicrobials. C. Wu, C. Jang, M. Guo

General Papers
Pennsylvania Convention Center Room 110B Section C
N. P. Seeram, Organizer, Presiding W. Liu, H. Ma, Presiding
8:00 Introductory Remarks.
8:05 274. Applications of the polysaccharide-polypeptides nanocomplexes in multi-platforms for nutraceuticals encapsulation. Y. Jiang, Q. Huang
8:30 275. Interaction and structure formation between α-lactalbumin and chitosan grafted with poly(ethylene glycol) chains. J. Du, O. G. Jones
8:55 276. Depolymerization of lignin via co-pyrolysis with 1,4-butadienel in a microwave reactor. P. Tarves, C. A. Mullen, A. Boateng
9:20 Intermission.
11:20 281. Analysis and reduction of possible carcinogenic 4(5)-methylimidazole in a caramel colorant model system. K. G. Lee
11:40 Concluding Remarks.

Who Should Regulate Pesticides in Our Food?
Sponsored by AGRO, Cosponsored by AGFD and ETHC

THURSDAY AFTERNOON August 25 Pennsylvania Convention Center Room 110A Section A
International Student Symposium Molecular Definition of Food Quality
P. Schmidberger, R. Tardugno, Organizers, Presiding 1:00 Introductory Remarks.
1:05 282. Decoding the taste of foods: What makes that cheese taste so good? M. Salger, T. Hofmann
1:30 283. Changes in the key aroma compounds of dried shitake mushroom induced by rehydration. P. Schmidberger, P. H. Schieberle
1:55 284. Evaluation of chiral heterocyclic key aroma compounds in cooked Allium-varieties - A case study regarding organoleptic and quantitative characteristics. M. Flaug, M. Granvogl
2:20 Intermission.
3:05 286. Differentiating cultivation locations and flowering stages of chrysanthemum by UPLC fingerprints combined with chemometric data analysis techniques. L. Yanfang, W. Lu, L. L. Yu
3:30 Concluding Remarks.

General Papers
Pennsylvania Convention Center Room 110B Section C
N. P. Seeram, Organizer, Presiding W. Liu, H. Ma, Presiding 1:00 Introductory Remarks.
1:05 287. Lateral flow assay exploiting aptamers for the extremely rapid detection of the anaphylactic allergen ß-conglutin. C. O’ Sullivan, M. Jauset, M. Svobodova
1:30 288. Portable optoelectronic nose for rapid monitoring of meat freshness. Z. Li, K. S. Suslick
2:45 Intermission.
3:00 291. Variations in the enantiomeric composition of thujone-containing essential oils. J. D. Williams, K. A. Anderson, J. A. Yazarians, G. R. Boyce
3:25 292. Improved method for determination of biofuel sugars by HPAGE-PAD. S. Patil, J. Rohrer
4:15 294. Estimation of total phenolic compounds in leaf tissues of American chestnut (Castanea dentata), Chinese chestnut (Castanea mollissima), and their back-cross breeding generations. J. She
4:40 295. Microwave-induced chemical synthesis of oxidized lanosterol and cholesterol derivatives using KMnO4-CuSO4 catalyst: Potential target molecules for clearing up protein aggregation in diabetes patients suffering from cataract formation. B. Dayal, J. Chou
5:05 Concluding Remarks.

Who Should Regulate Pesticides in Our Food?
Sponsored by AGRO, Cosponsored by AGFD and ETHC
AGFD Abstracts - 252nd ACS National Meeting in Philadelphia

AGFD 1 Protein engineering using bioorthogonal and combinatorial chemistry Yoshihiro Ito1,2, y-ito@riken.jp. (1) Nano Medical Engineering Lab, RIKEN, Wako, Saitama, Japan (2) Emergent Bioengineering Materials Research Team, RIKEN Center for Emergent Matter Science, Wako, Saitama, Japan Recently, protein engineering has been extended into bio-orthogonal protein engineering by the development of specific chemical or enzymatic modification technologies. The combinatorial approach of molecular evolutionary engineering (or in vitro selection) has also provided a new design tool for functional peptides. These methodologies have enabled the development of various new proteinaceous materials for biological and medical applications. Here, we will discuss recent progress in the molecular design of proteins with respect to the preparation of binding growth factors, which are of increasing importance in the biomaterials field.

AGFD 2 Design of biodegradable injectable polymer formulation exhibiting temperature-responsive covalent hydrogel formation Yuichi Ohya, yoha@kansai-u.ac.jp, Yasuyuki Yoshida, Keisuke Kawahara, Akinori Kuzuya. Dept of Chemistry and Materials Engineering, Kansai Univ., Osaka, Japan Biodegradable polymers exhibiting temperature-responsive sol-gel transition between room temperature and body temperature are expected to be applied as injectable polymer (IP) systems in biomedical applications. IP solution containing drugs or living cells can be injected by simple syringe injection at the target site in the body to form a hydrogel acting as sustained drug releasing depots or scaffolds for tissue regeneration. For example, Lee et al. reported ABA-type triblock copolymer of poly(lactide-co-glycolide) and poly(ethylene glycol) (PEG) as biodegradable injectable polymer. We also reported several biodegradable IP systems using block copolymers of aliphatic polyesters and branched PEG. However, such IP systems forming physically cross-linked hydrogel are likely to dissociate to sol state under highly wet condition such as intra-peritoneal space. To overcome the problems, we developed an injectable polymer formulation forming chemically cross-linked hydrogel in response to temperature change. We synthesized poly(caprolactone-co-glycolic acid)-b-poly(ethylene glycol)-b-poly(caprolactone-co-glycolic acid) (PCGA-b-PEG-b-PCGA) triblock copolymer bearing succinimidyl groups on its termini (CP-OSUs). The copolymer was mixed with water-soluble polymer bearing amine groups, such as poly-L-Lysine (PLys), which can form covalent bonds with the functional groups on the triblock copolymer termini. The mixture solution showed irreversible sol-to-gel transition and covalent bond formation in response to temperature change. The obtained hydrogel showed longer duration time of the gel state in aqueous solution.

AGFD 3 Plant cell-inspired hydrogel consisting of a poly(ethylene glycol) hydrogel and polyurethane foam Naozumi Teramoto, teramoto.naozumi@it-chiba.ac.jp, Mitsuru Harima, Keisuke Wakayama, Toshiaki Shimasaki, Mitsuhito Shibata. Chiba Inst of Tech., Narashino Chiba, Japan A hydrogel is one of promising materials as a biomaterial for regenerative medicine. Hydrogels are formed by a hydrophilic polymer network and large amount of water, and the distinguished advantage of hydrogels is biocompatibility and diffusibility of solutes in hydrogel. Though hydrogels are attractive for biomaterials, most traditional hydrogels are mechanically weak and brittle. We have proposed a novel strategy for reinforcing hydrogels with polyurethane foam based on the inspiration from the framework of plant cells, and we found that the mechanical properties of hydrogels could be significantly improved by the reinforcement with polyurethane foam in the previous study. In the present study, we prepared a poly(ethylene glycol) (PEG) hydrogel and it was reinforced by open-cell type polyurethane foam. Poly(ethylene glycol) diacrylate, which was polymerized using 2,2'-azobis(2-methylpropionamidine) dihydrochloride (V-50) radical initiator, was used for the preparation of hydrogel. Without polyurethane foam, the PEG gel was broken at the compression stress of around 100kPa. On the other hand, the PEG gel reinforced with polyurethane foam did not show the evident break point, and the composite gel material endured the high compression stress around 2 MPa. We used two types of polyurethane foam with different cell size. The compression modulus were influenced by the cell size. When the polyurethane foam with a small cell size was used for preparation of the composite gel, the compression modulus of the composite gel was higher than that of the composite gel with the polyurethane foam with a large cell size. We also observed the cyclic recovery from the 70% compression. The mechanical properties of our composite gel in the compression test are comparable to tough hydrogels developed recently.

AGFD 4 Preparation and analysis of functional oligosaccharides from rice bran arabinoxylan Brett J. Savary2, bsavary@astate.edu, Keat (Teoh)1, Ningning Zhang1, Jianfeng Xu2, Fabricio Medina-Bolivar2, Shiguang Yu2, Sun-Ok Lee4, Ya-Jane Wang1. (1) Arkansas Biosciences Inst., (2) Arkansas State Univ., Jonesboro (3) Biological Sciences, Arkansas State Univ., (4) Food Sci., Univ. of Arkansas, Fayetteville As a cereal grain processing byproduct, rice bran represent a large reservoir of largely underutilized functional biopolymers that may be mobilized for improved feed, food, and nutraceutical uses. Hemicellulosic chains of arabinoxylan are largely locked within the fiber complex, notably through dehydrodiferulate cross-links. Ferulic acid is a potent antioxidant ester linked at the O-5 position of arabinofuranoside branches. The degree of substitution, branching, and branch-distribution profiles appear to vary considerably for different tissues and between different cereal species. This implicates differences in their metabolism and their texture and processing properties. We are investigating feruloylated arabinoxylan oligosaccharides (FAXOs) generated from insoluble rice bran fiber. A better understanding of bioavailability and structure-activity relationships will determine FAXO’s dietary utility and may identify effective processing technologies for formulating safe, high quality rice bran products enriched with FAXOs in a sustainable manner. This presentation will highlight our progress to isolate and characterize rice bran FAXOs and to evaluate their ability to modulate tight-junctions in a colon epithelial cell model.

AGFD 5 Sulfation pattern of fucose branches affects the anti-hyperlipidemic activities of sea cucumber fucosylated chondroitin sulfate Shiguo Chen1,2, handle@zju.edu.cn, Xingqian Ye3. (1) Dept of Food Sci., Zhejiang Univ., Hangzhou, China (2) Food Sci. and Nutrition, Zhejiang Univ., Hangzhou, China Fucosylated chondroitin sulfates (FCSs) are glycosaminoglycans extracted from sea cucumbers, consisting of chondroitin sulfate E (CSE) backbones and sulfated fucose branches. The biological properties of FCSs could be affected by the sulfation pattern of their fucose branches. In the present study, two FCSs were isolated from sea cucumber Isostichopus badionotus (ICS-Ib) and Pearsonothuria graeffei (ICS-Pg). Their monosaccharide compositions were as follow: glucuronic acid (GlcA), N-acetylgalactosamine (GalNAc), and fucose (Fuc). Their degree of sulfation and their anti-hyperlipidemic activities were investigated. Our results have shown that the efflux of cholesterol from HepG2 cells was highly dependent on the sulfation of their fucose branches.

AGFD 6 Absorption and excretion of fucosylated chondroitin sulfates (fCSs) in vivo and in vitro Shiguo Chen1,2, handle@zju.edu.cn, Xingqian Ye3. (1) Dept of Food Sci., Zhejiang Univ., Hangzhou, China (2) Food Sci. and Nutrition, Zhejiang Univ., Hangzhou, China Fucosylated chondroitin sulfates (FCSs) are glycosaminoglycans extracted from sea cucumbers, consisting of chondroitin sulfate E (CSE) backbones and sulfated fucose branches. The biological properties of FCSs could be affected by the sulfation pattern of their fucose branches. In the present study, two FCSs were isolated from sea cucumber Isostichopus badionotus (ICS-Ib) and Pearsonothuria graeffei (ICS-Pg). Their monosaccharide compositions were as follow: glucuronic acid (GlcA), N-acetylgalactosamine (GalNAc), and fucose (Fuc). Their degree of sulfation and their anti-hyperlipidemic activities were investigated. Our results have shown that the efflux of cholesterol from HepG2 cells was highly dependent on the sulfation of their fucose branches.
flavonones hesperidin, eriocitrin and eriodictyol (100, 200 and 200 mg/kg body weight) for 4 weeks to induce oxidative stress, protecting against metabolic disorders resulting from obesity. In the present work we studied the effect of fCSs, especially fCS-Pg, could be used as a potential antihyperlipidemic drug.

AGFD 6 Advances in food packaging films from milk proteins

Laetitia Bonnaillie1, laetitia.bonnaillie@ars.usda.gov, Lucy Aburto1, Michael H. Tunick2, John Mulherin3, Monica Du4, Raymond Kwoczak5, Serife Akkurt6, Peggy M. Tomasula7, (1) Dairy & Functional Foods Research Unit, USDA, ARS, Wyndmoor, Pennsylvania (2) Food Sci., Rutgers Univ., New Brunswick, NJ (3) Chemical Engineering, Univ. of Delaware, Newark Most commercial petroleum-based food packaging films are poor oxygen barriers, do not biodegrade, and some are suspected to leach compounds into the food product. For instance, three-perfluorinated coatings were banned from convenience food packaging earlier this year. These shortcomings are a problem particularly with high-fat foods, which may solvate leached compounds faster and tend to oxidize. Packaging films made from milk proteins are excellent oxygen barriers, up to 500 times better than LDPE, and completely food-safe. In addition, they are hydrophilic and repel grease, can be eaten with the food product, and dissolve easily in hot or cold water. For these reasons, milk-based films are ideal candidates to coat convenience food packaging; layer between synthetic films to block oxygen; coat products to preserve them and carry additional nutrients; or, form increasingly-popular single-serve pouches, which can be either eaten or dissolved, generating zero waste. This presentation reports ARS' recent advances in strengthening casein-based, edible packaging films, to physically protect food products, as well as mediate their hydrophilicity to customize their resistance to environmental conditions and/or rate of dissolution and enable a broad range of applications, from cheese-stick wrappers to healthy cereal glace. The rheological, mechanical, thermal, structural, barrier and functional properties of solvent cast casein-based films and coatings are characterized using state-of-the-art, environmentally-controlled instrumentation such as DMA-RH, vapor-sorption analysis (VSA), oxygen permeability analysis, water vapor transmission, microscopy, and more. Due to the complex, charged, 3D structure of protein monomers, casein films are sensitive to many formulation and processing parameters, including the caseinate type (calcium or sodium) and concentration, polysaccharide cross-linkers, alkalinity of the suspension, film-casting parameters, and the environmental conditions during drying, storage and testing conditions are critical to the mechanical properties and shelf-life of these hygroscopic, versatile edible polymers.

AGFD 7 Establishing a working intestinal microbiota community in multi-phase structure from biopolymers

Lin S. Liu1,2, linshu.liu@ars.usda.gov, Jenni Firrmann3, Peggy M. Tomasula1,2, (1) USDA ARS ERRC, Wyndmoor, Pennsylvania (2) Dairy & Functional Foods Research Unit, Wyndmoor, Pennsylvania The in vitro investigation of foods or food ingredients on the human intestinal microbial ecology requires a stable working intestinal microbiota community, which only can grow in a multi-phase structure. The preliminary study evaluated the genotypic response of human gut microbiota to the change in the composition and ratio of bacteria the structure, as well as the extrusion and survival of a genetically modified bacterium in the host community.

AGFD 8 Triterpenoids from the Chinese hawthorn (Crataegus cuneata) fruits: Extraction, structure, quantification, and bioactivity

Tao Yuan, chinayuantao@hotmail.com. Xinjiang Technical Inst. of Physics and Chemistry, Chinese Academy of Sciences, Urumqi, Xinjiang, China Crataegus cuneata is a species of Chinese hawthorn, which was consumed as fresh fruits and its manufactured product, juice, in China. However, there is paucity of data on its constituents and bioactivity. The current study aims to optimize the extraction methods for total triterpenoids from the fruits of C. cuneata, identify (using MS and NMR) and quantify triterpenoids in the optimization extracts, and evaluate their anti-tyrosinase activity. The experiments revealed that ultrasound extract with the 95% methanol had the highest triterpenoid content (25.5 mg/g). Ultrasound extract was further enriched in the Sephadex LH-20 column chromatography. Seven triterpenoids (1-7) were isolated and identified from the enriched extract.

AGFD 9 - Withdrawn

AGFD 10 Alkaln suppression of the enzyme tyrosinase

Anne Murray1, afmurray@berkeley.edu, Hiro Satoaka1, Kuniyoshi Shimizu1, Warinthon Chavasin2, Isao Kubo1. (1) UC Berkeley, California, (2) Chulalongkorn Univ., Bangkok Essential oil from the leaves of Polygonum odoratum (Polygonaceae), commonly known as Vietnamese coriander a spice herb, inhibited tyrosinase (EC 1.14.18.1) catalyzed oxidation reactions. Tyrosinase (EC 1.14.18.1), a copper containing oxidase, is responsible for catalyzing the first steps of the melanin formation pathway. Twenty five scent compounds were characterized in the essential oil by GC-MS analysis. The alkalans dodecanal (55.49%) and decanal (11.57%) were the two most abundant in the essential oil, followed by anisaldehyde (6.35%). Dodecanal and decanal inhibited the oxidation of both L-tyrosine and L-3,4-dihydroxyphenylalanine (L-DOPA) catalyzed by mushroom tyrosinase. The enzyme was inactivated when the concentration of these alkalans in the reaction mixture exceeded a certain concentration. This is supported by changes in inhibition activity when both dopachrome formation and stirring oxygen consumption were monitored. When alkalans were tested below this concentration the inhibition activity was absent. There was also a strong time dependence, if the enzyme was preincubated with the alkalans below this concentration the activity was reversible. The alkalan tyrosinase inhibitory activity was surfactant like, in that there was a concentration dependent nonspecific disruption of the tertiary structure of tyrosinase.

AGFD 11 Citrus flavonones decreases oxidative stress in the liver and blood serum caused by highfat diet feeding in C57BL/6J mice

Paula S. Ferreira1, paula22@msn.com, Ana Lucia M. Nasser1, John A. Manthey2, Danielle Goncalves2, Thais B. Cesar2. (1) Food and Nutrition, Univ Estadual Paulista - UNESP, Araraquara, Sao Paulo, Brazil (2) USDA ARS, Fort Pierce, Florida High-fat diet and adipose tissue accumulation commonly leads to an increased oxidative stress and inflammation, contributing to the development of chronic diseases observed in obesity, such as diabetes mellitus and cardiovascular diseases. Citrus flavonoids have biological properties capable of attenuating oxidative stress, protecting against metabolic disorders resulting from obesity. In the present work we studied the effect of the citrus flavonones hesperidin, eriocitrin and eriodictyol (100, 200 and 200 mg/kg body weight, respectively) over oxidative stress in the blood serum.
and liver of C57BL/6J male mice fed highfat diet (45% kcal from saturated fat) for 30 days. Mice fed highfat diet showed visceral fat accumulation and increased TBARS levels in the blood serum (80%) and in the liver (57%), while hesperidin, eriocitrin and eriodictyol increased the serum total antioxidant capacity (7%, 9% and 6%, respectively) and decreased the TBARS levels in the liver (50%, 57% and 64%, respectively). Eriocitrin and eriodictyol also decreased the blood serum TBARS levels in 48% and 47%, respectively. In addition, the liver fat accumulation and damaged hepatocytes (observed by histology analyses) was efficiently reduced by hesperidin and eriodictyol, and the serum levels of LDLC was reduced in 28% by hesperidin. These results showed that hesperidin, eriocitrin and eriodictyol have protective effect against oxidative stress caused by high-fat diet feeding in mice, as indicated by reduced liver damage, liver fat accumulation, and TBARS levels in the liver or serum, making them potential candidates to prevent tissue damage and the development of metabolic dysfunction associated to chronic diseases caused by obesity.

AGFD 12 Bioactive glucitol-core containing gallotannins from red maple (Acer rubrum) inhibit melanogenesis via down-regulation of tyrosinase and melageneic gene expression in B16F10 melanoma cells Hand Ma, hang_ma@uri.edu, Jialin Xu, Liangran Guo, Wei Lu, Navindra P. Seeram. Biomedical and Pharmaceutical Sciences, College of Pharmacy, Univ. of Rhode Island, Kingston Our group has previously isolated a series of bioactive glucitol-core containing gallotannins (GCCs) from the red maple (Acer rubrum L.) species, namely ginnalins A-C and several new compounds, named maplexins A-I, with potent antioxidant capacities. Herein, we investigated the cosmetic skin lightening/whitening applications of a standardized red maple leaf extract (Maplica™), contains ca. 45-50% ginnalin A and other GCCs in enzyme and cell based assays. Pure ginnalins A-C (used as representative GCCs in Maplica™) were assayed for their inhibitory effects on melanin production in murine melanoma B16F10 cells. At 50 µM test concentrations, ginnalin A (contains 2 galloyl groups) reduced the melanin content whereas ginnalins B and C (contain 1 galloyl group each) showed only minor anti-melanogenic effects. The mechanisms of the inhibitory effects of ginnalins A-C on melanogenesis in B16F10 cells were elucidated by real-time PCR and Western blot experiments. The results indicated that ginnalin A-C down-regulated the expression of MITF, TYR, TRP-1 and TRP-2 gene levels in a time and concentration-dependent manner and significantly reduced the protein expression of the TRP-2 gene. Our findings suggest that GCCs derived from red maple leaves possess anti-melanogenic effects and thus may have cosmetic skin-whitening applications.

AGFD 13 Binding of polyphenols to transport proteins William Butler, wb1016@wildcats.unh.edu, Salwa Harbi, Joe A. Vinson. (1) Chemistry, Univ. of Scranton, Dalton, Pennsylvania (2) Univ. of Scranton, Chemistry Dept., Penns. The importance of polyphenols for disease prevention is becoming well-known to the public and increasingly studied by chemists. Our group’s hypothesis is that these compounds, the major antioxidants found in plant-derived foods, aid in the prevention of cancer, diabetes, cardiovascular, and neurodegenerative diseases due to their ability to stabilized free radicals in the body. Polyphenols, which upon absorption are metabolized in the gastrointestinal tract by microbial and hepatic enzymes, are carried to cells and tissues by proteins in the plasma; most notably albumin, the major protein in plasma, and the lipoproteins LDL and HDL. There are published reports that such binding protects the lipoproteins from in vivo oxidation as the polyphenols are powerful antioxidants. We have indirect evidence from plasma spiking experiments with pure polyphenols and beverages which showed that the LDL is protected from ex vivo oxidation. Also we have done a beverage and fruit juice human supplementation experiment where the LDL obtained from plasma post-consumption was more protected from ex vivo oxidation than that from pre-consumption. Our research group has used a new affinity column method to separate protein-bound polyphenols in an ex vivo porcine plasma model. We have shown that Quercetin, a flavonol, spiked at 10 µM, is carried in plasma by albumin 60%, 21% by HDL and 18% by HDL. Catechin, a flavanol, is carried by albumin 37%, 15% by LDL and 48% by HDL. Thus the protein distribution of bound polyphenols is critically dependent on the polyphenol structure.

AGFD 14 Internal exposure of hemoglobin adducts of glycidamide enantiomers and acrylamide and the chemoprevention effect by catechins in rats Qiao Wang, wangqiao8577@zju.edu.cn, Jun Cheng, Yu Zhang. (1) Dept. of Food Sci. and Nutrition of Food Sci. and Nutrition, College of Biosystems Engineering and Food Sci., Zhejiang Univ., Hangzhou, Zhejiang, China (2) Zhejiang Key Lab for Argo-Food Processing, Zhejiang R & D Center for Food Tech. and Equipment testing, Zhejiang Key Lab for Argo-Food Processing, Zhejiang R & D Center for Food Tech. and Equipment, Fuli Inst. of Food Sci., Zhejiang Univ., Hangzhou, Zhejiang, China. Hemoglobin (Hb) adducts of acrylamide (AA) and its oxidative metabolite glycidamide (GA) are important biomarkers for evaluating the mid-term internal exposure of acrylamide toxicity in vivo. Few study focused on the chemoprevention of AA and GA in their forms of Hb adducts in mammal. Taking pentafluoro-2-methylphenyl isothiocyanates of N-(2-carbamoylethyl) valine (AA-VAL-PTh) and N-(2-carbamoyl-2-hydroxyethyl) valine (GA-VAL-PTh) as target analytes, we developed an isotope dilution ultra-high performance liquid chromatograph tandem mass spectrometry (UHPLC-MS/MS) method for the simultaneous determination of AA and GA Hb adducts under the electroscopy ionization negative (ESI-) mode in the present study. Among them, enantiomer pairs GA-VAL-PTh were firstly identified and successfully separated at baseline level. The limit of detection (LOD) and limit of quantification (LOQ) of the analytes ranged 1.6-1.8 ng/mL and 5.4-6.0 ng/mL, respectively. Acceptable within-Lab reproducibility (RSD < 11.17%), reliable pretreatment procedures, favorable spiking recovery (97.0%-111.2%) and short analysis time (12 min per sample) substantially supported the employment of this proposed method as an quantitative tool for the analysis of AA and GA Hb adducts. For mid-term internal exposure evaluation of acrylamide, Sprague-Dawley rats were orally administered with 1 mg/kg b.w., 10 mg/kg b.w. and 50 mg/kg b.w. of acrylamide, resulting in 0.39-0.48 nmol/g Hb, 1.43-2.42 nmol/g Hb and 10.31-14.21 nmol/g Hb for AA adduct, respectively, and 0.65-0.73 nmol/g Hb, 4.89-5.14 nmol/g Hb and 16.41-19.18 nmol/g Hb for GA adduct, respectively. The ratio of GA adduct to AA adduct ranged 1.4-3.6. For the chemoprevention work, rats were administered with acrylamide exposure (10 mg/kg b.w.) and intervened with either of catechins [extract of tea polyphenols, epicatechin (EC) or epigallocatechin gallate (EGCG)]. Compared to adduct levels in control group (10 mg/kg b.w. via oral gavage), the GA and total Hb adduct levels in blood of male rats in the EC intervention group significantly decreased by 23.3% and 18.6%, respectively. Our study revealed that EC mainly contributes to the decrease of acrylamide hemoglobin adducts via its oxidation pathway in male rats rather than female rats. This finding indicated that the 3-hydroxyl functional group of flavonoids may play an important role in the chemoprevention of acrylamide in vivo.

AGFD 15 Inhibitory effects of a phenylacetaldehyde-flavonoid adduct, 6-(E-phenylethenyl)naringenin, on human colon cancer cells Yueliang Zhao, yueliang2013@hotmail.com, Mingfu Wang. School of Biological Sciences, The Univ. of Hong Kong. Inhibition of mutagenic PhIP formation with the addition of a flavonoid naringenin gives rise to a novel adduct 6-(E-phenylethenyl)naringenin (6-
However, despite storage at low temperatures, even after short periods, a loss in freshness and changes in the aroma profile from concentrate by remixing and addition of water. An AGFD 20 Changes in key orange juice aroma compounds during chilled manufacture juice and aroma fractions, which are finally used to manufacture juice.

Blueberry cultivars (‘Bluecrop’ and ‘Elliot’) were isolated using solvent wash Column, ethyl 2-pyrroline (2AP). The most accurate ones among these are based on stable isotope dilution analysis (SIDA). In SIDA, an isotopically labeled internal standard (both deuterium- and 13C-labeled 2AP have been used) is spiked into the matrix and allowed to equilibrate prior to extraction. This insures that the ratio of natural substance (unlabeled target compound) and the labeled internal standard is maintained throughout the entire analysis procedure, including analysis by GC-MS. Even with SIDA, one must also consider the chemical stability of both the unlabeled target compound and isotopically labeled internal standard, as well as the extraction efficiency for tightly bound or matrix entrapped 2AP molecules. This is especially problematic in the case of rice, where temperatures above the gelatinization temperature of rice starch are required to release 2AP. Another concern is that it is not possible to equilibrate the labeled internal standard in rice matrix prior to the extraction procedure. Over the last few decades, researchers have developed procedures for maximum 2AP extraction from rice, but the accuracy of these methods has not been demonstrated. This study evaluated the accuracy and precision of a procedure developed nearly two decades ago for the high throughput extraction and analysis of 2AP in aromatic rice [Cereal Chem 2000, 77, 454-458]. The updated procedure includes SIDA, employing 13C2-2AP as the internal standard. Both stability and extraction efficiency for 2AP were evaluated. It was found that that 2AP, spiked at 500 ppb in a non-aromatic rice, was stable during extraction for up to 120 to 150 min. Meanwhile, maximum extraction of 2AP from an aromatic rice was achieved after 120 min. Therefore to achieve the most accurate determination of 2AP in aromatic rice by this method an extraction time of 120-150 min is recommended. Results of studies relating this method with other previously published methods used for determination of 2AP in rice will be discussed.

AGFD 19 Odor active compounds and their chiral compositions in Bluecrop and Elliot blueberry Danni Zhang1,2, YanPing L. Qian3, yan.ping.qian@oregonstate.edu, Michael C. Qian1. (1) Oregon State Univ, Corvallis (2) Crop and Soil, Oregon State Univ., Corvallis (3) College of Food Sci. and Tech., Nanjing Agricultural Univ., China The increased interest in the health benefits of antioxidant compounds in blueberries has promoted research to address the fruit quality of blueberry, especially in flavor quality. Odor active compounds in two blueberry cultivars (‘Bluecrop’ and ‘Elliot’) were isolated using solvent-assisted flavor evaporation, and aroma compounds and their chiral isomer aroma composition were characterized using aroma extract dilution analysis on a ZB-wax column and a CycloSil-B chiral column. Overall, the aroma intensity in ‘Bluecrop’ was higher than that in ‘Elliot’. According to flavor dilution factor (FD value) determined on the ZB-wax Column, ethyl 2-methylbutyrate, ethyl 3-methylbutyrate, 1-octen-3-one, methional, linalool, 2,6-nonadienal, α-terpineol, β-damascenone, geraniol, phenethyl alcohol, eugenol and vanillin were found to be the prominent contributors in these two blueberry cultivars. AEDA-chiral contribution analysis showed that (R)-linalool had higher FD value than (S)-linalool, although (S)-linalool was dominate in both blueberry cultivars.

AGFD 20 Changes in key orange juice aroma compounds during chilled storage of NFC juice Peter H. Schieberle, peter.schieberle@lrz.tum.de, Veronika Mall, Ines Sellami. German Research Center for Food Chemistry, Freising, Germany Due to its characteristic aroma and taste, orange juice belongs to the most demanded fruit juices in Europe and in the US. To guarantee its availability throughout the year, the juice is often concentrated to obtain a concentrate and aroma fractions, which are finally used to manufacture juice from concentrate by remixing and addition of water. Another option is storage at low temperatures in aseptic tanks to obtain the NFC juice. However, despite storage at low temperatures, even after short periods, a loss in freshness and changes in the aroma profile is often observed.
Numerous investigations were already performed to clarify such changes in the organoleptic properties of orange juice during processing and storage on a molecular basis. However, up to now, in particular the fate of important juice odorants, such as aldehydes, still remains open. To get an insight into the changes in key aroma compounds, changes in the concentrations of selected key aroma compounds were monitored by application of the Sensomics concept over a period of one year. To clarify the reason for the degradation of e.g., saturated aldehydes as well as of 1-pentene-3-one, systematic model studies were carried out using isotopically labelled precursors. The structures of the new degradation products identified by means of LC-MS/MS and NMR experiments will be discussed in detail.

AGFD 21 Shelf-life challenge of savory snacks with colored vegetables C. T. Shao1, Tony.shao@fritolay.com, Vincent A. Elder1. (1) R&D, PepsiCo, Inc., Plano, Texas, (2) R&D, PepsiCo, Inc., Plano, Texas Global snack sales totaled $374 billion annual ending March 2014, and Europe ($167 billion) and North America ($124 billion) were the major regions (Nielsen, 2014). Health is an important snack selection criterion for half of adults (Technomic 2014b). Salty snack sales in US reached $22 Billion in 2015 (Packaged Facts, 2016). Healthy snacks with vegetables, such as spinach or green beans, contain phyto-nutrients and contribute to daily servings of green vegetables. Sweet potato chips contain fiber, beta-carotene and antioxidants. However, the shelf-life of snacks with colored vegetables is normally shorter than similar snacks without colored ingredients. If exposed to light in clear packaging, photooxidation of snacks with green vegetables is rapid because chlorophyll is a potent photosensitizer. Metalized packaging film with low light transmission does not completely eliminate photooxidation if package is exposed to light during shelf life. Beta-carotene in sweet potato is considered to be an antioxidant. However, beta-carotene can also act as a pro-oxidant after light exposure during processing resulting in rapid auto-oxidation during storage. There are many approaches to maintain the desirable shelf-life for savory snacks with vegetables, such as using aluminum foil to minimize light transmission or maintaining low oxygen content in the package. However, packaging requirements for shelf life will add to product cost. To maintain the desired shelf-life and include healthier ingredients in practical way can be a challenge.

AGFD 22 Oiling-out effect of aroma compounds Hiroshi Tamura1, tamura@ag.kagawa-u.ac.jp, Shoko Ueno1, Azusa Naka1, Ami Fukuzumi1, Stephany Ho1, Mala Nattawadee1,2, Sujinda Sriwattana2, Lina Yonekura1. (1) The Graduate School of Agriculture, Kagawa Univ., Takamatsu, Japan (2) Faculty of Agro-Industry, Chiang Mai Univ., Chiang Mai, Thailand Aroma compounds in oily foods such as edible oils, butter, sesame oil, olive oil and other oils are hard to isolate because of the similarity of the polarity of volatile compounds with oils such as triglycerides and phospholipids. Distillation technique such as SDE, SAFE, vacuum distillation and headspace gas analysis using SPME adsorbents are considered as nicer systems of the isolation matter. However, top notes and/or base notes of the aromas might be lost by the distillation system. So, solvent extraction with methanol and hexane as a mild separation technique for isolation of aroma compounds in edible oils was developed for the characterization. So, solvent extraction method coupled with a porapack Q column will be reported as an efficient separation method for volatile compounds. It was found that the solvent extraction method was applicable for ordinal aroma extraction of natural plants, meaning that it is quite one of general extraction methods with a wide range of application.

AGFD 23 Identification of bioactive components in wheat bran: An example of team science Shengmin Sang, ssang@ncat.edu. Lab for Functional Foods and Human Health, Center for Excellence in Post-Harvest Technol, North Carolina AT State Univ., Kannapolis What are the active components in a specific food is a complex scientific question to answer. Often time, it requires a cross-disciplinary team science approach, which aims at enhancing the processes and outcomes of team-based research. In this lecture, I would like to use our study on the bioactive components in wheat bran as an example to demonstrate the complexity of the phytochemicals in a specific food and the importance of collaborative research. We used a comprehensive approach to elucidate the active components in wheat bran including bioassay-guided purification, natural product chemistry, synthetic chemistry, analytical chemistry, and biological assays. We have identified 14 alkylresorcinols, 19 sphingolipids and 21 steroids from wheat bran, established their chemical profiles, and elucidated colon cancer preventive effects. These results help us to pinpoint the major components and the active components in wheat bran for colon cancer prevention.

AGFD 24 Characterization of oligomeric anthocyanins and proanthocyanidins from red grape pomace by mass spectrometry (MALDI-TOF and ORBITRAP ESI-MS) Erika Salas, esalas@uch.ac.mx. Facultad de ciencias Quimicas, UACH, Chihuahua, Mexico Phenolic compounds are essential for the quality of food products derived from fruits, especially in wine; phenolic compounds are responsible for the color and astrignency of red wines. Red grape pomace by-product, usually considered a waste from red winemaking, was used as a source of phenolic compounds. 2 phenolic extracts were made, one from red grape pomace and another from grape seed, and were fractionated first by liquid-liquid extraction with hexane. The aqueous fractions were fractionated by low-pressure chromatography on Toyopearl HW-40 gel and on C18. Different fractions were obtained by sequential elution with aqueous/organic solvents, and then analyzed by mass spectrometry. The polyphenolic composition of red wine pomace, and the fractions obtained from it, was characterized by the means of mass spectrometry analysis using two different techniques: MALDI-TOF-TOF MS and ORBITRAP MS (coupled to an HPLC/DAD), phloroglucinolysis was also performed on each grape seed fraction in order to estimate a mean degree of polymerization. HPLC/DAD/MS is very complementary to MALDI-TOF-TOF analysis. On one hand HPLC/DAD/MS provides the means to make peak assignments and acquire quantitative data by relying on UV-VIS data and mass spectra data. On the other hand MALDI-TOF-TOF analysis is the ideal technique for the analysis of complex mixtures as it produces only a singly charged molecular ion for each parent molecule. Red wine pomace is a good source of anthocyanin-based pigments (both native and derived), mass spectrometry analysis showed that one of the late eluting fractions (obtained with 100% organic solvent in low pressure chromatography) was particularly enriched in less hydrophilic pigments. This fraction was mainly composed of coumaric derivatives of anthocyanins (monomers and oligomers). Mass spectrometry (MALDI-TOF) methodology was developed in order to optimize the detection of oligomeric anthocyanins hence oligomers of coumaroylated anthocyanins (up to trimers) were detected.

AGFD 25 Development of specific dietary biomarkers to better capture whole grain wheat exposure and beneficial health effects Yingdong Zhu, yzhul@ncat.edu. Center for Excellence in Post-Harvest Technol, North Carolina AT State Univ., Kannapolis Whole grains (WG) are recognized for their potential roles in preventing risk of major chronic diseases, such as cancers, cardiovascular disease, and type 2 diabetes. However, findings are inconsistent due possibly to recall bias and measurement errors. For this reason, there is a pressing need for
dietary biomarkers to better capture exposure. In addition, the mechanisms underlying protective effects of WG intake are not fully understood yet. We isolated and identified that 5-alk(en)ylresorcinols (ARs) as the major active components in wheat bran (WB) inhibit growth of human colon cancer cells HCT-116 and HT-29, and further demonstrated anticancer properties of ARs based on synthetic short-chain ARs and analogues. Continuing along this line of research, we revealed that sphingolipids in WB may be implicated in colon cancer prevention as a component of this bioactive food. Likewise, we determined that oxyphytosterols in wheat may greatly contribute to the observed health effects of WG consumption. In light of the specificity of bioactive ARs in wheat and rye, we investigated the metabolism of ARs in humans and in mice, and unveiled two new AR metabolites as potential biomarkers for WG consumption in a diet-controlled trial. We further explored specific dietary biomarkers and endogenous changes in humans after WG consumption, using a combination of nontargeted and targeted metabolomics approach. In conclusion, we developed a panel of markers consisted of WG phytochemical metabolites as specific biomarkers to better capture WG intake, and also determined endogenous changes that are linked to health effects of WG consumption.

**AGFD 26 Integrating traditional disciplines to develop novel technologies to address agricultural and environmental issues** Rong Li, Rong.Li@deq.idaho.gov. Idaho Dept. of Environmental Quality, Boise This presentation will provide an overview of integrating traditional disciplines to develop novel technologies to address agricultural, environmental, and societal issues. Pesticides have adverse effects on human health, and recent research raised new concerns about low-dose pesticides because they were linked to the decline of bees that are important pollinators. We developed a multi-media fate and chemical transport modeling system for pesticides. Our modeling system is used to identify the major sources of pollutants to water resources. The pollutants in water resources have local sources such as leaching and surface runoff from nearby poorly managed agricultural fields, as well as remote sources from which pollutants can be emitted and transported through the atmosphere and deposited into the watershed. However, accurate quantification of the long-range transport and deposition of pollutants has been a challenge. Our modeling system was used to quantify long-range transport and deposition of pesticides from agricultural ecosystems and soils to sensitive water resources. The modeling system also provides the spatial distribution of pesticides that may be important for risk assessments of bees. In addition, we will introduce a coupled terrestrial and land modeling system that can be used for studying ecosystem-climate interaction. We also studied interactions among climate, hydrological cycle, wildfires, and air quality. These studies demonstrate that integrating multiple disciplines is required in order to address complex agricultural and environmental issues.

**AGFD 27 Structural and functional studies of ice nucleation protein and its applications in food industry** Li Zhang, zhanglingjau@gmail.com. Food Sci , Rutgers Univ. , Edison, NJ Erwina herbicola is Gram-negative bacteria that causing severe frost injury to economically important plants, and this is due to surface located ice nucleation protein (INP). INP's function as ice nucleators that help shorten freezing time while increase nucleation temperature. However, it has not been wildly used in food industry for little is known about the structure and its mechanism to facilitate ice formation. Also, its pathogenic property poses great concerns to food safety. In this study, we construct a new plasmid that carries the inaA gene that expressed in E.coli system through molecular methods. Through investing different parameters such as expression temperature, competent cells and etc., high yield of INP could be achieved. And it could be further purified through Histag column. Based on this, different models could be created to test INP effects in frozen foods.

**AGFD 28 Understanding the ligand specificity of bitter taste receptors in humans and cats** Joseph Rucker¹, jrucker@integralmolecular.com, Anu Thomas¹, Jason Goodman¹, Michelle Sandau², Chidananda Sulli¹, Thomas Charpentier¹, Edgar Davidson¹, Nancy Rawson¹. (1) Integral Molecular, Philadelphia, Pennsylvania, (2) AFB International, St. Charles, Missouri Bitter taste perception is mediated by the highly divergent TAS2R receptor family of G protein-coupled receptors (GPCRs). TAS2Rs expressed in taste and other chemo sensory cells detect the extraordinary diversity of bitter compounds found naturally in foods and toxins, translating that detection into gustatory perception via G protein coupled signaling. The lack of direct structural information for TAS2Rs (and most GPCRs) limits our understanding of the structural features responsible for ligand binding and signaling. Using high-throughput shotgun mutagenesis mapping we created a comprehensive mutation library for human TAS2R16 with defined mutations at every residue, and screened each mutant’s functional activity in response to unique ligands, both agonists and inhibitors, using a calcium-flux signaling assay. We identified residues whose substitution abrogated signaling for all agonists, as well as residues important for the activity of only specific ligands. These critical residues define both the binding sites for various TAS2R16 ligands as well as motifs important for signal transduction, increasing our structural understanding of TAS2R function. In a complementary approach to understanding TAS2R structure and function, we have cloned the sequences for domestic cat TAS2Rs and deorphanized many of these receptors using our calcium-flux signaling assay. We demonstrate that the response profiles of cat TAS2R38 and TAS2R43 are distinct from those of their human homologs. Human and feline TAS2R38 both respond to phenylthiocarbamidate (PTC), the prototypical TAS2R38 ligand, but show drastically different sensitivities to other known TAS2R38 ligands. Similarly, both human and feline TAS2R43 respond to aloin but differ in sensitivity and specificity to other TAS2R43 ligands. Comparative studies of the human and cat receptors should allow a better understanding of the residues important for ligand specificity. Future work will deorphanize additional cat bitter taste receptors and test identified compounds perceptually in cats.

**AGFD 29 Single-site catalysts in the production of polyolefins for food contact applications** Raymond Briñas³, raymondpeter.brinas@fsa.hhs.gov, LaShonda T. Cureton¹, Allan B. Bailey². (1) Center for Food Safety and Applied Nutrition, FDA College Park, Maryland (2) Center for Food Safety and Applied Nutrition, FDA College Park, Maryland Single-site catalysts (SSCs) are those whose metal ion is in a constrained geometry that allows for specific access by the monomer to the active site, resulting in more reproducible and defined structures. SSCs include metallocene and post-metallocene catalyst systems. Recently, we have reviewed several food contact notifications that employed SSC in the manufacture of polyolefins (PO) used for food packaging. Our reviews prompted several fundamental questions on their fate in PO manufacture, including the safety of decomposition products. As part of our post-market evaluation of food contact materials, FDA has initiated a project to gather information, available in Agency files and the open literature, on the identities of SSCs used in PO manufacture, their decomposition products, migration levels in food or food simulants, and estimates of consumer exposure. Our findings based on our survey of the open literature and Agency files regarding the decomposition behavior and fate of the decomposition products of SSCs will be discussed in this presentation.
AGFD 30 Enhanced anti-inflammatory efficacy of Calebin-A encapsulated in modified starch Lynn Perera, flynn_acatanoe@yahoo.com, Min-Hsiung Pan, Yu-Wen Ting. Inst. of Food Sci. and Tech., National Taiwan Univ., Taipei, Taiwan Calebin-A is a natural phytochemical from the rhizomes of turmeric (Curcuma longa) that has anti-cancer and anti-adipogenesis properties. However due to its exceedingly low aqueous solubility, the therapeutic potential of calebin-A is greatly limited in the animal body due to its poor absorptivity and low bioavailability. To deliver the hydrophobic calebin-A into an aqueous environment, it was encapsulated with food-grade hydrophobically modified starch to form polymer micelles and thereby increase the bioavailability and efficacy. It was shown that encapsulated calebin-A has increased aqueous solubility compared to native calebin-A. In mice with dextran sulfate sodium (DSS)-induced colitis, encapsulated calebin-A placed in drinking water significantly reduced the protein level of COX-2, iNOS and decreased the secretion of TNF-α. Encapsulated calebin-A ameliorated the colonic structure of the colitis mice while native compound showed rare improvement. These results indicated that the bioaccessibility and anti-inflammatory efficacy of calebin-A could be significantly improved through encapsulation with a food-grade biopolymer system. This finding will be a good reference to future development of delivery system for hydrophobic compound into food matrix.

AGFD 31 Role of novel multi-starter on the generation of volatile compounds in buckwheat (Fagopyrum sculentum) soksungjang according to fermentation period Min-Kyung Park, Hye-Sun Choi, Young-Suk Kim, In Hee Cho, inheecho@vku.ac.kr. (1) Department of Food Sci. and Engineering, Ewha Womans Univ., Seoul, Korea (2) Division of Food and Environmental Sciences, Wonkwang Univ., Iksan-city, Jeonbuk, Korea (3) Dept. of Food Sci. and Engineering, Ewha Womans Univ., Seoul, Korea (4) Dept. of Agrofood Resources, National Academy of Agricultural Science, Wanju-gun, Jeonbuk, Korea. Fermented soybean products have been enjoyed for hundreds years in Asia. Buckwheat soksungjang (BS) is one of Korean traditional fermented soybean products, and generally manufactured with buckwheat and soybeans during relative short fermentation period unlike other Korean soybean products (e.g., Deonjang, Gochujang, and soy sauce). To study on the role of starters on the generation of volatile compounds in BS, we compared volatile profiles between BS traditionally manufactured and newly manufactured by inoculating with novel multi-starters, Aspergillus oryzae (PS03) and Bacillus subtilis (RD7-7), which were isolated from Korean traditional fermented soybean products, and generally manufactured with buckwheat and soybeans during relative short fermentation period unlike other Korean soybean products (e.g., Deonjang, Gochujang, and soy sauce). It was performed to assess changes in the volatile compounds according fermentation periods. Both BS had different patterns on the change in the volatile compounds according to fermentation period. In the early stage of fermentation (0d→1w→2w), volatiles contributed to the change of traditional BS were butanal, dimethyl carbonate, and pentyl propionate, whereas 3-hydroxy-2-butanoic (acetoin), dimethyl carbonate, ethyl formate and 2-ethyl-1-hexanol were major compounds in BS with novel multi-starter. On the other hand, volatile compounds mainly associated with later stage of fermentation (2w→5w) in traditional BS were benzeneethanol, 2-methyl-1-propanol, 3-methyl-1-butanol, and 2-methoxy-4-vinylphenol, but, methyl-4-methyl-3-pentenoate, methyl tridecanoate, tetramethylpyrazine, and 2-phenylpropenal were important contributors to the change in later stage of fermentation (2w→5w) of BS with novel multi-starter.

AGFD 32 Preparation of carbon adsorbent from apple pomace waste aiming removal of estriol from water bodies Suzimara Rovani, susziquimica@gmail.com, Amanda G. Rodrigues, Leonardo Medeiros, Renato Cataluna, Eder Lima, Andrea N. Fernandes. (1) Material Science, Federal Univ. of Rio Grande do Sul, São Paulo, Brazil (2) Inst. of Chemistry, Porto Alegre, Brazil (3) Center for Chemical and Environmental Tech. (CQMA), Nuclear and Energy Research Inst., Sao Paulo, Brazil (4) Inst. of Chemistry, Federal Univ. of Rio Grande do Sul, Porto Alegre, Rio Grande do Sul, Brazil. Carbon adsorbents (CA) are known as an excellent material for removal of organic contaminants due to its large adsorption capacity, but due to its high costs of production, nowadays there is an interest for organic matrix precursors alternatives to reduce the total cost of production of the CA. Agro-industrial wastes have shown promising results for production of carbon adsorbents, because of their availability at low cost. Many organic contaminants can be potentially actives in the biological systems, promoting alterations in human beings and animals, such as the endocrine disruptor compounds (EDC): estriol (E3), estrone (E1), 17β-estradiol (E2). These compounds have shown adverse effects on fishes in environmental in contaminations in the range of ng L⁻¹. This way, a new carbon adsorbent was prepared from apple pomace waste (APW) by pyrolysis at 800°C and subsequent acid wash with HCl 6 mol L⁻¹. The material was characterized by a combination of spectroscopic and chemical techniques. Furthermore, APW carbon prepared was used as adsorbent in the removal of E3 from aqueous solutions. Factors that can affect the adsorption process as pH, initial E3 concentration and contact time have been investigated. The results of characterization of the APW carbon manufactured showed the material presents potential to be employed as adsorbent. The microscopy images showed the carbon has a high surface roughness. The value of the point of zero charge (pH_ROC) of the APW carbon was ~5, above this value the carbon has a negative surface charge and positive below. The maximum E3 removal was found at pH values between 6.0 and 9.0. The adsorption kinetic study was carried out in a pH 6.5 solution. As regards applicability of APW carbon, the percentage of E3 removal from aqueous solution was 75% in 24 h of contact time. These aspects demonstrate the potential of the agro-industrial wastes as new adsorbents for removal of endocrine disruptor compounds from aqueous solution.

AGFD 33 Comparison of mineral contents in vegetables (white cucumber, red paprika, water parsley and kohlrabi) undergoing different cooking methods Jinhoong Hwang, hwangjh@kfri.re.kr, Dongwon Seo, dwseo@kfri.re.kr, Soyoung Kim, mwsh324@naver.com, Eun-joo Park, Park.Eun-Joo@kfri.re.kr, Hyun-Jeong Kim, sarikhj@kmu.ac.kr, Sam-Pin Lee, splee@kmu.ac.kr, Mi-Ok Yang, miokyang@wvu.ac.kr. (1) Food Analysis Research, Korea Food Research Inst., Seongnam, Gyeonggi, Korea (2) Traditional Microorganism Resource, Keimyung Univ., Daejeon, Korea (3) Medicine & Healthcare Dean of Graduate School, Wonkwang Digital Univ., Iksan, Korea. This study attempted to compare minerals contents in vegetables undergoing eight cooking methods such as raw materials, boiling, pan-frying, stir-frying, deep-frying, steaming, roasting and microwave. The vegetable samples, including white cucumber, red paprika, water parsley and kohlrabi were provided by Ministry of Food and Drug Safety (MFDS). The sample was prepared with different cooking methods and then it was digested with 8 mL of HNO3 and 2 mL of H2O2 using the microwave. This solution was cooled and diluted with deionized water. Diluted solution was injected into the inductively the coupled plasma optical emission spectrometry (ICP-OES) and the inductively coupled plasma mass spectrometer (ICP-MS) to determine minerals (Na, Ca, K, P, Mg, Fe, Mn, Se, Cu and Zn). Most minerals of water
parsley showed the highest content among the samples. The highest content was found in the samples cooked by deep-frying. However, the lowest content was in raw water parsley and the other samples cooked by boiling. Potassium for macro-minerals and iron for micro-minerals had the highest content. Hence, it is expected that the mineral contents could be used as nutritional food ingredient database for national health promotion. *This research was supported by a grant (15162MFD039) from Ministry of Food and Drug Safety in 2015.

AGFD 34 Edible packaging: improved strength and thermal stability of casein films with citric pectin Lucy Aburto, munhel@gmail.com, Laetitia Bonnaillie, Peggy M. Tomasula. Dairy & Functional Foods Research Unit, USDA, ARS, Wyndmoor, Pennsylvania  Calcium Caseinate-Glycerol (CaCN/Gly) based films show promising viability as non-toxic, 'green' and edible packaging to protect foods during transport and storage; especially with the addition of citric pectin (CP). In previous works, dynamic mechanical analysis of CaCN/Gly films under controlled humidity (DMA-RH) demonstrated their strength but high sensitivity to T and RH, with a melting point as low as 46°C at 50% RH. In another study, CP displayed complex molecular interactions with CaCN, depending on CP content and formulation of the film-forming suspension. DMA-RH is employed here to quantify the thermo-mechanical response of dried CaCN/Gly/CP films at 50% RH when CP concentration of the suspension is adjusted. Absolute values and shifts of the storage modulus (E'), loss modulus (E''), phase angle (tan-δ) and creep-displacement (D) of films during a slow 5°C-90°C temperature ramp reveal changes in the molecular network and its viscoelastic properties during heating. As with CaCN/Gly films, CaCN/Gly/CP possess two secondary transitions temperatures and a melting point (T_m). Adding 2 to 5% CP progressively raises E' and lowers tan-δ, indicating a denser, more elastic network; and lengthens the E'' and D plateaus before melting, suggesting improved thermal stability, before rupture of the main inter-molecular bonds around T_m. Microscopy confirms these results and shows markedly smoother film surfaces with increased %CP. However, above 4% CP, excessive viscosity renders the suspensions difficult to process and cast. Optimally, the addition of 3% CP increases T_m of CaCN films by over 10°C and considerably strengthens and stabilizes the films, enabling a broad variety of possible applications.

AGFD 35 Determination of structural amino acids in bamboo shoot, tomato and corn undergoing different cooking methods using automated amino acid analyzer Dongwon Seo1, dwseo@kfr.re.kr, Won-Jin Yoon1, Hyunjun Lee1, Jinbong Hwang1, Mi-Ok Yang2. (1) Food Analysis Center, Korea Food Research Inst., Seongnam, Gyeonggi, Korea (2) 2Dept. of Oriental Medicine & Healthcare Dean of Graduate School, Wonomwang Digital Univ., Ilsan-si, Jeolla, Korea  The goal of this study was to analyze the structural amino acids (aspartic acid, serine, glutamic acid, glycine, histidine, threonine, arginine, alanine, proline, tyrosine, valine, methionine, lysine, isoleucine, leucine, phenylalanine) contents in bamboo shoots, tomatoes and corns. The eight kinds of different cooking methods were conducted with raw materials, boiling, pan-frying, stir-frying, deep-frying, steaming, roasting and microwave. Analysis of amino acid in foods were hydrolyzed with 6N HCl and then analyzed using automated amino acid analyzer. The automated analysis of the amino acids was performed on an ion-exchange packed column separation with a visible detector. In bamboo shoots, the contents of aspartic acid ranged from 308.4±24.3 (boiling) to 736.8±85.1 (deep-frying) mg/100g. The amounts of glutamic acid detected in tomatoes ranged from 462.3±89.7 (boiling) to 552.6±69.9 (deep-frying) mg/100g. For corns, the concentration of glutamic acid ranged from 477.3±27.9 (raw materials) to 652.1±69.8 (deep-frying) mg/100g. The highest content was found in the samples cooked by deep-frying. However, the lowest content was in raw corns and the other samples (bamboo shoots and tomatoes) cooked by boiling. * This research was supported by a grant (15162MFD039) from Ministry of Food and Drug Safety in 2015.

AGFD 36 Aroma composition of kale (Brassica oleracea L. Var.) tea In Hee Cho1, inheecho@wkku.ac.kr, Jeongyoon Oh2. (1) Division of Food and Environmental Sciences, Wonkwang Univ., Iksan-city, Jeonbuk, Korea (2) Dept. of Food Sci. and BioTech., Wonkwang Univ., Iksan-city, Jeonbuk, Korea  In recent, there has been an increasing demand by consumers for food products having health benefits, food safety, and desirable organoleptic qualities. Kale, one of vegetable cultivars within the plant species Brassica oleracea, has been known as a super food due to not only low calorie but also high level of nutrition, such as fiber, iron, calcium, vitamin A, B, C, and K, antioxidants (carotenoids and flavonoids), omega-3 fatty acids, and so on. It has been mainly consumed as raw material, e.g., salad or saasm (literally meaning ‘wrapped’ and referring to a dish in Korean cuisine), in the world. In our group, kale tea (aqueous extract of kale leaves roasted by thermal processing) was developed and has more attractive flavor characteristics and longer shelf life compared with fresh one. In general, a thermal treatment can improve flavor characteristics and extend the shelf life of vegetable-based food materials. In this study, kale leaves were roasted at three different temperatures and compared the preference by consumer test for appropriate roasting condition. And then, the aroma composition of kale tea was profiled using GC-MS. A total of 78 volatile compounds were identified in kale tea, including 23 acids and esters, 16 pyrazines, 11 alcohols, 9 other nitrogen-containing compounds, 7 carboxyls, 4 sulfur-containing compounds, 2 oxygen-containing compounds, and 5 miscellaneous compounds. Noticeably, N-(including pyrazines), S-, and O-containing compounds, and carbonyls, which could be formed via thermal degradation and/or thermal interactions between components in kale leaves, were quantitatively main compounds of kale tea, whereas allyl isothiocyanate in kale seeds and sprouts and norisoprenoids, alcohols, and carbonyls in kale leaves had been predominantly major in previous studies.

AGFD 37 Heat-stabilized rice bran metabolome reveals biochemical contents and metabolic pathways with medicinal properties Iman Zarei, iman.zarei@colostate.edu, Elizabeth P. Ryan. Dept. of Environmental and Radiological Health Sciences , CSU, Fort Collins, Colorado, Rice bran is a functional food that includes both nutritional and medicinal benefits across the lifespan, and has shown protection against major chronic diseases (e.g. obesity, diabetes, cardiovascular disease and cancer) in animal and human studies. Identification of the phytochemical diversity of rice bran associated with medicinal properties is possible through global metabolome investigations and will aid this global dietary solution to be further tested for disease control and prevention. This study was performed to establish the medicinal roles for rice bran compounds across diverse metabolic pathways using metabolomics. The aim of this study was to perform a non-targeted global metabolite profile of rice bran from three US rice varieties and compare then to a global-grown set of 16 varieties from 7 different geographical locations using Ultra-performance liquid chromatography mass-spectrometry (UPLC-MS). The evaluated rice bran metabolome contained ~446 phytochemicals, of which 217 phytochemicals were associated with the following metabolic subclasses: Amino acids, Cofactors & Vitamins and Xenobiotics. This analysis revealed 76 rice bran metabolites that merit consideration for pharmacological and medicinal properties. Some of the medicinal compounds with varying relative abundance in rice bran included gamma-aminobutyric acid (GABA), 5-oxoproline, rhapontigenin, trans-urocane, N-acetylleucine, gentisate, N-acetylserotonin, N-acetyl histidine, 2-piperidinone,
stigmastanol and luteolin. These molecules have established health benefits such as anti-convulsive, improving blood circulation, anti-hyperlipidemic, UV protectant, vertigo treatment, anti-inflammatory, anti-insomnia, anti-cataract formation, anti-hypertensive and cancer chemopreventive, respectively. Human clinical trials that evaluate the medicinal potential and bioavailability of these rice bran compounds are thus warranted. Global rice varietal differences may contribute to inconsistent results on the biochemical numbers and structures of rice bran with medicinal actions, and reported results will further incorporate genetic and environmental variability into the presentation.

AGFD 38 Simultaneous analysis of the fenthion and its oxidative metabolites in rice, chili pepper and mandarin using LC-MS/MS
Jong-Hwa Lee, Jung Hak Lee, Ji-Ho Lee, Yongho Shin, Min Woo Jung, Eunhye Kim, Jeong Han Kim, kjh2404@snu.ac.kr. Dept. of Agricultural BioTech., Seoul National Univ., Seoul, Korea. The simple and rapid method for simultaneous analysis of organophosphorous insecticide, fenthion and its five oxidative metabolites (fenthion-oxon, fenthion-oxon sulfide, fenthion-oxon sulfone, fenthion sulfoxide and fenthion sulfone) in rice, chili pepper and mandarin was developed with liquid chromatography tandem mass spectrometry (LC-MS/MS, SHIMADZU LCMS-8050TM). The target compounds were analyzed on LC-MS/MS with positive electrospray ionization and selected reaction monitoring. For the best sensitivity in LC-MS/MS, acidified deionized water and methanol with formic acid (0.1 %) were selected for mobile phase in LC gradient elution. For optimization of the sample preparation, two QuEChERS extraction methods were compared by preliminary recovery test at spiking levels of 0.10 mg/kg. The citrate buffered QuEChERS (EN 15662) showed better recoveries of all analytes in samples than unbuffered QuEChERS extraction. To validate the optimized method, recovery tests were carried out with untreated rice, chili pepper and mandarin at spiking levels of 0.01, 0.10 and 0.20 mg/kg (n=3). At all fortification levels the accuracy and precision results satisfied between 70 and 120% associated with relative standard deviation of ≤10% for fenthion and all metabolites. Quantification of each analyte was performed using matrix matched calibration curves at concentration ranged from 0.005 to 0.200 mg/kg. Correlation coefficients (R²) of calibration curves was >0.99 for all the target compounds. The method limit of quantification (MLOQ) was 0.01 mg/kg for all compounds. As a result, the simultaneous analytical method developed in this study was proved to be efficient and rapid for the analysis of fenthion residues in rice, chili pepper and mandarin.

AGFD 39 Bisphenol A in breast milk from nursing Cavalier King Charles Spaniels: A preliminary study
Melissa B. Cichowicz, mcichowicz@wcupa.edu, Leslie B. Slusher, Clarissa Martin, Jenn Poshkus. Chemistry, West Chester Univ. of PA, King of Prussia. BPA (Bisphenol A) is a known endocrine disruptor and its presence in various body fluids and tissues has been linked to numerous negative health conditions in animal models. Previous research on other mammals has shown detectable levels of BPA in breast milk, as well as in the blood and urine of newborns. Little research has been conducted in canines and so this study endeavored to measure the levels of BPA in breast milk from nursing Cavalier King Charles Spaniels. Milk samples were solicited from a variety of breeders at a national Cavalier King Charles Spaniel show, so that dogs from different parts of the country were represented. Health surveys are also being conducted with the breeders, through the Cavalier Health Foundation, to track the incidence of stillbirths and birth defects (particularly cryptorchidism) as well as kennel practices, including use of plastic versus metal food storage containers and dispensers, use of plastic versus metal fencing and gates, and whether BPA-containing plastic chew toys were allowed. The results of the study are being used in an attempt to correlate the detectable BPA levels with use of plastic products in housing and feeding, versus incidence of pregnancy issues and birth defects. The method of detection involves an LC-tandem MS method with little pre-treatment of the milk sample. The method has been tested and shown to be independent of the method of sample storage or age since BPA does not degrade, and the LC-MS-MS limit of detection was sufficiently sensitive that BPA levels were measurable in virtually every sample. A wide range of BPA concentrations have been found in the limited number of samples tested to date, and so further study will require a larger number of samples to be solicited for evaluation. Future plans involve measurements of BPA levels in the blood and urine of the puppies, to establish a correlation with levels in the breast milk of the respective mothers, and for other dog breeds to be studied.

AGFD 40 Rapid screening and determining natural and synthetic steroid hormones in baby formulas using gas chromatography – tandem mass spectrometry
Jason Tang, tang@nsf.org, Timothy Baker, Kerri LeVanseler. Chemistry Lab, NSF International, Ann Arbor, Michigan. There always have been concerns about the presence of naturally occurring steroids in dairy products and the abusive or illegal use of synthetic steroids in dairy practices. Since intake of these steroid hormones may pose a great risk to endocrine disruption or cancers for children, it is important to develop fast and sensitive methods to screen and determine multi-residues of endogenous and exogenous estrogens and steroids in dairy products. A rapid and sensitive method has been developed for the simultaneous analysis of 85 natural and synthetic estrogens and steroids in baby formulas using gas chromatography coupled with tandem quadrupole mass spectrometry (GC-MS/MS). Baby formula samples first were wetted and homogenized with water containing 1% acetic acid, then were extracted with acetonitrile in a sonicator, and were centrifuged at 4°C. An aliquot of acetonitrile supernatant was cleaned with dispersive SPE sorbents of C18, PSA, and Z-Sep, then was dried at 70°C by a gentle nitrogen flow. The dry residues of extracts were reconstituted in water containing 1% acetic acid and were extracted with mixture of pentane/ether/MTBE (2/1/1, v/v/v). The solvent mixture of pentane/ether/MTBE were cleaned by an Agilent 7890B-7000C QQQ gas chromatography–tandem mass spectrometer in MRM mode with overall analysis time of 21 min. The limits of detection and limit of quantification for the targeted compounds were below 5 or 10ng/g and average recoveries were greater than 70% for the most spiked compounds. The results showed that the method was suitable for simultaneously screening and determining multi-residues of both natural and synthetic estrogens and steroids in baby formula samples.

AGFD 41 Understanding sodium diffusion in turkey breast meat
Janam K. Pandya, kmpandya@umass.edu, Amanda J. Kinchla. Food Sci., Univ. of Massachusetts, Amherst. In recent days, people of the US have become concerned about sodium intake in their diet. Research studies show that an average American takes 3,400 to 4,500 mg/day of sodium in their diet against dietary recommendation of 1,500 to 2,300 mg/day. Studies also show that 70-75% of sodium in the diet comes from the processed food. Excess sodium in the diet can potentially cause health issues such as hypertension, heart attack, kidney failure and bone problems. With a view of that the hypothesis of our study is to understand the sodium diffusion in different model foods and to determine the possibilities to limit it by changing the process variables. After studying potatoes as a simple starch model in the first part of the study, the present study focuses on Turkey Breast Meat as a
protein model. Since proteins are a complicated system and there are very limited research studies available on meat in this area, it is necessary to determine the trend of sodium diffusion in the meat while cooking in presence of salt at different temperature followed by analyzing the change in the diffusion in presence of different anions larger than sodium chloride. Since, protein denaturation can have great impact on diffusion process, the denaturation profile for turkey breast meat protein was analyzed by Differential Scanning colorimetry (DSC). Obtaining results from the DSC analysis, the processing temperature of 4°C, 23°C, 50°C and 70°C was implemented to obtain the diffusion trend in co-relation with the denaturation. 1 inch meat cubes were cooked in 5% (0.86M) salt solution at with different time temperature combination. Sodium analysis were performed on Ion Selective Electrode and the results were confirmed by ICP-OES. The trend showed that the diffusion increases with increase in cooking temperature in a dramatic way. Also cooking loss increased rapidly while cooking above 50°C. Processed samples were analyzed on Scanning Electron Microscopy (SEM) and compared with control raw meat to visually quantify the protein denaturation effect of sodium diffusion. The future work of this research will focus on examining the effect of sodium salts having anions larger than chloride on the diffusion of sodium in the turkey breast meat. It will also look into effect of different salt concentration on diffusion while cooking.

AGFD 42 Development of lecithin emulsion gels system: Influence of formulation parameters on physicochemical properties and digestion kinetics Wei-Jing Huang, 181483433@qq.com, Yu-Wen Ting. Institution of Food Sci. and Tech., National Taiwan Univ., Taipei, Abstract Emulsion gel is a solid-like system similar to the organogel that has exceptional control release property when encapsulating hydrophobic ingredients. Unlike organogel composed solely of organic solvent (lipid in most food system), emulsion gel is formed by droplet flocculation in a solidified continuous network. In this work, we used lecithin as the emulsifier to disperse the lipid into the aqueous continuous phase and then, at specific compositional ratio, transformed into a semi-solid structure thorough physical entanglement between lecithin molecules. To develop an emulsion gel system with optimum physicochemical properties, the effect of formulation parameters, such as excipient oil, lecithin concentration, and aqueous phase ratio, were investigated. To determine the effect of excipient oil, pseudo-ternary phase diagrams were constructed using three different oils including medium chain triglyceride (MCT), soybean oil, or olive oil as oil phase to indentify the region that would result in a gelled structure. The result showed that oil type had a major impact on phase behavior where soybean oil and olive oil could form a homogeneous emulsion gel with lower lecithin concentration (< 1%) than MCT (> 3%). The rheological properties and texture of the emulsion gel formed with lecithin concentration from 1 – 10% were evaluated systematically. In general, higher lecithin concentration resulted in more viscoelastic and firmer gel structure. This finding then corresponding to the later in vitro lipolysis study where firmer gel structure delayed the lipid digestion in the emulsion gel indicating the digestion kinetic could be modulated through varying the formulation parameters. The results from this study show that rational design will allow the development of lecithin emulsion gel system with desirable control release property when used as encapsulation system for bioactive ingredients. Moreover, the semisolid property makes it a suitable system to partially replace fat in food of similar stuture, such as mayonnaise or cake dressing, where thoughtful formulation design could increase the usefulness of such system in food industry.

AGFD 43 In vitro release, anti-proliferative and antimicrobial activity of carnosic acid nanoemulsion Huijuan Zheng, huijuanzheng87@gmail.com, Qiongrong Huang . (1) Food Sci., Rutgers Univ, New Brunswick, New Jersey, (2) Food Sci., Rutgers Univ., New Brunswick, New Jersey The aim of this work is to develop a carnosic acid nanoemulsion delivery system for food application. An oil-in-water nanoemulsion was prepared by high pressure homogenization method with lecithin as emulsifier. The emulsion was characterized by size, zeta potential, storage stability, in vitro digestion bioaccessibility, anti-proliferative effect on various cell lines and antibacterial effect on Gram positive bacteria. Results showed the prepared nanoemulsion has a high loading efficiency and good stability. In vitro release of carnosic acid from nanoemulsion by simulated gastric and intestine fluid studies showed that the slow release of carnosic acid from the nanoemulsion increased its bioavailability. Anti-proliferative on cancer cells were conducted on HepG2 and Caco-2 cell lines, which showed a dose and time dependent manner. Antimicrobial study showed carnosic acid nanoemulsion possess inhibition effect on Staphylococcus aureus and Listeria monocytogenes.

AGFD 44 Stability of beta-carotene and alpha-tocopherol in cooked Moringa oleifera leaves, By HPLC-UV Arianne Vasilatis, aa51@scarletmail.rutgers.edu. Plant Science, Rutgers Univ. , New Brunswick, New Jersey Moringa oleifera leaves are commonly incorporated into many African and Asian dishes partly due to their high mineral and vitamin content. In this study, Moringa oleifera leaves were subjected to temperatures ranging from 40-70°C for 15, 30, and 45 minute intervals to evaluate the effect of cooking on their β-carotene and α-tocopherol content. After heating duration elapsed, β-carotene and α-tocopherol content was measured using HPLC-UV. A strong decrease in both beta-carotene and alpha-tocopherol content was observed in all samples subjected to elevated temperatures compared to unheated sample. β-carotene content of samples subjected to elevated temperatures for 15, 30, and 45 minutes was found to be 102µg/g, 105 µg/g, and 160 µg/g respectively while α-tocopherol content ranged from 447µg/g, 481 µg/g, and 466µg/g respectively.

AGFD 45 Physical characterization of mushrooms as taco filling extender Kristin Wong, kmwong@umass.edu, Amanda J. Kinchla. Food Sci. , Univ. of Massachusetts, Amherst Although diet can significantly reduce the risk of heart disease, American consumers continue to eat detrimental diets high in fat and sodium. Products need to be made that decrease fat and sodium intake while still delivering acceptable taste. Mushrooms have the potential of being healthy meat extenders due to their low fat and sodium contents. The objective of this research was to investigate the physical properties of taco fillings using varied ratios of mushrooms and beef. Formulas were evaluated for cook yield, moisture, color, and texture. Each formula varied in mushroom type (white button vs. portobello), preparation (blanched vs. non-blanched), particle size (small vs. large), and usage (25, 50, 75, and 100% mushrooms by weight). Results showed that usage levels 50% and higher displayed significant moisture, color, and texture differences from the control, thus setting the difference threshold at 50%. The control exerted a max pressure of 17.00 kPa and was similar to the 25% mushroom formula which exerted 16.71 kPa, however the 50, 75, and 100% mushroom formulas exerted lower pressures of 14.27 kPa, 8.81 kPa, and 5.02 kPa respectively. A second set of tests was conducted on formulas with lower usage (15, 30, and 45%) to confirm the threshold. All formula variables were similar to the control across all tests except color. The control received an L* value of 37.86. The white button formulas received values of 37.92, 36.86, and 36.71 while portobello formulas received values of 36.83, 33.22, and 30.89 (15, 30, and 45% respectively). A paired-preference study was held
confirming acceptance of a 45% mushroom filling against the all-meal control. This indicates that mushrooms may be suitable healthy meat extenders while still achieving consumer acceptance.

AGFD 46 Total polyphenol antioxidants in the US diet Joe A. Vinson, joe.vinson@scranton.edu. Chemistry, Univ. of Scranton, Dalton, Pennsylvania  Polyphenols are now considered the major antioxidants in plants and hypothesized to be beneficial in decreasing the risk of chronic diseases. This hypothesis has primarily been tested by epidemiology studies and short-term supplementation studies. A greater amount of dietary antioxidants are associated with a less atherogenic blood profile (Kim et al., 2016). Free polyphenols can be measured by extraction and either colorimetric methods or more expensive LC-MS analysis. The latter is available in the USDA database which measured flavonoids but omitted phenolic acids. Phenol Explorer is a more comprehensive online database for all classes of polyphenols. Many plant foods contain fiber and this matrix may contain covalently bound polyphenols which are not tested in the aforementioned methods which measure free polyphenols. Some of the bound polyphenols are released during in vivo digestion due to enzymes and pH changes. Also there may be degradation of polyphenols during digestion such as occurs with anthocyanins. These free polyphenols or free polyphenols from food are available for absorption (bioaccessible) into the bloodstream and are then metabolized and carried to cells, tissues and organs throughout the body leading to beneficial systemic effects by a variety of mechanisms. We have developed a simple selective colorimetric method using the Folin reagent and catechin as the standard. The sample was extracted and underwent acidic hydrolysis (fruits, vegetables, spices, oils) or basic hydrolysis (nuts, coffee, tea, grain-based foods). Fruit juices contained only free polyphenols due to processing. We then used the USDA database which lists the per capita consumption and determined from total polyphenols and consumption data the polyphenol contribution of each food and beverage. Beverages contributed over half the polyphenols in the diet. Per capita daily consumption (maximum bioaccessible amount) is over 2g of total polyphenols in the US diet.

AGFD 47 Effects and molecular mechanisms of soy foods or soy isoflavones in prostate cancer prevention Chan Ho Jang, chano@udel.edu, Changqing Wu. Animal and Food Sci., Univ. of Delaware, Newark, Prostate cancer is the most commonly diagnosed cancer and the second leading cause of cancer deaths in American men. Due to its high incidence rate, serious side effects from current cancer treatments, a more practical approach to reduce risk of prostate cancer should be found and cancer prevention might be considered as one of alternatives to decrease the prostate cancer incidence rate. Regular intake of soy foods or soy isoflavone supplements is well-known for helping to reduce a risk of prostate cancer through increasing epidemiological and Lab evidence. Nevertheless there are limited data to prove such relationship and the underlying molecular mechanisms. To understand the preventive effects of soy foods or soy isoflavones, it is essential to study the impact of complex bioactive compounds contained within soy foods using a relevant animal model. In this study, the prostate cancer incidence rate and gene expression patterns were hypothesized to vary among Pten-/- male mice with the different soy diet composition, i.e. cooked and raw soy foods, isoflavone combination and genistein for 25 weeks. Our current findings have showed that 25-week dietary treatment of mixture of daidzein and genistein reduced a hyperplasia/Prostatic Intraepithelial Neoplasia/Carcinoma in Situ (PIN/CIS) incidence rate up to by 40% compared with the genistein or DMSO carrier solvent treatments. In addition, 25-week dietary treatment of raw soy food had a 17.5% lower hyperplasia/PIN/CIS incidence rate and 0% hyperplasia/PIN/CIS/ invasive carcinoma rate compared with the cooked soy food or water treatments. The dietary treatment of mixture of daidzein and genistein exhibited a significantly lower body weight of Pten-/- male mice after 144-day old compared with the genistein or DMSO carrier solvent treatments. The findings suggest that the combination of daidzein and genistein or soy food might be more efficacious to prevent the prostate cancer. RNA sequencing (RNA-seq) research is now used to search for novel information about underlying molecular mechanisms of prostate cancer prevention through different gene expression patterns of Pten-/- male mice with the different soy diet composition.

AGFD 48 Isolation and identification by high-performance liquid chromatography of bioactive metabolites of polymethoxylated flavones in rat urine Danielle Goncalves, danigoncalves_123@yahoo.com.br, Marilia Rodrigues, Thais B. Cesar, John A. Manthey. (1) Food and Nutrition, Sao Paulo State Univ., Araquara, Brazil (2) USDA ARS, Fort Pierce, Florida (3) Food and Nutrition, Univ Estadual Paulista - UNESP, Araquaraq, Sao Paulo, Brazil  The polymethoxylated flavones (PMFs) are a subclass of flavonoids in citrus, which are known for their potential antioxidant, anti-inflammatory and anticancer actions to human health; as well as high bioavailability compared to other flavonoids. Recent studies show that metabolites of PMFs are also biologically active, and in fact, may have stronger effects compared to those of the parent compounds. Therefore, the objective of this study was to identify and isolate PMFs metabolites in rat urine with active biological properties. Thirty adult male Wistar rats were separated into 3 groups with ten animals in each, and they were administered with 200 mg/kg/day of PMF during 20 days. Each group received tangeretin (TAN), nobiletin (NOB) or 3',4',3,5,6,7,8-heptamethoxylavone (HMF). 24 hours urine of each group was collected and the metabolites were extracted with ethyl acetate, identified by high-performance liquid chromatography (HPLC) and then isolated using preparative liquid chromatography. Many of the PMF glucuronide metabolites were initially detected by their characteristic UV spectra during HPLC analyses, then later seen by mass spectrometry (ESI-MS) coupled to HPLC. Analyses included detection of the protonated molecular ions [M+H]^+, and detection of the ion mass of the aglycone fragment ions. PMF glucuronides of these latter ions are shown by a neutral loss of 176 amu [glucuronic acid-H2O]. Successful isolation of the PMF metabolites have made possible the performance of biological assays using these metabolites individually and a thorough study of their courses of action to human body.

AGFD 49 Nondestructive analysis of vitamin C content in dietary supplement tablets by using terahertz time-domain spectroscopy Ju Hee Kang, Kyungwon Kwak, Hyang Sook Chun, jschn@cau.ac.kr. (1) Food Sci. and Tech., Chung-Ang Univ., Anseong, Korea (2) Chemistry, Chung-Ang Univ., Seoul, Korea  Recently, vitamin C consumption has increased as our concern and interest in health issues have increased. However, recent reports have revealed that some dietary supplement tablets that are available on markets contain less vitamin C than the declared content. The purpose of this study was to demonstrate the potential use of terahertz time domain spectroscopy (THz-TDS) for nondestructive analysis of vitamin C content in dietary supplement tablets. Spectral fingerprints of vitamin C were identified in the frequency range of 0.1-3 THz with the aid of density functional theory (DFT) calculations. The influence of factors such as thickness, minor ingredients, surface roughness, and curvature radius on the analysis of vitamin C content was examined. Finally, the calibration model that can be used to measure the content of vitamin C in dietary supplement tablets was generated. THz absorption peaks of L-ascorbic acid were detected at 1.08, 1.47, 1.79, 2.01, and 2.32 THz. Factors that influence the analysis of vitamin C content in dietary supplement tablets were
considered to construct the calibration model. The generated calibration curve of L-ascorbic acid had a good regression coefficient of >0.995, and its root mean square error of prediction (RMSEP) was 2.19%. Furthermore, the average vitamin C content and relative standard deviation values in the commercial tablets (n = 50) analyzed by THz-TDS method were in good agreement with those determined by reference HPLC method.

AGFD 50 Fabrication of oil-in-water nanoemulsions by dual-channel microfluidization using natural emulsifiers: saponins, phospholipids, proteins, and polysaccharides Long Bai1,2, longbai2011@hotmail.com, David McClements2. (1) Northeast Forestry Univ., Harbin, China (2) UMASS Dept of Food Sci, Amherst US. Nanoemulsions are utilized within the food, pharmaceutical, and personal care industries because of their unique physicochemical properties and functional attributes: high optical clarity; prolonged stability; enhanced bioavailability. For many applications, it is desirable to utilize natural ingredients to formulate nanoemulsions so as to create label-friendly products. In this study, we compared different natural emulsifiers for fabricating nanoemulsions with dual-channel microfluidization method. These emulsifiers were either amphiphilic biopolymers (whey protein and gum arabic) or biosurfactants (quillaja saponin and soy lecithin). The interfacial properties of the natural emulsifiers at planar oil-water interfaces were characterized using interfacial tension measurements. The influence of emulsifier type, concentration, and homogenization pressure on the efficiency of nanoemulsion formation was examined. The long-term storage stability was also monitored at ambient temperature. For all of the natural emulsifiers, nanoemulsions could be produced by dual-channel microfluidization, with the mean particle diameter decreasing with increasing emulsifier concentration and homogenization pressure. Whey protein isolate and quillaja saponin were more effective at forming nanoemulsions containing fine droplets than gum arabic and soy lecithin, with a lower amount of emulsifier required and smaller droplets being produced. This effect was attributed to faster emulsifier adsorption and a greater reduction in interfacial tension leading to more efficient droplet disruption within the homogenizer for the saponins and whey proteins. This study highlights the potential of using dual-channel microfluidization to efficiently produce label-friendly nanoemulsions from natural emulsifiers.

AGFD 51 Bioactive peptides released during of digestion of processed milk Michael H. Tunicl,2, Michael.Tunick@ars.usda.gov, Diane L. Van Hekken1,2, Peggy M. Tomasulas1,2. (1) USDA ARS, Wyndmoor, Pennsylvania (2) Dairy & Functional Foods, E. Regional Res. Ctr., Wyndmoor, Pennsylvania Most of the proteins contained in milk consist of αs1-, αs2-, β-, and κ-casein, and some of the peptides contained in these caseins may impart health benefits. To determine if processing affected release of peptides, samples of raw (R), homogenized (H), homogenized and pasteurized (HP; 72°C for 15 s), and homogenized and ultra-high pasteurized (HU; 135°C for 2 s) milk were subjected to in vitro gastric and intestinal digestion. LC/TOF mass spectrometry analysis of peptides revealed that gastric digestion resulted in the release of several small phosphopeptides (<6 kDa) from αs1- and β-casein after HP and HU treatment, but intestinal digestion led to the release of >30 phosphopeptides from all four caseins. Different processing treatments often led to the same peptides being generated, with R and H producing the most. Some of these peptides have been identified in the literature as exhibiting bioactivity. Processing of milk influences the appearance of bioactive peptides in the small intestine, which should provide insights into the digestion of milk by humans.

AGFD 52 High throughput analysis of caffeine In beverages using 2.3 μm analytical reversed phase chromatography column with dual functionality for use both in HPLC and UHPLC Atis Chakrabarti, Crystal Benner, crystal.benner@tosoh.com. Tosoh Bioscience LLC, Wallingford, Pennsylvania Reversed phase liquid chromatography (RPC) is the analytical technique most widely used in the Research and Development (R&D) and Quality Control (QC) Dept.s of the food and beverage industry. Many popular soft drinks have a high percentage of caffeine as a stimulant. The Food and Drug Administration does not regulate caffeine content of soft drinks, although the agency does require that the presence of caffeine is disclosed on labeling for energy drinks and cold coffee beverages. In this era of high throughput analysis, the need to obtain sooner retention times while maintaining or improving resolution is very important for quality control analysis. We report the separation of caffeine found in popular soft drinks using a TSKgel ODS-140HTP column with dual functionality, useful for both in conventional HPLC and UHPLC. UV-VIS and CAD (Charged Aerosol Detector) were used as detectors in this analysis. The study shows that Caffeine can be analyzed reproducibly using 2.3 μm analytical Reversed Phase chromatography Column in both HPLC And UHPLC.

AGFD 53 Investigation of the antiproliferative constituents of Linociera ramiflora collected in Vietnam P. Annéce Benathreina1, benathreina.1@osu.edu, Li Pan1, C. Benjamin Naman1, Hee-Byung Chai1, Tran N. Ninh1, Dijaja D. Soejarto2,3, L. Harinantenaina Rakotondraibe1, Alan D. Kinghorn1. (1) College of Pharmacy, The Ohio State Univ., Columbus (2) College of Pharmacy, Univ. of Illinois at Chicago (3) Science and Tech., Field Museum, Chicago, Illinois (4) Inst. of Ecology and Biological Resources, Vietnam Academy of Science and Tech., Hanoi, Viet Nam. In an effort to discover new lead anticancer agents from natural sources, tropical plant samples have been collected in Vietnam rainforests and tested for their cytotoxicity in a preliminary screening against the HT-29 human colon cancer cell line. A sample of the branches of Linociera ramiflora (Roxb.) Wall. ex G. Don, a plant belonging to the olive family (Oleaceae), showed the cytotoxicity in this bioassay, and thus was further investigated for its bioactive secondary metabolite content. L. ramiflora, previously known as Chionanthus ramiflorus, is native to Southeast Asia and has been reported to grow predominantly in mainland China, Vietnam, Taiwan, and the Philippines. Partial DNA sequence analyses have previously confirmed the close phylogenetic relationship between this plant and the well-known olive tree (Olea europea). Due to the economic and dietary importance of the latter, its phytochemistry has been heavily studied. Conversely, phytochemical reports on L. ramiflora have been limited. In the present study, one new and three known arylglycerol lignan derivatives have been isolated so far from this plant. The chemical characterization through various chromatographic and spectroscopic methods and the biological activity against HT-29 cells of these isolates as well as the isolation and structure determination of compounds from the remaining antiproliferative subfractions will be described.

AGFD 54 Investigation of the lymphatic transport of solid-lipid curcumin particles (Longvida®) in comparison to curcumin extract in rats Thomas Eidenberger1, Nikeeta Kheradia2, nikeetakheradia@yahoo.com, Sonya Cropper1, scropper@vs-corp.com. (1) Belan Ziviltechniker-GmbH , Wels, Upper Austria, Austria (2) Pharmaceutical Sciences, Butler Univ., Noblesville, Indiana (3) Verdure Sciences, Noblesville, Indiana. It is well-known curcumin has a low, apparent bioavailability in humans mainly due to its instability in physiological pH-conditions in the small intestine and extensive first-pass metabolism. Majority of previous human studies indicate that a major part of
curcumin appears in blood as its metabolite curcumin-glucuronide. Only a minor part is detected in plasma as unglucuronidated curcumin. The pharmacokinetic profile provides a hypothesis for the lack of efficacy observed in many clinical studies, in which even high doses of curcumin administered orally yielded negligible unconjugated curcumin plasma levels. Further, in recently published in vivo studies the efficacy of curcumin is most likely correlated with circulating levels of free (unglucuronidated) curcumin. In a small human pilot trial, it could be shown that curcumin from the solid-lipid curcumin particles (Longvida®) yields substantially higher levels of free circulating curcumin when compared to conventional curcumin formulations. To further investigate these encouraging results the pharmacokinetic, with special emphasis laid on lymphatic absorption, of curcumin from either a standard curcumin extract or from Longvida® was investigated in rats. Following the previously published design, five rats received a single oral administration of 75 mg curcumin/kg body weight of either Longvida® or standard curcumin (suspended in aqueous solution). Following oral administration, the mesenteric lymph and plasma samples were collected up to 5 hours after administration. Analysis of free curcumin and glucuronidated curcumin were performed by HPLC with UV-detection coupled to MS according to published methods. Both plasma and lymph concentrations of unglucuronidated curcumin were substantially higher after administration of Longvida® when compared to the standard curcumin suspension. The study results strongly indicate that curcumin after oral administration in the form of solid-lipid curcumin particles (Longvida®) circumvents the liver and the first-pass metabolism yielding substantially higher concentrations of circulating free curcumin when compared to conventional curcumin formulations.

AGFD 55 Chemical composition and anti-hyperglycaemic effects of triterpenoids enriched Eugenia jambolana Lam. berry extracts

Yuanyuan Li, Jialin Xu, Chunhui Yuan, Hang Ma, hang_ma@uri.edu, Tingting Liu, FeiFei Liu, Navindra P. Seeram, Li Han, Xueshi Huang, Liya Li. (1) Inst. of Microbial Pharmaceuticals, Northeastern Univ., Shenyang, China (2) Biomedical and Pharmaceutical Sciences, College of Pharmacy, Univ. of Rhode Island, Kingston (3) Inst. of Biochemistry and Molecular Biology, College of Life and Health Sciences, Northeastern Univ., Shenyang, China In our investigation on anti-hyperglycaemic constituents of Eugenia jambolana L. (Jamun), one new triterpenoid, 2-O-cis-p-coumaroyl maslinic acid, along with thirteen known triterpenoids were isolated from the fruit methanol extract. The structures of compounds 1-14 were elucidated on the basis of MS, 1D and 2D NMR spectroscopic data analyses. The profile of triterpenoid-enriched Jamun fruit extracts (TJFE) was determined by HPLC-DAD analysis, and six major components were quantified. Animal studies demonstrated that TJFE (total triterpenoids content 48.7%) decreased blood glucose content in C57BL/6 mice (P < 0.05) upon sucrose challenge and improved mouse glucose tolerance following 2 weeks of treatment by oral gavage (100 mg/kg body weight). The current study advances scientific knowledge of Jamun constituents and suggests that triterpenoids may play an important role in the anti-diabetic properties attributed to this edible purple berry.

AGFD 56 In vitro anti-neuroinflammatory effects of urolithins, ellagitannin-gut microbial metabolites

Nicholas DaSilva, NickDasilva91@gmail.com, Pragati P. Nahar, Hang Ma, Angela Slitt, Navindra P. Seeram. Biomedical and Pharmaceutical Sciences, College of Pharmacy, Univ. of Rhode Island, Kingston Our group has previously reported that urolithins (hydroxybenzopyran derivatives), formed from the gut microbial biotransformation of ellagitannins, may be the relevant bioactive compounds responsible for the neuroprotective effects of pomegranate, an ellagitannin-rich fruit. Neuroinflammation is implicated in several neurodegenerative pathologies and frequent activation of microglia (resident macrophages of the brain) by chronic inflammation, leads to reactive microgliosis and secretion of pro-inflammatory biomarkers (NO, PGE2, IL-6, TNFα) which causes neuronal death by the activation of pro-apoptotic pathways. Herein, several urolithin analogs (at 10 μM) were shown to decrease NO, IL-6, PGE2, and TNFα (by 33, 31, 65 and 75%, respectively) levels in murine BV-2 microglia cells. In addition, in a non-contact co-culture cell model, differentiated SH-SY5Y (human neuroblastoma) cells were exposed to conditioned media from the urolithins- or lipopolysaccharide (LPS)-treated BV-2 cells. The urolithins-BV2 treated media maintained SH-SY5Y cell viability greater than LPS-BV2 treated cells for 24 h (100% cell viability treated vs. 84% untreated) and 48 h (92% cell viability treated vs. 67% untreated) post-treatment. Therefore, the anti-neuroinflammatory effects of urolithins may play a role in the overall neuroprotective effects attributed to ellagitannin-rich foods such as pomegranate.

AGFD 57 Inhibitory effects on the formation of advanced glycation endproducts by hydroponically grown Moringa oleifera

Shelby Johnson, shelby.johnson@salve.edu, Weixi Liu, Hang Ma, Susan M. Meschwitz, Jameson Chace, Navindra P. Seeram. (1) Chemistry, Salve Regina Univ., Sauderstown, Rhode Island (2) Biomedical and Pharmaceutical Sciences, Univ. of Rhode Island, Charlestown (3) Chemistry Dept., Univ. of Rhode Island, Kingston (4) College of Advanced Pharmacy, Univ. of Rhode Island, Kingston (5) Biology, Salve Regina Univ., Newport, Rhode Island Alzheimer’s disease is ranked as the 6th leading cause of death in the US, with over 5 million diagnosed cases. Natural products high in phenolic content have recorded high antioxidant potential, and high inhibition rates in the formation of Advanced Glycation Endproducts (AGEs). The bioaccumulation of AGEs have been linked to several chronic human diseases such as diabetes, inflammation, and neurodegenerative diseases. Moringa oleifera was grown in a hydroponics system to determine if the leaves and flowers would yield high concentrations of polyphenols, possess high antioxidant and AGE inhibition. Leaves and flowers were extracted to yield four fractions: crude, ethyl acetate, water, and butanol. These fractions were subjected to HPLC, Total Phenolic Content, DPPH (antioxidant), and AGE fluorescence assays. HPLC yielded the presence and relative concentrations of known polyphenols. Total phenolic content assay showed higher concentrations than previously reported for all fractions. The ethyl acetate fractions contained the greatest amount of polyphenols, 19,600 (leaves) and 12,367 mg/100g of GAE (flowers). The ethyl acetate fractions also showed highest antioxidant potential, yielding IC50 values of 1.83μg/ mL (leaves) and 71.14μg/ mL (flowers). On day 21, AGE inhibition was seen in the crude, ethyl acetate and butanol fractions for both leaves and flowers at 100 PPM. Leaf extracts showed 39% crude, 50% ethyl acetate and 2% butanol inhibition of the formation of AGEs at 100 PPM. The crude flower extract showed 50% inhibition, the ethyl acetate showed 11% inhibition, and butanol showed 30% inhibition at 100PPM. These results show that the flower extracts exhibit similar inhibitory properties as the leaves. Therefore, it was concluded that both the leaf and flower extracts from hydroponically grown Moringa oleifera have high potential to inhibit the formation of AGEs and thus inhibit the progression of many diseases related to oxidative stress.

AGFD 58 Natural anthraquinones inhibited protein glycation and amino acids side chain modification by protecting protein structures

Weixi Liu, weixi_liu@my.uri.edu, Hang Ma, Joel A. Dain, Navindra P. Seeram. (1) Biomedical and Pharmaceutical Sciences, College of Pharmacy, Univ. of Rhode Island, Kingston (2) Chemistry Dept., Univ. of Rhode Island, Kingston Protein glycation plays a
critical role in the pathology of diabetes, cancer, and neurodegenerative diseases. Herein, we investigated the anti-glycative effects of seven natural anthraquinones, namely, rhein, emodin, aloes-emonin, aloin, physcion, chrysophanol and anthraquinone. In a model reaction containing human serum albumin (HSA) and D-fructose, the anthraquinones (10-100 μM) reduced the formation of glycation products as measured by intrinsic fluorescence. Aloin (100 μM), showed the highest inhibitory effect and reduced HSA glycation by 92.3%, followed by rhein (80.2%), emodin (78.5%), anthraquinone (68.3%), chrysophanol (68.2%), physcion (43.8%) and aloes-emonin (20.6%). In contrast, the positive control aminoguanidine (AG; 100 μM) only reduced HSA glycation by 10.4%. In addition, the anthraquinones inhibited carbonyl species (methylglyoxal; MGO) induced protein glycation. The most potent inhibitor was emodin (100 μM) which reduced HSA-MGO glycation by 94.0% followed by aloin (56.4%) and rhein (45.1%). The other anthraquinones showed slightly lower inhibitory effects ranging from 33.4-16.8%, which were more potent than AG (12.8%). Moreover, these compounds reduced lysine and arginine modifications caused by glycation, as measured by fluorescein and 9,10-phenanthrenequinone assays. By protecting amino acids side chains, the anthraquinones maintained HSA secondary structure (characterized by circular dichroism), which might contribute to their anti-glycation effects. Overall, this study compared the inhibitory effects of seven anthraquinones on HSA glycation. A mechanistic study revealed that their anti-glycation effects may be due to their protective effects on protein side chains and secondary structures.

AGFD 69 Isolation and structure elucidation of diterpenes from *Euphorbia saudiarabica* Abdullahi T. J. Bin Muhsinah1, pharmakkua@hotmail.com, Yongqiang Liu1, Hang Ma1, Nicholas DaSilva1, Hesham Soliman2, Abdulrhman Alsayari2, Navindra P. Seeram1.
(1) Biomedical and Pharmaceutical Sciences, College of Pharmacy, Univ. of Rhode Island, Kingston (2) College of Pharmacy, King Khalid Univ., Abha, Saudi Arabia *Euphorbia saudiarabica* Fayed & D. Al-Zahrani (family, Euphorbiaceae) is a previously uninvestigated plant which is endemic to Saudi Arabia. Herein, *E. saudiarabica* aerial parts (collected in Saudi Arabia) were extracted with methanol and further fractionated by liquid-liquid partitioning with n-hexanes, acetonitrile, ethyl acetate, and n-butanol. All of the extracts were evaluated for cytotoxicity against a murine microglial cell line (BV2) by the (3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium, MTS) assay. The acetonitrile extract showed the most potent cytotoxicity and on further purification yielded several diterpenoids whose structures were elucidated on the basis of extensive NMR and mass spectroscopic data. Currently, the isolates are being evaluated for biological activities in our Lab.

AGFD 60 Bioactive glucitol-core containing galloandins and other phytochemicals from silver maple (*Acer saccharinum*) leaves Abdullahi T. J. Bin Muhsinah1, pharmakkua@hotmail.com, Hang Ma1, Tao Yuan1,2, Navindra P. Seeram1.
(1) Biomedical and Pharmaceutical Sciences, College of Pharmacy, Univ. of Rhode Island, Kingston (2) Xinjiang Technical Inst. of Physics and Chemistry, Chinese Academy of Sciences, Urumqi, Xinjiang, China Our Lab has previously investigated several maple (genus, *Acer*) species endemic to North America including the red maple (*A. rubrum*), sugar maple (*A. saccharum*), and sycamore maple (*A. pseudoplatanus*). In the course of these studies, we obtained a class of bioactive phenolic compounds, namely, glucitol-core containing galloandins (GCGs), which show a wide range of bioactivities including antioxidant, anti-cancer, anti-α-glucosidase, and anti-glycative effects. Since GCGs have been reported from members of the maple genus, herein, we focused our attention on the silver maple (*A. saccharinum*) species which is also endemic to North America. Using authentic GCG standards (previously isolated from the red maple), several GCGs were identified from silver maple leaves by HPLC-DAD analyses including ginalmins A-C, and maplexins B, and D-F. Additionally, three other phenolic compounds, namely, methyl syringate, methyl gallocate, and 3-methoxy-4-hydroxyphenol 1-β-D-(6-galloyl)-glucopyranoside, and a sesquiterpenoid, namely, puberuroid A, were isolated and identified (by NMR and HRESIMS). Therefore, among all of these North American maple species investigated to date, only the silver maple along with the red maple species produce GCGs. Also, this is the first phytochemical investigation of the silver maple species.

AGFD 61 Comparison of acidic collagen extraction methods of collagen from channel catfish skin Yuqing Tan, ytl142@msstate.edu, Sam Chang. Food Sci., nutrition and health promotion, Mississippi State Univ Due to the outbreak of bovine spongiform encephalopathy, transmissible spongiform encephalopathy and some religions considerations, the usage of collagen and its products of land animals is avoided by more and more people. Therefore, alternative sources of collagen like aquatic animals have attracted increasing attention. Mississippi ranks number one in catfish production and fillet processing. However about 60% of the original catfish mass from fillet making is waste such as skin, head and frame. Catfish skin was collected from a local catfish processing plant in Isola, MS. Catfish skins were pretreated by washing with iced water containing 1% NaCl (1:6 w/v). Minced skins were extracted twice with 0.5 M acetic acid to find the optimal combinations of extraction time, particle size and skin-to-solvent ratio. Then the selected optimal condition was applied to four different acids (citric acid, lactic acid, acetic acid and hydrochloric acid) with different pH (1.8, 2.1, 2.4, 2.7, 3.0) to further optimize extraction condition. SDS-PAGE analysis for extracted collagen was performed. Results showed that for first extraction step, collagen yield from minced skins extracted with 1:50 (w/v) ratio for 48 hours was the highest (18.94% based on wet weight of skins); For residue extraction, yield from minced skins extracted with 1:50 (w/v) ratio for 48 hours was the highest (12.04%). For four different acid extraction, yield from skins extracted with pH 2.4 HCl was the highest (24.56%) in first extraction step; in the second residue step, yield from skins extracted with pH 2.4 HCl was the highest (9.30%). SDS-PAGE showed that all collagen had similar pattern with α chain (123 KDa), α2 chain (113 KDa), β chain (225.7 KDa) and γ chain (338.5 KDa). Thus, HCl can be used as collagen extraction solvent for industries in terms of extraction efficiency and economy.

AGFD 62 Size exclusion enhancement of in-vitro digestion model Karen R. Conca, karen.r.conca.civ@mail.mil, Katherine R. Kensil, Jason L. Andresen. Combat Feeding Directorate Army Natick RD&E Ctr, Natick, Massachusetts Digestibility, or essential amino acids [EAAs] available for absorption during digestion, is an important factor in determining protein quality. Since protein quality can change during high temperature storage the Army is interested in studying these effects on protein digestibility of rations. A bench top in-vitro digestion model was studied as an alternative, to animal trials or TNOs TIM-1 (w/ dialysis), to determine the extent of protein breakdown and EAA absorption profiles. Since quantification of amino acids uses a severe acid hydrolysis that breaks down all proteins into amino acids, a size exclusion method was developed to separate out non-absorbable polypeptides/protein prior to hydrolyzing digested samples for quantification of EAAs. Model ration components were processed through synthetic digestive fluids to simulate breakdown of proteins/peptides during digestion to measure protein digestibility in stored samples. After rigorous filtration, 10ml samples were loaded onto
Sephadex packed column and various mobile phase formulations were tested. Fractions were collected, and concentrations for amino acids were analyzed using HPLC/FLD [EX340/EM450nm] after pre-column derivatization with o-phthalaldehyde. Acid hydrolysis of fractions was used to confirm size exclusion separation. A Sephadex-G-10 packed column [47cm x 2.5cm] with a 9:1 [40mM KHPO4 buffer-pH7, 150mM NaCl and 0.02% Na3: Isopropanol] mobile phase at a flow rate of 1.25ml/min over a 7.2 hour period was used to elute and separate large protein polypeptides from small digestible peptides and amino acids. Four bulk fractions were collected. The 1st [0-70min] fraction contained no amino acids, but after acid hydrolysis all amino acid levels increased significantly. Amino acids detected in the 1st size exclusion fraction verified presence protein polypeptides and confirmed that separation of large peptides [non- absorbable] from free amino acids cannot be removed by filtration alone. The 2nd fraction [70-210min], contained all amino acids, except for tryptophan, which was collected in the 4th fraction [290-430min]. By using size exclusion separation after in vitro digesting the result EAA absorption profiles will more closely represent in vivo protein digestibility. Methodology will ultimately be used to assess protein quality of rations during storage.

AGFD 63 Tyrosine nano-emulsion stability for supplementation of Army rations

Karen R. Conca, karen.r.conca.civ@mail.mil, Katherine R. Kensil. Combat Feeding Directorate Army Natick RD&E Ctr, Natick, Massachusetts

Tyrosine is being studied by the Army as a supplement to reduce the effects of stress on physical performance by maintaining muscle protein synthesis; reducing muscle losses during extensive physical activity, and for muscle recovery. However, high concentrations required for supplementation to achieve benefits also impact sensory quality of products. By using nanotechnologies such as micro-fluidized nano-emulsions, required concentrations can be reduced. In previous animal studies, Tyrosine Nano-Emulsions [TNE] have been shown to enhance tyrosine bioavailability. To incorporate TNE into a food, tyrosine load was optimized and a nano-emulsion spray-drying protocol was developed to produce a stable TNE-Powder [TNE-P]. To maximize tyrosine load while maintaining stability of the nano-emulsion a non-ionic ethoxylated dual-emulsification system was used. The tyrosine load in TNE was increased from 3 to 7.5% while maintaining a particle size of 38-58nm. Particle size analyses were conducted [Malvern Zetasizer nano series Zen 3600] to down-select TNE formulations and to also confirm retained particle size of reconstituted spray dried TNE-P. A stable powder was produced using spray drying parameters: [2:1] TNE: 50% Maltodextrin/water, inlet/outlet temperature of 155/60°C and a 2ml/min feeding rate. Spray-dried emulsions retained an average particle size of 58nm. Sieved TNE-P with a tyrosine concentration of 11.3% +/-0.4 was incorporated into Army dairy shake beverage powder at a 2% load. Accelerated military relevant storage studies were conducted for 4wk at 120F and 6M at 100F. HPLC analysis was conducted to assess TNE-P stability and sensory tests were conducted to determine acceptability of stored supplemented dairy shakes. HPLC analysis of reconstituted shakes showed 90.1% +/-2.75 tyrosine recovery before and 87.2% +/-2.58 and 90.7% +/-1.20 recovery after 4wk and 6M storage, respectively. There were also no significant differences in sensory quality scores [9-point hedonic scale] between the control [6.45] and the TNE-P supplemented [6.46] dairy shake which was acceptable after storage. Sensory and load/stability data complement previous bioavailability studies indicating that use of nanoTech. is effective for effective supplementation of tyrosine thereby benefiting soldier performance. Proven protocols for producing nano-emulsions/spray-dried powders will increase applicability for other compounds of interest.

AGFD 64 HPLC-ESI-MS analysis of poly methoxylated flavone metabolites in human urine

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The pharmacokinetics and bioavailability of orange juice flavonoids were studied in the urine of healthy human volunteers that consumed single doses of orange juice prepared by either conventional fruit extraction or by fresh fruit processing. The orange juice (POJ) processed by conventional fruit extraction contained higher levels of the flavanone glycosides originating from a fraction [290-430min]. By using size exclusion separation after in vitro digesting the result EAA absorption profiles will more closely represent in vivo protein digestibility. Methodology will ultimately be used to assess protein quality of rations during storage.

AGFD 65 Expression and characterization of a thermostable endo-1,5-α-arabinanase (TS-ABN) in Pichia pastoris for biocatalytic solubilization of bioactive feruloylated arabinobio-oligosaccharides from sugar beet pulp Ningning Zhang, ningning.zhang@s@mail.astate.edu, Jianfeng Xu, Brett J. Savary. Arkansas Biosciences Inst., Arkansas State Univ., Jonesboro Sugar beet pulp generated from beet sugar processing is rich in the highly functional cell wall polysaccharides pectin and associated arabinans. The arabinan core chain consist of α-(1,5)-linked L-arabinofuransyl units and ferulic acid substitutions at O-2 L-Araf and more rarely, terminal O-5 L-Araf. Ferulate dehydrodimers between chains cross-link arabian into the insoluble fiber fraction. We are investigating a thermostable endo-1,5-α-L-arabinanase (TS-ABN) from Geobacillus thermodenitrificans to determine its utility in alternative processing of beet biomass for industrial sugar fermentation and to improve the nutritional profile of sugar pulp used in food and feed products. The overall goal of this study is to evaluate TS-ABN as an efficient enzymatic platform for generating feruloylated arabinobio-oligosaccharides (FAOs) from sugar beet pulp. FAOs are targeted in food and feed applications for healthful colon functioning through modulating pro-inflammatory activities in the colon epithelium. We present results to characterize the TS-ABN expressed in Pichia pastoris cells. The recombinant enzyme’s properties are presented in terms of structure, biochemical properties (pH, salt activation, and temperature profiles), and action on defined substrates. We have applied rTS-ABN to autohydrolyzed beet pulp and recovered FAOs. The composition of the FAOs and their ability to modulate tight-junctions in T84 colonicoytes will be presented.

AGFD 66 Biochemical investigation into the functional properties of Delonix regia, Cassia fistula and Blighia sapida extracts

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Three tropical plant species, namely Delonix regia, Cassia fistula and Blighia sapida were selected for evaluation of their functional properties. D. regia and C. fistula are mainly ornamental in nature and currently underutilized in Jamaica. The pods and seeds of B. sapida are discarded after...
processing. Seed extracts of *D. regia* and *C. fistula* and fruit extracts of *B. sapida* were investigated. Extracts were evaluated for their antioxidant activity, free radical scavenging properties, total phenolics, fatty acid profile and iodine values. Antioxidant activity was determined by the 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay and total phenolics by the Folin-Ciocalteau assay. Lipids were Soxhlet extracted and characterized by gas chromatography/mass spectrometry and nuclear magnetic resonance spectroscopy. Fourier Transform Infrared Spectroscopy (FTIR) was utilized to assess chemical functionalities present. Of the samples evaluated, *B. sapida* pods had the highest antioxidant activity (1.81 ± 0.11 mg/g) and free radical scavenging properties (69.7 ± 1.3 %) and may be considered a moderate source of antioxidant activity. Palmitic acid was identified as the predominant fatty acid in *D. regia* (41.6 ± 3.2 %) and *C. fistula* (34.4 ± 6.4 %) seed extracts whereas gondoic acid (48.4 ± 9.1 %) was the major fatty acid present in acce seed. The aril of the acce fruit is a rich source of oleic acid (57.2 ± 8.8 %). *C. fistula* seed oil extracts are expected to be the most stable to oxidation with a predicted iodine value of 16. FTIR spectroscopy revealed a broad peak in the range of 3200-3500 cm⁻¹ for all samples investigated indicating the presence of phenolic compounds. *D. regia, C. fistula* and *B. sapida* extracts are a source of antioxidants and omega fatty acids which are known for their functional properties and potential health benefits. These extracts may be considered for use in nutraceutical applications.

**AGFD 67 Developing a thermally-tolerant pectin methyl esterase for improved sugar beet biomass processing** Jose C. Tovar, Megan Cease, Jianfeng Xu, Brett J. Savary, bsavary@astate.edu, Arkansas Biosciences Inst., Arkansas State Univ., Jonesboro Beets sugar production is an energy intensive process with high greenhouse gas emissions. Up to a third of total thermal energy consumed in a beet factory is used to dry beet pulp, the pectin-rich biomass left after sucrose extraction. We are investigating a *Citrus* fruit thermally-tolerant pectin methyl esterase (TT-PME) for application to reduce thermal energy inputs for beet pulp processing. We hypothesize that processive PME action can modify cell wall structure to improve mechanical separation of water from beet pulp prior to drying through a calcium cross-linking mechanism. Our project objectives are to: 1) determine if PME action can reduce water binding in beet pulp, 2) establish specific antibodies for TT-PME detection, and 3) demonstrate TT-PME recombinant expression in planta. Using a quantitative benchtop assay, we determined PME treatment reduced water binding in beet pulp by 25% over untreated controls. These results provided proof of concept that TT-PME expression in sugar beet roots may confer a novel processing benefit. As a tool for detecting TT-PME in transgenic plant tissues, we produced antibodies using a sequence-specific peptide antigen that differentially detected TT-PME. Towards developing an expression strategy for sugar beets, different TT-PME structural constructs were transiently expressed in *Nicotiana benthamiana*. TT-PME’s native signal peptide yielded high recombinant expression levels comparable to the well-established patain signal peptide, and active TT-PME expression required the PRO region. Results from these expression studies will direct future strategies for TT-PME expression in sugar beet taproots. Biotech beets expressing TT-PME is envisioned to deliver an innovative processing output trait providing economic and environmental benefits for beet sugar processing.

**AGFD 68 Simultaneous determination of unregistered pesticides in Korea for agricultural products using LC-MS/MS** Sang-Hyeob Lee¹, qgwe234@naver.com, Jeong-In Hwang², Min-su Kang², Moonik Chang³, Young D. Lee², Jang-Eok Kim², Gyu-Seek Lee¹, (1) Agr Chem Dept Daegu Univ, Kyungsan Kyungbuk, Korea (2) School of Applied Biosciences, Kyungpoob National Univ., Daegu, Korea (3) Food Safety Evaluation Dept., National Inst. of Food and Drug Safety Evaluation, Osong, Korea Positive List System (PLS) which has been used for safety management of imported agricultural products is a negative regulation, allowing below 0.01 mg/kg for unregistered pesticides residues. For establishing the PLS into Korea, it is required to develop rapid and sensitive methods that can simultaneously analyze unregistered pesticides in imported agricultural products using LC-MS/MS. In this study, Korean Pesticide Residue Analysis (KOPRA) method was developed to analyze 121 unregistered pesticides for three agricultural products, such as brown rice, orange, and green pepper chosen as representatives of fatty, non-fatty, and high chlorophyll-containing samples, respectively. Acetoneitrile was used for the extraction of pesticide residues in samples, and the dispersive solid phase extraction using primary secondary amine and anhydrous magnesium sulfate was employed for a clean-up. Concentrations of pesticide standards prepared for the matrix-matched calibration ranged from 0.002 to 0.5 mg/kg, and limits of quantification (LOQ) were below 0.01 mg/kg for all tested pesticides. Correlation coefficients of matrix-matched calibration curves were more than 0.9921. Recoveries of pesticides in fortification ranges of 0.05-0.5 mg/kg using the KOPRA method were between 70 and 130%, and relative standard deviations were below 30%. The number of pesticides amenable to the KOPRA method was more than 97. Therefore, these results show that the KOPRA method developed in this study could be used as a rapid and high-sensitive analysis method of pesticide residues for agricultural products with meeting the LOQ of below 0.01 mg/kg for the PLS in Korea.

**AGFD 69 Identification and quantification of phenolic acids and flavonoids in three phenolic-rich legume varieties as affected by thermal treatments** Yan Zhang, yzhang@fsnhp.mstate.edu, Sam K. Chang. Dept. of Food Sci., Nutrition and Health Promotion, Mississippi State Univ., Starkville Lentil, black soybean and black turtle bean have been reported to possess high antioxidant activities which can be however greatly changed by thermal treatments. However, the change of individual phenolics as affected by thermal treatments has not been studied. This study’s objective was to accurately identify and quantify selected individual phenolics of raw and cooked three legume varieties with purification and fractionation pretreatments. Lentil, black soybean and black turtle bean were steamed at 100 C for 10, 50 and 30 min, respectively. The cooked and respective raw legumes were extracted with acetone/water/acetic acid (70/29.5/0.5). The crude extract (CE) was semi-purified by removing sugar, organic acid and protein with XAD-7 packed column. The semi-purified extract (SPE) was further separated in LH-20 packed column through sequential elution by water, 50% ethanol and 50% acetone. Phenolic acids and flavonoids in CE, SPE and each column fraction were identified and quantified based on retention time and spectrum of 17 phenolic acid and 18 flavonoid standards. The results showed semi-purification and fractionation of phenolic extracts made accurate identification and quantification of individual phenolics possible by elimination of co-elution. Steaming treatments had a great impact on the contents of selected individual phenolic acids and flavonoids. Four, three, and three phenolic acids were identified in lentil, black soybean, and black turtle bean, respectively. One, two and six flavonoids were identified in these three legumes, respectively. Except protocatechuic acid in black soybean, the contents of other phenolic acids were significantly (p<0.05) increased by thermal treatments and some phenolic acids undetectable in raw samples were even made detectable by thermal treatments. Different flavonoids showed different change patterns during heating. In black soybean, heating made epicatechin and quercetin-3-O-glucoside undetectable. This study accurately quantified the effect of thermal processing on some individual phenolic acids and flavonoids through pretreatments of purification and fractionation.
Prebiotics and probiotics are functional foods. A probiotic is defined as a viable 
microbial dietary supplement that beneficially affects the host through its effects in the 
testinal tract. A prebiotic is defined as "a 
nondigestible food ingredient that beneficially affects the host by selectively stimulating the growth and/or activity of one or a 
limited number of bacteria in the colon" Food products that meet this definition are water-soluble carbohydrates such as GOS, FOS, and inulin. 
GOS are primarily composed of galactose and often terminate with a glucose residue at the reducing end. Both inulin and FOS are fructans, 
but they differ in polymerization. Inulin is a linear, highly polymerized fructan of degree of polymerization (DP) 11–60, consisting of a linear 
chain of fructose with β-(2 → 1) linkages and a terminal glucose unit. FOS has a degree of polymerization (DP) of 2–9 and is produced from 
inulin by controlled hydrolysis. In this work, the oligo- and polysaccharide distribution of FOS and GOS samples has been characterized by 
HPAE-PAD. In addition, HPAE-PAD profiling was demonstrated as a method to determine FOS/GOS content in samples where they are
added as a prebiotic and their change upon the addition of probiotics. For probiotics, we used Yakult® drink, a well-known probiotic dairy product. In this method, separation of individual oligosaccharides in FOS/GOS was achieved by HPAE using a Dionex CarboPac PA200 column with a sodium hydroxide/sodium acetate mobile phase. Oligosaccharides were detected using PAD with a gold working electrode; therefore, no sample derivatization is required.

AGFD 74 1,2,4-Trithiolane, found in stinky bean (Parkia speciosa), is a slow releasing hydrogen sulfide donor Dong Liang, doliangld@yahoo.com, Dejiang Huang. Dept. of Chemistry, National Univ. of Singapore Hydrogen sulfide (H2S) is a gasotransmitter with multiple cellular signaling functions, and large number of H2S donors has been reported for research and therapeutic applications. However, most of the H2S donors are synthtic compounds. Naturally occurring H2S releasing agents, especially those which can release H2S slowly, are still rare. On the other hand, polysulfides from fruit and vegetables, such as diallyl trisulfide and diallyl disulfide from garlic, are reported to be dietary H2S donors, while few research has been done on those dietary H2S donors. We found that 1,2,4-trithiolane (TTL), a cyclic polysulfide from stinky bean, a local ingredient in South East Asia, is a potent, slow releasing H2S donor. TTL was 6.35 times more effective than diallyl trisulfide (DATS) in terms of increasing the cellular H2S concentration in cultured cells. Moreover, TTL could release H2S in cultured cells for up to two days with apparent rate constant estimated (2.02 ± 0.38)×10−3 s−1. HPLC and LC-MS study revealed that TTL releases H2S through a slow reaction with glutathione (GSH), during which the thiolate attacks the carbon to open the trithiolane ring, resulting in H2S and a number of glutathione-methylene-sulfide conjugates. Our results suggest that stinky bean, may be of potential as functional food with H2S donation property because TTL is the major organosulfide compound.

AGFD 75 Development of multi-residue analysis methods of pesticides for red ginseng tea Min-su Kang1, mskms12@naver.com, Jeong-In Hwang1, Sang-Hyeob Lee1, Jun-Sang Ryu1, Hye-Hyun Jung1, Se-Youe Kwak1, Ja-Gun Kang1, Ho-Jin Kim1, Jang-Eok Kim1. (1) School of Applied Biosciences, Kyungpook National Univ., Daegu, Korea (2) Experiment Research Inst., National Agricultural Products Quality Management Service, Gimecheon, Korea With an interest in health from consumer, the demand for red ginseng (RS) products which are processed using ginseng is increasing in Korean market, so it is required to ensure the safety of pesticides from the RS products like a tea. However, there are no authorized analysis methods of pesticides for RS products. In this study, multi-residue analysis method of 78 pesticides for RS tea was developed using a liquid chromatography-tandem mass spectrometer (LC-MS/MS). According to this developed method, the small amount of RS was extracted with acetonitrile, and the extract was evaporated to obtain the low limits of quantification (LOQs). The clean-up of samples was followed by a dispersive solid phase extraction method using the primary secondary amine and magnesium sulfate. The analytical method developed in this study was amenable to 40 of 78 tested pesticides. Using the developed method, the LOQs of the amenable pesticides for RS tea were between 3 and 70 ng mL−1 and their matrix-matched standard calibration curves to the RS tea had the high correlation coefficients of > 0.9880. In addition, the recoveries of 40 pesticides for RS tea were acceptable with the range of 76.9 to 124.5%, with standard deviations 0.5~16.0%. Therefore, the analytical method developed in this study could be used as a quick and sensitive analysis tool of pesticides for RS tea.

AGFD 76 Design, synthesis and herbicidal activity of novel triketone compounds Hui-Chao Li1,2, Ai-Ying Guan1,2, Zhongyuan Yao1,2, Xiao-Li Xia1,2, Zheng-Hang Wang2, Hong-Juan Ma1,2, Chang-Ling Liu1,2, liuchangling@sinochem.com. (1) State Key Lab of the Discovery and Development of Novel Pesticide, Shenyang Sinochem Agrochemicals R&D Co., Ltd., Shenyang, China (2) Shenyang Research Inst. of Chemical Industry Co. Ltd., Shenyang, China In 2014, world pesticide expenditures totaled about $56.7 billion, herbicides account for 42.6% of those sales and constituted the biggest portion, followed by insecticides, fungicides, and other types. Triketone herbicide is a member of the class of HPPD inhibitors, which all work by inhibiting the plant enzyme 4-hydroxyphenylpyruvate dioxygenase. Sulcotrione was the first commercialized herbicide in this class, while mesotrione was the best-selling one, they are both used to control of broad-leaved weeds post-emergence in maize. To improve the activity profile and selectivity, we designed and synthesized a series of new triketone compounds by the approach of Intermediate Derivatization Methods (IDM). 2,6-dichlorotoluene (1) was employed as the starting material and then conducted successive reactions to obtain the key intermediates substituted 3-aminoethylbenzoic acid (2), which was then used to replace the benzoyl moiety of sulcotrine and mesotrine to generate the target compounds. Their structures were confirmed by 1H NMR, MS and elemental analysis. Bioassays demonstrated that some of the title compounds exhibited excellent herbicidal activity against broadleaf and gramineous weeds, such as Solanum nigrum, Echinochloa crusgalli, Digitaria sanguinalis. The results of this study suggested that further design and structural modification of the triketone compounds as herbicides is worthwhile.

AGFD 77 Development of an absorbent to reduce pesticide residue in ginseng Shin Byeung Koon1, sbkon1@korea.kr, Jang-Eok Kim1. (1) Dept. of Agricultural Chemistry, Kyungpook National Univ., Daegu, Korea (2) NAQS, Daegu, Korea Ginseng (Panax ginseng C. A. Meyer) is one of the typical medicinal plants using a root. Featuring 4- to 6-year long growth duration and shade growth, Ginseng has weak disease endurance and thus pesticides are extensively used to prevent disease in Ginseng. If pesticides are applied to the upper parts of ginseng while growing, a considerable amount of pesticide residues also get accumulated on the head of ginseng after they are applied on its leaves and stems. This study focuses on developing an absorbing filter attached to the stem of Ginseng to absorb flowing pesticides, in order to prevent pesticides from getting accumulated on the head of ginseng. The filter surface is composed of Hanji, traditional Korean paper, to improve hygroscopy and air permeability, and activated carbon is used as an inner insertion. The filter size is 4cm in length and the amount of its inner insertion is 2g. The size of particles consists of four elements, such as 8 mesh, 16 mesh, 30 mesh and 100 mesh. Six components (Dimethomorph, fluquinconazole, pyraclostrobin, pyrimethanil, tebuconazole and trifloxystrobin) of pesticides were applied to the upper part of ginseng with the filter device five times in 1-week intervals from August 9, and ginseng spices harvested in October were analysed to measure pesticide residues by means of analytical instruments, including LC/MS/MS. As a result of the analysis, the most consistent and effective reduction in pesticide residues was found in the filter with the 30-mesh particle size of activated carbon. As compared with the control group with no the filter designed to reduce pesticide residues, the reduction ranged from 60.1% to 79.0%, in accordance with pesticide components, which could be considered to be remarkably effective in reducing pesticide residues. The results indicated that the reduction filter attached to the stem of ginseng could contribute to significantly reducing the pesticide residues accumulated in ginseng.
AGFD 78 Tyrosol-based liposomal behavior: size, zeta-potential, TEM, QCM-D and fluorescence analysis Kervin Evans¹, abqsaxophone@gmail.com, David L. Compton¹. (1) NCAUR ARS USDA, Peoria, Illinois (2) Neaur-Ars-USDA, Peoria, Illinois. In our continued efforts to create biobased antibacterial for the food industry, we have used phospholipase D from Streptomyces sp. to create hydroxytyrosol and tyrosol phospholipids. Extrusion methods proved that both hydroxytyrosol phospholipids and tyrosol phospholipids each formed liposomes that were pH-dependent in size. zeta-potential analysis demonstrated that the surface charge was well below the threshold of -25 mV for stable nanoparticles. Transmission electron microscopy (TEM) analysis demonstrated that both types of liposomes were spherical and had a single bilayer characteristic. Quartz crystal microbalance with dissipation monitoring (QCMD) analysis demonstrated that both types of liposomes could be supported bilayers under proper condition (Ca²⁺) and pH conditions. Fluorescence anisotropy measurements indicate that melting temperatures of both lipids were below 4 °C, suggesting that adsorption behavior and liposome formation was limited by electrostatic interactions and not gel-state transformation of phospholipids.

AGFD 79 Cellulose-bodipy nanohybrids for singlet oxygen production Prashant Chauhan¹, prashant.tillu@yahoo.co.in, Ning Yan². (1) Univ. of Toronto, Toronto, Ontario, Canada (2) Faculty of Forestry, Univ. of Toronto, Canada A new hydrophilic bodipy dye was synthesized and well characterized by different spectroscopic methods. The water soluble (sulfonated) groups where introduced on the carboxylated bodipy using Chlorosulfonic acid. The novel bodipy was covalently attached to amino nanocellulose NC using carbodiimide linkage. At last the resulting nano material was well characterized by IR, UV-visible, TEM, XPS, TGA analysis. Being easily to suspend in water, the potential of this material was demonstrated to act as an efficient photosensitizer in producing singlet oxygen in presence of light source; which in turn can be termed as an excellent candidate for therapeutic applications.

AGFD 80 Accuracy of volatile quantification using isotopically labeled internal standards for SPME Vanalysis of a grape mapping population Elizabeth A. Burzynski¹, cab54@cornell.edu, Imelda Ryona², Bruce I. Reisch³, Gavin L. Sacks¹. (1) Food Sci., Cornell Univ., Ithaca, NY (2) Q2 Solutions, Ithaca, NY (3) Horticulture, Cornell Univ., Ithaca, NY. Volatile profiling of plant populations, is frequently performed via solid-phase microextraction (SPME) coupled to GC-MS. SPME is well-known to suffer from matrix effects, and best practices recommend the use of well-matched (e.g. isotopically labeled) standards. However, because of the large number of volatile targets in profiling studies, researchers commonly use a single surrogate standard, with the assumption that matrix effects are consistent across a population. However, this variation in matrix effects has not been quantified across a plant population. Using a set of isotypically labeled standards, we assessed the variation in matrix effects during SPME-GC-MS analyses of a hybrid grapevine (Vitis sp.) family (140 individuals) used for purposes of chromosome mapping. Our analysis of the berry juice extracts demonstrated high variability in the relative responses of internal standards across individuals in the population. For example, the ratio of responses for [U-¹³C]hexanal to [U-¹³C]hexanol showed a log normal distribution with a 95% confidence interval spanning greater than two orders of magnitude with a maximum difference of responses of 1000 fold between two individuals. Of the 15 internal standard pairwise comparisons, 12 had a 95% confidence interval spanning more than 25 fold. A sub-sample of grape individuals were verified, and a much stronger predictive model could be generated for hexanol in finished wines based on hexanal in the original grapes when appropriate isotopically labeled standards were used ($r^2 = 0.88$ vs. $0.41$). These results indicate that volatile profiling studies on mapping populations should not assume homogeneous matrix effects, and should employ multiple well-matched internal standards to achieve accurate measurements.

AGFD 81 Solid phase mesh enhanced sorption from headspace (SPMESH) coupled to DART-MS/MS for high throughput quantification of trace-level odor-active volatiles Jillian A. Jastrzembski¹, jaj239@cornell.edu, Gavin L. Sacks¹. Food Sci., Cornell Univ., Ithaca, NY. The most commonly employed method for volatile analysis is gas chromatography – mass spectrometry (GC-MS), as it is the only technique offering enough selectivity and sensitivity for the detection of trace-level compounds in complex matrices. A major drawback of GC-MS is its low throughput of 30-60 minutes per sample, which is poorly suited to many GC-MS applications such as routine detection of pesticides, drugs, toxins or natural components in biological samples or foodstuffs, as well as phenotyping for objective flavor characterization. In contrast, Ambient Ionization (AI) techniques like Direct Analysis in Real Time (DART) – MS require less than one minute of instrument time per sample, but the omission of the chromatography step necessitates adequate off-line sample preparation such as solid-phase microextraction (SPME) to compensate for the loss of sensitivity and selectivity. We report a method in which extraction and pre-concentration can be performed in parallel and coupled to DART-MS/MS as a high-throughput replacement for GC-MS quantification of odor-active volatiles in complex matrices. Since the traditional SPME fiber is configured for a GC port and poorly suited to AI desorption, commercial meshes for use with DART-MS were coated with a non-polar sorbent (polydimethylsiloxane) and used for Solid Phase Mesh Enhanced Sorption from Headspace (SPMESH) of linalool and 2-isobutyl-3-methoxypyrazine (IBMP). Calibration curves were prepared for both compounds using isotopically labelled internal standards. The new method achieved good linearity for both linalool and IBMP ($r^2=0.99$, 0.96, respectively) as well as detection limits approaching the sensory threshold for both compounds (71 ng/L, 21 ng/L, respectively). Quantification was also demonstrated for recovery spikes in grape macerate with excellent precision (3.8-9.5% RSD). This technique has the potential to acquire GC-MS-like data at a rate of 100 samples per hour.

AGFD 82 Effect of microstructure on the barrier property of water and oxygen in hydroxypropyl starch (HPS)/SiO₂ nanocomposites films Siyuan Liu¹,², sliu.scut@hotmail.com, Xiaoxi Li³, Ling Chen¹, Lin Li¹, Bing Li¹. (1) Food Sci., South China Univ. of Tech., Guangzhou, China (2) Food Sci., Rutgers, New Brunswick, New Jersey. The limited barrier property of starch-based biodegradable material restricted its application in packaging. In this study, the addition of SiO₂ nanoparticles into starch matrix has been proven to effectively reduce the permeation of water and oxygen gases. SiO₂ particles prolonged the transfer path and it was generally accepted that “tortuous path” was the main reason for resistant property improvement in nanocomposites. However this study found that only the prolonged path contributed by the SiO₂ nanoparticles cannot precisely explain the decreased permeation of water and oxygen as the results deviated from Nielson Model. The aggregation state of HPS/SiO₂ nanocomposites films could have a vital influence on the barrier property. Moreover, the requirement for the microstructure was not the same for the lowest permeation of water and oxygen molecules. The increase size of micro-ordered region favor the barrier effect of water and the compact structure of this region contributed to the oxygen prevention. The effect of aggregation structure on mass transfer could be a proper supplement to “tortuous path” for the interpretation of the improvement in resistant.
property. Also, the aggregation state of HPS/SiO₂ nanocomposites can be used as effective factor to control “selective transfer” of water and oxygen molecules.

AGFD 83 Fully automated sample extraction and analysis of mycotoxins in foods by online SFE-SFC-MS William Hedgepeth, wahedgepeth@shimadzu.com, Kenichiro Tanaka, Tairo Ogura. Shimadzu Scientific Instruments, Columbia, Maryland  Mycotoxins are low-molecular-weight natural products produced by fungi and are capable of causing disease and death. They are strictly regulated around the world because of their strong carcinogenic effects. A simple and reliable method to analyze mycotoxins is required to ensure food safety. The current methods require time-consuming sample pretreatment. Here we report a fully automated online sample extraction and analysis of mycotoxins in foods by online SFE-SFC-MS. Several mycotoxins such as Afla (aflatoxin B₁, B₂, G₁ and G₂), OTA (ochratoxin A), ZON (zearalenone), DON (deoxynivalenol) in foods were analyzed in this study. 1g of wet food samples were mixed with 1g of absorbent before loading to the extraction vessels, while 1g of dried food samples were put into the vessels as is. The vessels were set on the online SFE-SFC-MS system. They were extracted on the SFE unit and then transferred to a 4.6 x 250mm column. The mycotoxins were detected by a triple quadrupole mass spectrometer. The food samples were purchased from a local supermarket. Mycotoxins were spiked in, and the spiked samples were analyzed as calibration standards. The mycotoxins in corn grits and peanut butter were successfully extracted from the samples using the online SFE-SFC system, analyzed on a Cosmosil pi-NAP column, and detected by a triple quadrupole MS. Four mycotoxins (ZON, OTA, Afla B₁, DON) were spiked in corn grits and two (Afla B₁ and B₂) in peanut butter and analyzed to check reproducibility and linearity. 1ppb of ZON, OTA, and Afla B₁ and 100ppb of DON were detected in corn grits, and 0.1ppb of Afla B₁ and B₂ in peanut butter was able to be detected. Reproducibility was checked at this concentration (n=5). As a result, 12.2-32.9% relative standard deviation of peak areas were obtained. Linearity was checked ranging from 1-100ppb for ZON, OTA, Afla B₁ and 100ppb-10ppm for DON in corn grits, and 0.1-10ppb for Afla B₁ and B₂ in peanut butter. The coefficients of determination were greater than 0.99 for all the mycotoxins except for DON in corn grits (0.988).

AGFD 84 Microbiological and physicochemical analysis of pumpkin juice fermentation by the basidiomycetous fungus Ganoderma lucidum Jing Zhao, zhaoj10@rpi.edu. Rensselaer Polytechnic Inst., Troy, New York. A new protocol for processing of pumpkin juice was set up which included fermentation by the basidiomycete Ganoderma lucidum at 28 °C for 7 d. The growth curve of G. lucidum in pumpkin juice was successfully (R² = 0.99) fitted by a 4-parameter logistic model and the ideal highest biomass was estimated to be 4.79 g/L. G. lucidum was found to have a significant acidification effect on pumpkin juice. The lowest pH (4.05 ± 0.05) and highest total titratable acidity (14.31 ± 0.16 mL 0.1 M NaOH/100 mL) were found on the 4th day during fermentation. Sugars in pumpkin juice fermented with G. lucidum showed a significant decrease, especially glucose and fructose. On the contrary, the release of exo-polysaccharides and free amino acids greatly enriched the pumpkin juice. The variation of color index and viscosity also mirrored the above behavior. Based on headspace solid phase microextraction and gas chromatographymass spectrometry, 68 volatile compounds were identified, including 17 esters, 14 alcohols, 13 phenyl compounds, 11 aldehydes, 8 ketones, 3 acids, 1 furan, and 1 benzothiazole. The pumpkin juices fermented for different days were markedly differentiated with principal component analysis and the fermentation process was tentatively divided into 3 periods: the booming (1st to 4th day), steady (5th to 6th day), and decline (7th day) period.

AGFD 85 Design, synthesis and biological activity of novel substituted diamides derivatives containing thiophene ring Miao Li¹,², Lin Li³, Baoshan Chai², Ji-chun Yang², Yuqiao Song², Chang-Ling Liu², liuchangling@sinochem.com. (1) State Key Lab of the Discovery and Development of Novel Pesticide, Shenyang Sinochem Agrochemicals R&D Co., Ltd, Shenyang Liaoning, China (2) Shenyang Research Inst. of Chemical Industry Co. Ltd., Shenyang, China (3) State Key Lab of Fine Chemicals, Dalian Univ. of Tech., Dalian, China (4) Dept. of Pharmaceutical Chemistry, Hebei Medical Univ., Shijiazhuang, China A new class of insecticidal anthranilic diamides has been found which exhibit their action by binding to ryanodine receptors and activating the uncontrolled release of calcium stores. Whole organism symptoms include feeding cessation, lethargy, paralysis, and death. To discover novel diamides derivatives with high insecticidal activity, a series of new substituted diamides derivatives containing thiophene ring 1–3 were designed by introducing thiophene ring to diamides derivatives utilizing intermediate derivatization methods (IDM). The compounds were identified by 1H nuclear magnetic resonance (NMR), IR and elemental analysis. Preliminary bioassays indicated that compounds 1 exhibited excellent insecticidal activities against Plutella xylostella and showed 100% mortality at 600 mg L⁻¹ concentration. Compounds 1a and 1e showed above 60% mortality at 20 mg L⁻¹. Compounds 1 and 3 attained by changing the pyrazole ring in diamides derivatives have no insecticidal activity, which illustrated that pyrazole ring in diamides derivatives is very important.

AGFD 86 Changes of polyphenolic compounds level in artichoke (Cynara scolymus L.) grown in Korea during cultivation Kyu-Won Hwang¹, duddjhwa@naver.com, Daniel Son², ChunHwan Kim², Ki Cheol Seong², Joon-Kwan Moon¹. (1) Hankyong National Univ., Ansan, Korea (2) Agricultural Research Center for Climate Changes, NIIHSS, Jeju, Korea The levels of polyphenolic compounds in two varieties of artichoke (Cynara scolymus L.) grown in Jeju island, Korea. Violeto di Chioggia and Green glove cultivated depend on harvest time of Green glove variety, 5-17mg/g artichoke, and comprising 38.4-71.6% of the total polyphenolic compounds in Green glove.

AGFD 87 Changes of organic acids level in coffee during roasting Kyu-Won Hwang, duddjhwa@naver.com, Joon-Kwan Moon. Hankyong National Univ., Ansan, Korea Five coffee beans were roasted at different condition (235°C, 10 min; 245°C, 13 min; 250°C, 15 min; 250°C, 19 min) and were brewed with hot water for the analysis of organic acids. Organic acids were separated and quantified through the post column analysis method using HPLC in brewed coffees. Seven different organic acids (acetic acid, citric acid, formic acid, lactic
acid, malic acid, phosphoric acid, quinic acid) were detected and quantified from the roasted beans. The total organic acids content went from 0.39 ug/mL to 0.32 ug/mL, with donor two the concentrations went from 2.80 ug/mL to 0.24 ug/mL and with donor three the concentrations went from 5.66 ug/mL to 5.68 ug/mL, respectively. These results suggest that the type of intestinal microbiota is directly related to the metabolism and hence intestinal stability of grape derived products.

**AGFD 90** 5-hydroxytryptophan, cyanoglycoside, and flavonoid content of *Griffonia simplicifolia* populations Daniel Giurleo1,2, giurleod1@gmail.com, Rodolfo Juliani1, Larry Hwang3, Julie Asante-Dartey1, Qingli Wu1,2, James Simon1,2, (1) New Use Agriculture & Natural Plant Products Program, Dept. of Plant Biology and Pathology, Rutgers Univ., New Brunswick, New Jersey (2) Dept. of Medicinal Chemistry, Rutgers Univ., Piscataway, New Jersey (3) College of Agriculture and Sustainable Development, Cuttington Univ., Suacoco, Bong County, Liberia (4) Agri-Business in Sustainable Natural African Plant Products- Ghana, East Legon, Ghana *Griffonia simplicifolia*, a member of the Leguminosae family, is a tree climbing shrub distributed throughout the forests of Sub-Saharan West Africa ranging from Liberia to Gabon. The seeds of this species are known to accumulate an unusually high amount of 5-hydroxytryptophan (5-HTP), a widely consumed alternative treatment for depression and other conditions involving serotonin imbalance. In this study, the 5-HTP content of seeds from 10 different *G. simplicifolia* populations originating from various regions across Ghana and Liberia was measured using HPLC-UV. This data could be useful in identifying genetic features and/or growing conditions that favor 5-HTP production in *G. simplicifolia* seeds. Since 5-HTP is an important product of commerce, maximizing its output can have a significant economic impact on locals in the Sub-Saharan region of Africa. In addition, the minor cyanoglycosides in the seeds and flavonoids in the leaves of each *G. simplicifolia* population were quantified by HPLC-UV. Significant accumulation of any of these compounds could expand commercial interest and the economic value of this crop.

**AGFD 91** HPLC-UV analysis of α-tocopherol and β-carotene in amaranth, spider plant, and nightshade accessions grown in New Jersey Daniel Giurleo1,2, giurleod1@gmail.com, Bo Yuan1,2, by114@scarletmail.rutgers.edu, Arianne Vasilatis1, a.vasilatis@gmail.com, Bernard Somers1,2, bws43@scarletmail.rutgers.edu, David Byrnes1, James Simon1,2, Qingli Wu1,2, (1) New Use Agriculture & Natural Plant Products Program, Dept. of Plant Biology and Pathology, Rutgers Univ., New Brunswick, New Jersey (2) Dept. of Medicinal Chemistry, Rutgers Univ., Piscataway, New Jersey (3) Dept. of Food Sci., Rutgers Univ., New Brunswick, New Jersey Amaranth (*Amaranthus spp.*), spider plant (*Cleome spp.*), and nightshade (*Solanum spp.*) are popular indigenous vegetables in sub-Saharan Africa, India and in many Latino countries yet little information is available on their nutritional and phytochemical attributes. These crops are not only easy to grow, but preliminary studies indicate that they are also nutrient rich, and may serve as an available source of many essential micronutrients that are often limited in developing countries. In this study, an HPLC-UV method was used to measure the β-carotene and α-tocopherol content of 3 amaranth, 4 spider plant, and 8 nightshade genetic accessions grown in New Jersey. The results of this study will be used as a foundation to breed future accessions that contain higher amounts of micronutrients in support of efforts to combat malnutrition throughout Africa. The α-tocopherol content of amaranth accessions was found to range from trace levels to 1.13±0.02 mg/100g while β-carotene ranged from 1.00±0.45 mg/100g to 4.85±0.56 mg/100g. α-tocopherol content of spider plant accessions ranged from 3.04±1.77 mg/100g to 7.32±2.21
agricultural residues, dedicated energy crops, wood product wastes, and municipal solid waste, seem to be the largest and mos

AGFD 92 Design, synthesis, and biological activities of novel quaternary salts derivatives containing substituted aniline Qiao Wu¹², Ji-chun Yang¹², Hong-Juan Ma¹², Chang-Ling Liu¹², liuchangling@sinochem.com. (1) State Key Lab of the Discovery and Development of Novel Pesticide, Shenyang Sinochem Agrochemicals R&D Co., Ltd., Shenyang Liaoning, China (2) Shenyang Research Inst. of Chemical Industry Co. Ltd., Shenyang, China Aliphatic amines quaternary salt as fungicides have been widely used in industry. Substituent aminooacetanilide quaternary salt also have been reported as denaturants for organic substances and silver halide photographic light-sensitive material. However, the compounds of this kind had not been published with agrochemicals. To further discover novel biological activity compounds a series of new substituent aminooacetanilide quaternary salt were designed and synthesized by introducing the herbicide carboxylic acid into substituent aminooacetanilide compounds via the intermediate derivatization method. The structure-activity 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. Most of these compounds displayed more than 80% control against Zinnia elegans Jacq., and Abutilon theophrasti Medic. at 150–300 g (a.i.)/hm². In particular, compound No.63 showed 100% post-emergence herbicidal activities against Zinnia elegans Jacq., Abutilon theophrasti Medic., Setaria viridis, and Echinochloa crusgalli, and it was safe to corn at this dose. The present work demonstrates that quaternary salts derivatives can be used as potential lead compounds for developing novel herbicides. Further syntheses and structure optimization studies are in progress.

AGFD 93 Determination of nepetalactones and dihydronepetalactones in catnip by LC/MS Xujuan Dong, William Reichert, williamreic@gmail.com, James Simon, Qingli Wu, qw@aesop.rutgers.edu. Plant Biology, Rutgers Univ., Annandale, New Jersey Ten different Nepeta cataria (catnip) lines were analyzed for the monoterpenyl nepetalactones and dihydronepetalactones to evaluate insect repellent activity. Using a newly developed LC/MS method, 4 stereoisomers of nepetalactones and dihydronepetalactones were successfully separated and identified based on the UV and MS data, and in comparison with the purified standards. The major monoterpenes including Z, E-nepetalactone, E, Z-nepetalactone and a dihydronepetalactone were isolated from the hydrodistilled essential oil using various chromatographic methods and their structures were elucidated by UV, MS and NMR. Using MS detection under MRM mode, the 8 monoterpenes were quantified and their chemical profile was compared each other. The results show that the chemical profile among different catnip lines and the total monoterpen level are significant different ranging from 0.71% to 2.03% for total nepetalactones and from 1.47% to 4.76% total dihydronepetalactones.

AGFD 94 Design, synthesis and biological activity of thienopyrimidine derivatives Fan Yang¹², Chang-Ling Liu¹², liuchangling@sinochem.com, Ai-Ying Guan¹², Zhongyuan Yao¹², Zhihuan Li¹², Yuyuan Song¹². (1) State Key Lab of the Discovery and Development of Novel Pesticide, Shenyang Sinochem Agrochemicals R&D Co., Ltd., Shenyang, China (2) Shenyang Research Inst. of Chemical Industry Co. Ltd., Shenyang, China Compared with many other kinds of heterocyclic compounds, the thienopyrimidines as an important member with both excellent biological and pharmacological activities has been deeply favored by many leading agrochemical companies especially the Dow chemistry continuously for many years. DOW has many publications about the thienopyrimidines among which the compound 137 in the patent US 20060089370 issued in 2006 was revealed with better fungicidal activity at 200mg/L. In order to develop novel agrochemicals with higher efficiency from this kind of compounds, the terminal group replacement method which is one of three classic connotations of Intermediate Derivatization Method(IDM) was applied by introducing arxyoxypyridine moieties which possess reactive group as key intermediates to be connected with the thienopyrimidines. A series of compound 137(US 20060089370) analogues with novel structures were synthesized and bioassayed aiming at exploring the structure-activity relationship. The results of bioassays revealed that many of the compounds have been found with excellent fungicidal and/or insecticidal activity at the tested concentrations especially C-63. It showed 90% control of puccinia polysara at 6.25mg/L, second only to fenaminstrob in the same doses. Besides fungicidal activity, C-56 was found 100% fatality rate to myzus persicae at 10 mg/L as well. So these compounds with both novel structure and high biological activities are worthy of further research and development as lead compounds. The Chinese patent of this kind of compounds has been filed, further research is still in progress.

AGFD 95 Molecular modeling of plant ripening receptors and their interactions with ethylene and ripening inhibitors Jon Gold, jgold@esu.edu, Eric Rosa, ehr8450@live.esu.edu, Richard S. Kelly, rskelly@po-box.esu.edu. East Stroudsburg Univ., Pennsylvania The plant growth regulator ethylene is a crucial hormone in fruit ripening, flower senescence, seedling growth, and seed germination. Ethylene is produced naturally by many plant tissues, is often regulated by internal signals within the plant and acts in response to environmental stress. It is believed that there is a Cu(I) cofactor responsible for the binding of ethylene in the ethylene receptors known as ETR1. In the ETR1 receptor, there is an identified binding location in a 128 amino acid sequence that contains three alpha helices. There are four identified amino acids in the sequence that may ligate the Cu(I) cofactor: histidine, aspartic acid, cysteine, and tyrosine. Very little is understood about how the ethylene binds to the Cu(I) in ETR1. Likewise, very little is known about how 1-MCP inhibits ethylene in the binding site. In this work, the bonding interactions between Cu(I) coordination complexes with ethylene and 1-MCP are investigated. Density functional calculations (B3LYP/6-32G*) were performed utilizing Spartan ’14 software (Wavefunction Inc.). Cu(I) complexes were modeled with varying ligands focusing on their interactions with 1-MCP and ethylene. The complexes studied involved coordination of 2, 3 and 4 ligands. These ligands included CN, CO, H₂O, NH₂, and benzene. The amino acids included in this study were histidine, cysteine, aspartic acid, and tyrosine. The carbon-carbon π-bond lengths, bond-angle of directly bonded hydrogen atoms, HOMO-LUMO energy gaps, and predicted IR spectra were modeled in order to determine likely ligands involved in the binding at the active site.

AGFD 96 Dual-enzyme nano-biocatalyst for the cascade conversion of cellulose-derived oligomers to fructose via a glucose pathway Hao-Hsin Chi, Daniela R. Radu, Guinhal Ozbay, Cheng-Yu Lai, cylai@desu.edu, Delaware State Univ., Dover Biomass resources, such as agricultural residues, dedicated energy crops, wood product wastes, and municipal solid waste, seem to be the largest and most promising
future resources for biofuels and valuable chemicals production alternative to fossil fuel. To reach full potential for valuable chemicals, 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 through hydrolysis. Enzymatic hydrolysis is the key to cost-effective ethanol production from lignocellulosic substrates in the long run, as it is a very mild process, gives potentially high yields, and the maintenance costs are low compared to acid or alkaline hydrolysis (Kuhlai 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 in solid supported catalysis. 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. Current work demonstrates the proof-of-concept of dual-enzyme immobilization to achieve the following steps: transformation of cellulose-derived oligomers to D-fructose in one step by using a porous silica nanoparticle with pores in the range of 7-15 nm as support for: i) A beta-glucosidase enzyme, which converts cellulolic oligomers such as cellobiose to D-glucose; and ii) Glucose isomerase enzyme, which converts (isomerizes) D-glucose to D-fructose. Silica materials scaffolds synthesis and characterization for porosity, surface area and composition, along with enzyme immobilization and assessment of the efficiency of the cascade reaction, will be presented.

AGFD 97 Design, synthesis and fungicidal evaluation of novel substituted arylx pyridine compounds containing pyrimidinamine moiety Yi-Ai Guan1,2, Xu-Feng Sun2, Ji-chun Yang2, Yong Xie2,2,1, Qiao Wu1,2, Chun Yang1,2, Ai-Ying Guan1,2, Lanfeng Ban1,2. (1) State Key Lab of the Discovery and Development of Novel Pesticide, Shenyang Sinochem Agrochemicals R&D Co., Ltd., Shenyang, China (2) Shenyang Research Inst. of Chemical Industry Co. Ltd., Shenyang, China. Downy mildew, a worldwide destructive disease, is one of the core problems to be resolved in crop protection field. Pyridine-containing intermediates have been applied widely as the raw material for agrochemicals or pesticides including fungicides, insecticides/acyaricides and herbicides, due to their bearing reactive groups like halogen, active H or COOH, etc. which can easily be modified. In this study, for discovering a novel candidate to protect crops and F&V from downy mildew, relying on Intermediate Derivatization Methods, the substituted 2-chloro-5-(chloromethyl)pyridine was employed as the starting material and then conducted successive reactions to achieve the key ethylamine intermediates, which was then used to replace 2-(4-(trifluoromethoxy)phenyl)ethanimine of insecticide flufenoxuron delivering a series of substituted arylx pyridine analogues containing pyrimidinamine moiety. Their structures were confirmed by 1H NMR, MS and elemental analysis. Bioassays demonstrated that some of the title compounds exhibited excellent fungicidal activity against cucumber downy mildew at 6.25 mg L⁻¹. The relationship between structure and fungicidal activity is reported as well. The present work demonstrates that substituted aryloxy pyridine compounds containing pyrimidinamine moiety can be used as possible lead compounds for further optimization.

AGFD 97 Design, synthesis, and the structure-activity relationships of novel N-substituted piperazines derivatives Yong Xie1,2, Chang-Ling Liu1,2, liuchangling@sinochem.com, Ying Xu1, Ai-Ying Guan1,2, Lanfeng Ban1,2. (1) State Key Lab of the Discovery and Development of Novel Pesticide, Shenyang Sinochem Agrochemicals R&D Co., Ltd., Shenyang, Liaoning, China (2) Shenyang Research Inst. of Chemical Industry Co. Ltd., Shenyang, China. Pytophagous mites, such as Tetranychus cinnabarinus, Panonychus citri and Panonychus ulmi are most important and highly polyphagous pests of a wide range of field and greenhouse crops worldwide. They attack glasshouse as well as field crops causing serious damage by direct feeding or by transmitting plant pathogens and viruses. At present, spider mites such as Tetranychus urticae have developed resistance to virtually all chemical classes to control them. Thus, discovering and exploiting acaricidal compounds with new modes of action becomes an important way to overcome resistance problems. Hence, a series of novel N-substituted piperazines derivatives were designed and synthesized by intermediate derivatization methods and their acaricidal activities were evaluated. The acaricidal activity in greenhouse tests showed some compounds exhibited significant acaricidal activity in controlling adults of Tetranychus cinnabarinus. Compound 623 in particular was found to be the best potential candidate acaricide and proved more active than the contrast spirodiclofen and pyridaben. The results of acaricidal activities against larvae and eggs of Tetranychus cinnabarinus indicated that compound 623 possessed equivalent larvicidal activity to spirodiclofen. Meanwhile, compound 623 showed more ovicidal activity than spirodiclofen. Then, the structure-activity relationships (SARs) of was studied. The present work indicates that compound 623 may be a novel acaricide candidate for spider mites control.

AGFD 99 Design, synthesis and herbicidal evaluation of novel N-[3-(pyridin-2-yl)-phenylsulfonylcarboxamides Ji-chun Yang1,2, Qiao Wu1,2, Ai-Ying Guan1,2, Hong-Juan Ma1,2, Chang-Ling Liu1,2, liuchangling@sinochem.com. (1) State Key Lab of the Discovery and Development of Novel Pesticide, Shenyang Sinochem Agrochemicals R&D Co., Ltd., Shenyang Liaoning, China (2) Shenyang Research Inst. of Chemical Industry Co. Ltd., Shenyang, China. Weeds continue to evolve resistance to all the known modes of herbicidal action, and no herbicide with a new target site has been commercialized in nearly 20 years. So, Much research has focused on discovering novel compounds with structures different from those of commercial herbicides. In previous works, we have synthesized a series substituted 3-(pyridin-2-yl)benzenesulfonamide derivatives, of which some compounds gave excellent herbicidal activities against velvet leaf, youth-and-old age, barnyard grass and foxtail using herbicidal activity assay in greenhouse tests. While, Amide herbicides are highly effective and selective against many kinds of weeds, such as dифлуфенокс. Novel N-[3-(pyridin-2-yl)-phenylsulfonylcarboxamides were designed and evaluated in the search for new herbicides with improved biological properties, and the terminal group replacement method which was key type of Intermediate derivatization methods (IDM) was applied by introducing aroyl to modify the ethyl carbamate group of 3-(pyridin-2-yl)benzenesulfonamide derivatives. The herbicidal activity assay in greenhouse tests showed several compounds could efficiently control velvet leaf, youth-and-old age at 37.5 g a.i./ha, meanwhile, no hazard to crops such as wheat, corn and rice at 300 g a.i./ha. The results of this study suggest that further design and structural modification of the N-[3-(pyridin-2-yl)-phenylsulfonylcarboxamides derivatives as herbicides is worthwhile.

AGFD 100 Dietary exposure and toxicological effects of non-phtalate plasticizers from use in food contact materials LaShonda T. Cureton, Lashonda.Cureton@fda.hhs.gov, Omari J. Bandele, Omari.bandele@fda.hhs.gov, Allan B. Bailey, Adejoke Ogungbesan.FDA,
College Park, Maryland Plasticizers have long been used in the industrial manufacture of polymers for processing and increasing flexibility and toughness of the material. Plasticizers help balance performance and costs for the production of materials with mass versatility in the global market. Phthalates are the most commonly used plasticizers, accounting for >75% of the world’s consumption of plasticizers in 2012. The US consumption of plasticizers in 2012 was ~0.8 million metric tons, of which ~60% were phthalates. About 80-90% of the plasticizer market is devoted to polyvinyl chloride (PVC), which is a highly versatile thermoplastic used to produce both rigid and flexible products with a combination of engineering properties. While articles produced from rigid PVC do not contain plasticizers, those produced from flexible PVC traditionally include plasticizers to impart ductility, while maintaining strength. Given the substantial use of flexible PVC in many food-related commodities, the FDA is updating and evaluating dietary exposure estimates and toxicological information available on phthalates and non-phthalate substitutes, including epoxidized soybean oil (ESBO) and epoxidized linseed oil (ELSO). ESBO and the less frequently used ELSO are used in flexible PVC-based food contact film wraps and gaskets from which they can migrate into food. This technical review of the literature and agency files summarizes the identity, regulatory status, levels in food and food simulants, cumulative dietary exposure estimates, and toxicological information for the safety assessment of ESBO and ELSO. Based on this review, the cumulative dietary concentration (CDC) for ESBO and ELSO is 2.6 ppm and 65 ppb, respectively, which is estimated from uses in PVC-based films and gaskets. Migration of ESBO and ELSO increases with increasing plasticizer levels, food contact surface area, temperatures during food contact use and duration of contact with food. This review of all the available toxicological data has identified the most conservative no observed adverse effect level (NOAEL) for ESBO to be 140 mg/kg bw (2800 ppm) based on a 2-year study in rats. Similarities in the structure and toxicological profile of ESBO and ELSO suggest that their safety can be evaluated as a group. Combining the CDC for ESBO and ELSO from their use as plasticizers in PVC-based food contact materials, results in a CDC of 0.136 mg/kg bw/day and a calculated margin of exposure (MOE) of ~1030 relative to the NOAEL.

**AGFD 101** Total synthesis of novel flavan-alkaloids isolated from the African tea *Combretum micranthum* Jing Zhen, zhenjing89@gmail.com, Cara Welch1, Qingli Wu1,2, James Simon1,2. (1) Plant Biology, Rutgers Univ., New Brunswick, New Jersey (2) Medicinal Chemistry, Rutgers Univ., Piscataway, New Jersey A series of novel skeleton flavan-alkaloids were discovered in the leaves of the African shrub kinkeliba (*Combretum micranthum*), which is used as a popular herbal tea in Senegal and parts of West Africa. These flavan-alkaloids, which we name as kinkeloids in honor of the plant, consists of two major parts including a flavan moiety and an attached piperidine ring. Kinkeloids in *C. micranthum* are sub-divided into four series A-D and each group was isolated and characterized by UV, MS and NMR spectrometric methods. Each kinkeloids group has two constitutional isomers with piperidine ring attached at 6 or 8 position, and 2 to 3 chiral centers. Biological studies have shown that these kinkeloids from an enriched n-butanol extract exhibited promising glucose-lowering activity. To further develop applications of these novel natural products, the major flavan-alkaloids of Kinkeloids B were totally synthesized, and then spectral analysis and comparison with plant extracts further confirmed the structures and identities of these kinkeloids.

**AGFD 102** Assessment of dietary exposure to emulsifiers of regulatory interest for the US population Renata Kolanos, rkolanos@gmail.com, Romina Shah, Michael DiNovi, Antonia Mattia, Kotaro Kaneko. FDA, Center for Food Safety and Applied Nutrition, Office of Additive Safety, College Park, Maryland Dietary exposure assessment using food consumption data is an obligate part of assessing the safety of food ingredients. The dietary exposure estimate is compared to an experimentally determined upper limit of safe exposure, or Acceptable Daily Intake (ADI). Recently, two food additives classified as emulsifiers, sodium carboxymethylcellulose (CMC) and polysorbate 80 (P80), have received attention due to their potential putative adverse effects on gut microbiota. Currently, there are no published dietary exposure estimates for the US population for CMC, P80, and other commonly used emulsifiers. The current investigation focused on the estimation of dietary exposure to seven emulsifiers: CMC, P80, lecithin, mono- and diglycerides (MDG), stearyl lactylates (SSL) and calcium stearoyl lactylate (CSLL), sucrose esters, and polyglycerol polyricinoleate (PGPR). Maximum use levels of these emulsifiers were obtained from publicly-available sources. Dietary exposure to these emulsifiers was estimated for the U.S. population (aged 2 years and older) for two time periods (1999–2002 and 2003–2010) using both 2-day food consumption data from the National Health and Nutrition Examination Survey (NHANES), and 10–14 day food consumption data from the NPD Group, Inc. National Eating Trends-Nutrient Intake Database (NPD NET-NID). The present analysis indicated that the exposure to CMC is two to three times lower than lecithin and MDG; and the exposure to P80 is approximately half that of CMC. By examining two time periods (1999–2002 and 2003–2010), it was concluded that there is no evidence to suggest the exposure levels to emulsifiers have substantially increased during the time period examined. Our analyses indicate that the dietary exposure for these seven emulsifiers do not raise safety concerns at the current use levels.

**AGFD 103** Peptidolytic activity of three probiotic lactic acid bacteria for possible use as sourdough starters Humberto Hernandez-Sanchez, hherman1955@gmail.com, Mitzi Nava-Romero. Ingeniería Bioquímica, Escuela Nacional de Ciencias Biológicas - Instituto Politécnico Nacional, Ciudad de México, Mexico The aim of this work was to test the presence of peptidases in three probiotic lactic acid bacteria potentially capable of hydrolyzing Pro-rich peptides including the 33-mer peptide in gluten so a sourdough bread might be produced which could be tolerated by celiac sprue patients. Previous studies have indicated that some probiotics can digest gluten peptides. Three strains of commercial probiotics (*Lactobacillus casei* Shirota, *Lactobacillus plantarum* 299v, and *Lactobacillus rhamnosus* GG) were used in this study. Peptidase activities (PepN, PepI, PepX and PepO) on para-nitroanilide (p-NA) substrates were determined by measuring the increase in absorbance at 410 nm. The strains were also tested in their ability to use maltose to produce lactic acid in a modified MRS broth and in wheat dough. The three probiotics showed adequate growth and lactic acid production (pH<3.9) after 24 h at 35°C in broth. Good average peptidase activities were obtained for the three strains (0.202, 0.160, 0.179, and 0.347 U for PepN, PepI, PepX, and PepO respectively). Acceptable sourdoughs could be obtained with these microorganisms showing pH values between 3.7 and 3.9 after 12 h of fermentation at 35°C. These results showed that these microorganisms have the potential to digest the Pre- and Leu-containing peptides in gluten and could be included in a starter to produce sourdough bread for celiac sprue patients.

**AGFD 104** Explorative study to understand the chemical diversity in Maillard reactions Daniel Hemmler², daniel.hemmler@tum.de, Chloé Roullier-Gall², James W. Marshall¹, Michael Rychlik², Andy J. Taylor¹, Philippe Schmitt-Kopplin². (1) Waltham Centre for Pet Nutrition, Mars Petcare UK, Melton Mowbray, UK (2) Analytical Food Chemistry, Comprehensive Foodomics Platform, Technical Univ.
Maillard reactions refer to non-enzymatic reactions of reducing carbohydrates with amino compounds (amino acids, peptides or proteins). They play a crucial role in determining the aroma, taste and color of thermally processed food. Most knowledge of Maillard reactions to date has been deduced from the results of experiments in sugar / amino acid model systems. Furthermore, the discovery of the entire complexity and coherences arising from even simple model systems is still a challenge in analytical chemistry. In this particular study we present a methodology that exposes the amazing complexity of Maillard reaction products (MRPs) formed in aqueous model systems. Non-targeted ultrahigh-resolution mass spectrometry (FT-ICR-MS) in combination with mass difference network analysis enables a comprehensive investigation of non-volatile MRPs and the prediction of possible chemical transformations. Compounds arising from amino acid and sugar degradation were considered independently in order to identify pools of specific MRPs resulting only from the degradation of Amadori rearrangement products. The investigation of different treatment times, amino acid and sugar precursors allowed the visualization of a time-dependent and precursor specific evolution of MRPs. More than 700 distinct elemental compositions could be identified in a thermally processed ribose / lysine model system whereas more than 50% of the identifications were found to be specific to the amino acid lysine. Many of the identified compounds have formulas consistent with important precursors in the formation of aroma, taste and color compounds which also occur in real food samples.

AGFD 105 - Withdrawn

AGFD 106 Physico-chemical properties and stability of a soy protein isolate and peanut oil-based emulsion as affected by ultra-high pressure homogenization and pH Dipaloke Mukherjee, dm259@msstate.edu, Sam K. Chang. Dept. Food Sci., Nutrition and Health Prom, Mississippi State Univ. Soy protein isolate (SPI), a complex combination of proteins has long been used as an emulsifier in oil-in-water (O/W) systems, nevertheless its properties as affected by ultra-high pressure homogenization (UHPH), combined with changes in pH have not been fully assessed. The study aimed to investigate the physico-chemical properties and stability of SPI-based O/W emulsions, formulated using different levels of UHPH under various pH. The coarse emulsions, prepared using SPI (1%, w/v, the emulsifier) dispersed in potassium phosphate buffer [the continuous phase with three different pH (4, 6 and 7, respectively)] and fresh peanut oil (the dispersed phase) with a phase fraction (Φ) of 0.01] were subjected to UHPH of 70, 140 and 210 MPa, respectively. Mean globular particle size distribution (MPSD), droplet surface energy (SE), zeta potential (z-P) and surface hydrophobicity (SH) were analyzed for three weeks of refrigerated storage. Emulsions of pH 4 exhibited the least stability, indicated by significantly (P<0.05) lower SE and absolute z-P relative to the other emulsions (conceivably as pH 4 lies within the range of the isoelectric points of a considerable proportion of proteins in SPI, causing protein aggregation). The emulsion with pH 4 subjected to 210 MPa showed the best stability at the final week of storage, depicted by significantly (P<0.05) lower MPSD that was ~50% less, as well as 77 and 27% greater z-P than the emulsions with pH 4 and 6, respectively. UHPH being equal. It also had significantly (P<0.05) greater SE than emulsions with the same pH that were subjected to lower levels of UHPH, indicating a pressure dependent increase in SH, which was confirmed with 8-Anilinonaphthalene-1-sulfonic acid fluorescence assay. The study provided novel information depicting the potential of SPI for the development of stable emulsion systems for a wide range of beverages. Keywords: particle size, surface energy, zeta potential

AGFD 107 - Withdrawn

AGFD 108 Relationship between structural characteristics and digestibility of debranched starch Guodong Liu1, liuguodongwx@hotmail.com, Yan Hong2, Zhengbiao Gu3, Yike Jiang4. (1) Jiangnan Univ., Wuxi, China (2) Food Sci., Rutgers Univ., New Brunswick, New Jersey. Researches about the structure and digestibility of debranched starches (DBS) are meaningful and useful to design and product functional foods containing slowly digestible starch (SDS) and resistant starch (RS). We therefore aimed to establish statistical and causal relationships between starch fine structure and DBS digestibility and explored methods to generate modified starches with improved functional food potential. The results demonstrated that the content of RDS was significantly and positively correlated with the content and molecule size of amylopectin and partially debranched starches, while RS showed strong and significant positive correlations with amylose and linear-short amylose contents. DBS containing more amylose or with higher debranching degrees contain less RDS and more SDS and RS. Debranched high amylose starches (DB-HAS) were feasible to prepare high RS products, and debranched waxy starches (DB-WS) were an available source to prepare SDS. Amylopectin and partially debranched starch tend to be more easily and quickly hydrolyzed by amylase. Alignment and aggregation as well as recrystallization among amylose and linear-short amylose molecules contribute to the resistance to digestion. Summarily, pullullanase hydrolysis is a feasible method to obtain modified starches with low RDS and high SDS and RS.

AGFD 109 Alginate conjugated keratin for wound dressing materials Rong-min Wang, wangrm@nwu.edu.cn. Northwest Normal Univ., Lanzhou, China Keratin as a potential biopolymer has been applied for various biomedical fields due to its bio-compatible, biodegradability, eco-friendly and inexpensive characters. Here, keratin (FK), being extracted feather, was modified by conjugating with sodium alginate via EDC/NHS. Then, the keratin conjugated alginate sponge (FK-SA sponge) was prepared, and its properties as a wound dressing were measured. Its structure and properties were characterized FT-IR, TG/DSC and SEM. Their absorption capacity, water retention capacity and water vapor transmission were measured. Their antibacterial properties and release behaviors were also investigated. For FK-SA sponge, the cumulative release rate of model drug loaded keratin sponge reached 74 % in 13 hrs at pH 7.4. Meanwhile, FK-SA sponge loaded benzalkonium chloride has excellent antibacterial activity and exhibited unique biodegradation properties. This keratin conjugated alginate biopolymer sponge is expected to be used as a potential wound dressing in clinical nursing field as well as a sustained drug carrier in biomedical field.

AGFD 110 Triacylglycerol compositions of sunflower, corn and soybean oils examined with supercritical CO2 ultra-performance convergence chromatography combined with quadrupole time-of-flight mass spectrometry Boyan Gao1, raphaelgao1985@gmail.com, Yinghua Luo2, Weiying Lu1, Liangli L. Yu1. (1) Dept. of Agriculture and BioTech., Shanghai Jiaotong Univ., Shanghai, China (2) Univ. of Maryland, College Park (3) Univ. of Maryland, College Park The triacylglycerol compositions of sunflower, corn and soybean oils were examined using a supercritical CO2 ultra-performance convergence chromatography (UPC2) system combined with a quadrupole time-of-
flight mass spectrometry (Q-TOF MS). UPC² provided an excellent resolution and separation for the triacylglycerols, while the high performance Q-TOF MS system provide the accurate molecular weight and mass fragment ions information for triacylglycerol compound characterization. A total of 30, 29 and 30 triacylglycerols were detected and identified in sunflower, corn and soybean oils, respectively. The identification of these triacylglycerols based on their elementary compositions and MS² fragment ion profiles. The relative concentrations of these triacylglycerols in three oils were also estimated. The combination of UPC² and Q-TOF MS could determine triacylglycerol compositions for oils and fats, provide sn-position information for fatty acids, and important for food nutritional value and stability.

AGFD 111 Evaluation of hydrogen peroxide scavenging activity of phenolic acids by employing optical nanoprobes based on gold nanoshells Weiping Qian, wqian@seu.edu.cn. Southeast Univ., Nanjing, China. A series of phenolic acids were tested for their ability to scavenge hydrogen peroxide by using a novel enzyme-free, spectrophotometry assay. Gold nanoshells (GNSs) precursor composites were selected as the optical nanoprobes. The approach was based on the hydrogen peroxide-induced growth of GNSs, which combines nanoscience with food/health research as an innovative detection scheme. The addition of phenolic acids inhibits the formation of complete GNSs and the corresponding peak wavelength changes rationally, which could be used as an optical signature. Among the tested samples, caffeic acid is found to be the most efficient hydrogen peroxide-scavenger with its hydrogen peroxide scavenging activity, whereas transcinnamic acid exhibits the weakest activity. Results obtained were considered on the basis of structure-activity relationships. Additionally, several tea and herb extracts were also evaluated. The presented wavelength-based detection method shows superiority in evaluating coloured samples, which avoids background interference compared with the conventional absorbance based optical methods.

AGFD 112 Growth inhibition of bladder cancer cells is greater with quercetin-3-glucoside than with quercetin or quercetin-3-rutinoside Michael A. Lea, lea@njms.rutgers.edu, A astha Tandon, Charles desBordes. (1) Microbiology, Rutgers New Jersey Medical School, Newark, (2) Biology, Medgar Evers College, CUNY, Brooklyn New York. Cellular uptake and inhibition of growth by flavonoids is often greater with aglycones than with glycosides. However, we have seen previously in colon cancer cells that growth inhibition is greater with quercetin-3-glucoside than with quercetin. In the present study we investigated whether a similar observation can be made with bladder cancer cells. Eight human bladder cancer cell lines were studied: 5637, HT1197, HT1376, RT4, SW780, T24, TCCSUP and UM-UC-3 cells. Growth was monitored by staining with sulfonohadamine B after incubation in RPMI 1640 medium with 5% fetal calf serum for 72 hours. In all eight cell lines, growth inhibition was greater with quercetin-3-glucoside than with quercetin in the concentration range of 5-50 µM. In contrast, growth inhibition was greater with quercetin than with quercetin-3-rutinoside (rutin). Significant inhibition of growth was not seen in most of the cell lines when incubated with 50 µM rutin. The greater inhibition with quercetin-3-glucoside may relate to uptake of that molecule by a glucose transporter. We considered whether increasing the concentration of glucose in the medium might compete with transport of quercetin-3-glucoside and effect growth inhibition. Increasing the glucose concentration from 2 to 6 mg per ml did not significa ntly affect the growth inhibition by 50 µM quercetin-3-glucoside in six bladder cancer cell lines nor in two human colon cancer cell lines (Caco-2 and HT29). In conclusion, growth inhibition in bladder cancer cells was greater with quercetin-3-glucoside than with the aglycone and the role of glucose transporters in this difference remains to be defined.

AGFD 113 Soluble keratin from wool Eleanor M. Brown, elli e.brown@ars.usda.gov, Kalgi Pandya, Maryann M. Taylor, Cheng-Kung Liu. BOAC, USDA ARS ERRC, Wyndmoor, Pennsylvania. The U.S. sheep industry producing 40 million pounds of raw wool per year is an important component of the meat industry. New methods for the treatment of domestic wool with keratin isolated from the unmarketable fraction of wool, and functionalized for water, oil, or insect repellency are needed. As a first step in the process, we are evaluating the effectiveness of keratin solubilization via relatively benign methods that use thioglycolic acid or bisulfite to reduce disulfide bonds, peracetic acid to oxidize disulfides, or urea/thiourea as hydrogen bond disrupters. The procedures are compared in terms of quantity and quality of soluble protein and cost effectiveness. Successful completion of this project will provide the basis for commercial development of such methods, followed by functional modification of the soluble keratin, and its application to textiles.

AGFD 114 Synthesis and development of a new selective ryano dine receptor activator insecticide Won Hyung Lee, genius1982@nate.com. Central research Inst., Kyung Nong Co, Gy eong-jusi, Korea. Ryano dine receptor activator insecticides are recently developed by modifying the structure of the natural product ryano dine and its mode of action is known to inhibit ryano dine receptor, calcium-induced calcium release channel. Ryannodine combines the non-aqueous portion of the receptor that is distributed in nerve and muscle cells, thus it cause muscle contraction and inhibition of feeding activity on insects by disturbing the interaction between nerves. Insecticides in this group specially have strong e ffect on larvae of lepidoptera and low toxicity on mammals. Because of specificity like new mode of action, commercial registration is beginning. The purpose of this study is to synthesize and develop new compounds for selective activator of insect ryano dine receptors. A series of pyrazole amide derivatives possessing carbamate linker instead of anthralinic amide have been synthesized. Their biological activities against various harmful insects and safeties for beneficial insects including honeybee have been evaluated. A compound having the strongest activity is selected and commercialization is in progress with other tests, including toxicity and formulation.

AGFD 115 Fluorescence fingerprinting of antioxidants in sorghum and sugarcane Sophie M. Uchimiya, sophie.uchimiya@ars.usda.gov. CUR, USDA-ARS, New Orleans, Louisiana. Polyphenolic chromophores are found in various food products including sorghum and sugarcane, and underlie important functions such as antioxidant property and pest resistance. For example, polyflavanols (procyanidins), anthocyanins, and phenolic acids are known naturally-occurring antioxidants. Currently available standardized tannin methods are influenced by the experimental artifacts, including the kinetically controlled reactions, overlapping spectra near the detection wavelength, low sensitivity, and the reactivity of non-target structures. Structure-reactivity relationships are necessary to understand the influence of polyphenolic chromophore structures on the measurable tannin determined by the traditional calorimetric methods. This study will explore the utility of fluorescence EEM/PARAFAC to fingerprint polyphenols in sugar crops: sweet sorghum and sugarcane. Linear correlation was observed between (i) the antioxidant activity (ii) the amounts of procyanidins and flavonoids, and (ii) the aromaticity of fingerprint fluorescent structures.
AGFD 116 Starch modified by wet-milling process to stabilize Pickering emulsions Xuanxuan Lu\(^2\), Lauren Jackson\(^1\), John Hammerstone\(^1\), Rmargolskee@monell.org. (1) Monell Chemical Senses Center, Philadelphia, Pennsylvania (2) PepsiCo, Hawthorne, New York. The primary sweet sensor in taste cells for both sugars and non-calyoric sweeteners is the heteromeric combination of type 1 taste receptors 2 and 3 (T1R2=T1R3, encoded by TAS1R2 and TAS1R3 genes). This complex G-protein-coupled receptor has multiple ligand binding sites enabling it to respond to many different types of sweet compounds, from saccharin to sucrose. Activation of T1R2+T1R3 by either a sugar or a non-calyoric sweetener initiates a signal transduction cascade involving gustducin, phospholipase beta-2, Ca\(^{++}\) release and Ca\(^{++}\)-activation of the TrpM5 ion channel, ultimately leading to depolarization of the sweet taste cell. However, in the absence of T1R2+T1R3 (e.g., in TAS1R3 knockout mice), animals still respond to sugars, demonstrating the presence of a second T1R-independent sweet detection pathway. This second pathway utilizes glucose transporters and sodium glucose cotransporter-1 along with the ATP-gated K\(^{+}\) channel that serves as a metabolic taste. This T1R-independent sugar-specific sweet pathway functions similarly to how the gut and pancreas detect and respond to glucose and other metabolizable monosaccharide sugars based on their ability to generate ATP as an energy source. Recently we found that sweet taste cells also express multiple disaccharide-hydrolyzing enzymes (e.g., maltase-glucosaminylase and sucrase-isomaltase) previously known to occur only in the intestine’s “brush border”. This enables sweet-responding taste cells to detect disaccharide sugars by the second ("metabolic") pathway. Together with salivary amylase, these taste cell-expressed enzymes may locally break down dietary disaccharides and starch hydrolysis products into monosaccharides that could serve as substrates for the T1R-independent taste.
AGFD 121 Discovery, structure elucidation and efficacy testing of a natural compound used to improve low-calorie beverage sweet flavor quality William R. Bonorden, william.bonorden@pepsico.com, Tianying An, Phyllip Augustin, Shawn Ericson, Linda Flammer, Stephen Gravina, Keith Griswold, Thomas D. Lee, Samuel Lindberg, Laura Nattress, Jarvis Soto, Gerhard Zehentbauer, Christophe Galopin. PepsiCo Inc, Hawthorne, New York. A novel flavor molecule was discovered that improves the perception of sweet quality in low-calorie beverages. The plant material was identified through ethnohistorical history and an appropriate quantity obtained for ethanol/water extraction for preparative HPLC fractionation. Fractions were subject to bench top sensory evaluation screening for sweetener or sweetness modifying properties. No sweetener activity was discovered; however, one fraction displayed sweetness modifying properties and was subsequently purified via UPLC using ELSD and PDA detection. The active fraction contained a single compound whose structure was elucidated via NMR, LCMS and UV spectroscopy. The target compound was synthesized for physicochemical testing and a toxicological evaluation was conducted prior to continued sensory evaluation. Physicochemical testing included solubility, thermal stability, photo stability and a full kinetic analysis across a normal beverage pH range and potential commercial distribution temperatures. Sensory testing focused on demonstrating improvement of sweet flavor quality in low-calorie beverages. Physicochemical, kinetic and sensory data will be presented in more detail.

AGFD 122 Stevia innovation: Improved leaf extracts from advanced understanding of taste John C. Fry1,2, connectco@btinternet.com. (1) Director, Connect Consulting, Horsham, W. Sussex, United Kingdom (2) Principal External Consultant, Sweeteners, Cargill, Inc., Wayzata, Minnesota Stevia leaf extracts are important zero-calorie sweeteners, widely used to reduce sugars content of foods and beverages. Unwanted side tastes, such as bitterness and licorice, limit the use of such extracts, even when highly purified. Intensive investigations of taste interactions between steviol glycosides, coupled with mathematical modelling of these relationships, have revealed unexpected synergies. In appropriate combinations of glycosides these synergies act both to enhance sweetness potency and reduce side tastes. Such insights allows the selection of standardized leaf extracts of reliably superior taste that are now becoming commercially available.

AGFD 123 Dynamic proteome alteration and functional modulation of human saliva induced by dietary taste stimuli Matthias Bader1, Andreas Dunkel2, Guillaume Medard3, Estela del Castillo4, Amin Gholami2, Bernhard Kuster2, Thomas Hofmann2, thomas.hofmann@wzw.tum.de. (1) Food Chemistry and Molecular Sensory Science, Technical Univ. of Munich, Freising, Germany (2) Proteomics and Bioanalytics, Technical Univ. of Munich, Freising, Germany. In order to investigate the time-dependent influence of taste stimuli on saliva flow and the human salivary proteome, healthy individuals were challenged with sour, sweet, bitter, umami, salty, pungent, numbing and tingling stimuli. After evaluation of the influence on the saliva flow, the impact on the human saliva proteome was analyzed by SDS-PAGE, followed by tryptic digestion, nano-HPLC-MS/MS and a relative, label-free quantitation method. Each stimulus caused a specific modulation of the salivary proteome resulting in different proteins increased or decreased in abundance upon stimulation. As the effects of this study were observed instantaneously upon stimulation, any proteome modulation is very likely to result from the release of proteins from preformed vesicles and not from de novo synthesis. Functional pathway and gene ontology enrichment analysis, followed by functional test experiments revealed, that taste induced alterations of the saliva proteome trigger innate protective mechanisms like antimicrobial defence. Knowledge of these mechanisms will help to develop “tasty” oral health care products with enhanced functionality.

AGFD 124 Dietary fibers and associated phytochemicals in cereals Knud Erik Bach Knudsen, kmuderik.bachknudsen@anis.au.dk, Animal Science, Aarhus Univ., Tjele, Denmark. Epidemiological studies have linked whole-grain cereal consumption to a reduced risk of developing several chronic diseases including heart disease, arteriosclerosis, type-2 diabetes and colonic and breast cancer. The underlying physiological mechanisms behind the protective effects of whole-grains, however, are unclear but is most likely assigned to a concerted action of dietary fiber (DF) and a wide variety of phytochemicals. The DF fraction of cereals consists of non-starch polysaccharides (NSP), resistant starch, oligosaccharides (mostly fructans), and the non-carbohydrate polyphenolic ether lignin. The main NSP in cereals are arabinoxylan (AX), mixed linkages β(1-3; 1-4)-glucan (β-glucan) and cellulose, which vary significantly according to the cereal species but also between different tissues of the grains. Rye, triticale, wheat and corn are rich in AX, whereas barley and oats contain a high level of β-glucan. Physiologically, it is of importance that some of the cell wall polysaccharides, i.e. AX and β-glucan (soluble NSP) contribute to higher viscosity as this may influence rate and extent of digestion and absorption in the small intestine. Associated to the DF matrix of cereals, however, is also an array of non-nutritive non-carbohydrate constituents predominantly concentrated in the bran fraction. Of importance in a nutritional-health context is the phenolic components - benzoic acid and cinnamic derivatives and lignans. Of the phenolics only a small fraction is absorbed in the small intestine whereas the major part is passed to the large intestine. The colonic microbiota, along with the degradation and metabolism of DF to short-chain fatty acids and gases, also convert the phenolic compounds into a range of other metabolites that are absorbed to the body and with the capability of influencing the metabolism at the cellular level.

AGFD 125 Alkylresorcinols as dietary biomarkers of whole grain wheat and rye intake Rikard Landberg1,2, rikard.landberg@slu.se. (1) Dept. of Food Sci., Swedish Univ. of Agricultural Sciences, Uppsala, Sweden (2) Unit of Nutritional Epidemiology, Inst. of Environmental Medicine, Karolinska Inst.t, Stockholm, Sweden. Alkylresorcinols (AR) is a group of phenolic lipids almost exclusively found in the outer parts of wheat and rye grains among commonly consumed foods. The content in whole grain and bran products is high (200-4000 µg/g), whereas only trace-levels are detected in refined products. AR have therefore been suggested and evaluated as biomarkers for whole grain wheat and rye intake. In humans, plasma AR concentrations are typically in the range of nmol/L but may reach µmol/L immediately after whole grain wheat and rye product consumption. Habitual consumption of whole grain or bran-rich foods leads to accumulation of AR in adipose tissues. Elimination is mainly carried out through metabolism and subsequent urinary excretion of two main metabolites, 3,5-dihydroxybenzoic acid (DHBA) and 3-(3,5-dihydroxyphenyl)-1-propanoic acid (DHPPA). Recent studies have also identified minor metabolites such as DHB-glycine and 5-(3,5-Dihydroxyphenyl)pentanoic acid (DHPPTA). Results from human intervention studies as well
as studies in free-living populations have shown that plasma AR concentrations and their main metabolites can be used as biomarkers of whole grain intake from wheat and rye when intake is frequent and stable. Results from recent studies where plasma AR concentrations have been applied as dietary biomarkers to improve whole grain intake ranking and compliance will be presented. The validity and reproducibility of minor AR metabolites in urine will be presented along with novel data on the validation and application of AR in adipose tissue biopsies as long-term biomarkers of whole grain wheat and rye intake in relation to cardiometabolic risk factors among Swedish men and women.

AGFD 126 Biomarkers of whole grain wheat intake identified by targeted and non-targeted metabolomic approaches Yingdong Zhu1, yzhu1@ncat.edu, Wei Sha2, Pei Wang1, Shengmin Sang1. (1) Lab for Functional Foods and Human Health, Center for Excellence in Post-Harvest Technologies, North Carolina A&T State Univ., Kannapolis (2) Dept. of Bioinformatics and Genomics, Univ. of North Carolina at Charlotte, Kannapolis Increased whole grain (WG) consumption has been inversely associated with the risk for developing some diet-related disorders, such as type 2 diabetes, obesity, cancer, and cardiovascular diseases. Many epidemiological studies, however, have failed to generate consistent results on this topic due to a lack of accurate tools to assess dietary intake of whole grains. In addition, the underlying mechanisms of the observed beneficial health effects of WG intake are still largely unknown. Nutritional epidemiology research needs more reliable and quantitative methods for measuring dietary intake of specific foods. In this study, we found that the combination of the targeted and non-targeted metabolomic approaches is a powerful tool to identify the biomarkers of WG wheat intake. Using a targeted LC/MS based metabolomic approach, we established the metabolic fingerprints of the major phytochemicals in WG wheat in human urine including metabolites of alkylresorcinols, benzoxazinoids, lignans, and phytosterols, as well as microbial-derived metabolites. Using a non-targeted LC/MS based global metabolomic approach, we investigated the impact of WG wheat bread intake on the endogenous urinary metabolome. Metabolic profiling revealed a number of differences relating to the consumption of WG wheat bread vs. refined grain wheat bread, such as metabolites related to oxidative stress, cancer and cardiovascular diseases.

AGFD 127 Non-targeted metabolite profiling for characterization of bioactive compounds in cereals and their metabolic effects in different models Kati Hanhineva, kati.hanhineva@uef.fi. Univ. of Eastern Finland, Kuopio. Besides being an important source of dietary fiber, whole grains contain a plethora of phytochemical species that supposedly possess various bioactivities once harbored human body via diet. However, indication of the precise constituents responsible for any biologically relevant, health protective metabolic effect is difficult due to the large number of phytochemicals, including hitherto unknown compounds, present in the bran compartment. Furthermore, different processing methods during the food manufacturing modify quantitatively and qualitatively the phytochemical composition of the food product resulting in variation in bioavailability of bioactive compounds which ultimately may impact the biological outcome. Likewise, the complexity of the cellular metabolic processes the phytochemicals and their metabolites may perturb further complicates the task of elucidating the molecular mechanisms related to health protective effect of whole grain consumption. The non-targeted mass spectrometry-based metabolite profiling offers the possibility to monitor concomitantly the composition of wide array of metabolites both from plant and mammalian origin. We have analyzed phytochemicals present in whole grains and investigated how differentially processed rye and wheat bran fractions exert phytochemicals in a mouse feeding trial. The pattern of metabolites excreted in urine varied depending on the grain species and the bioprocessing method applied. Similarly, occurrence of phytochemical metabolites in plasma was differential, and interestingly, their accumulation pattern in various internal organs was also differential according to the feed. The phytochemical metabolites in organs are anticipated to potentially participate in cellular metabolism and cause fine tuning of metabolism eventually evidenced as improved metabolic health. For example, our results indicate that glycine betaine, which is abundant in both rye and wheat bran is metabolized, potentially by microbiota, resulting in various novel betaine compounds that are found both in biofluids and organ samples. Our preliminary results from human intervention trials indicate similar metabolic phenomena as found in the mouse studies.

AGFD 128 Avenanthramides and their microbial metabolites as the exposure markers for whole grain oat intake Pei Wang, wangpeijx@gmail.com, Huadong Chen, Aaron Verke, Shengmin Sang. Lab for Functional Foods and Human Health, Center for Excellence in Post-Harvest Technologies, North Carolina A&T State Univ., Kannapolis Oats have been cultivated for two thousand years in various regions throughout the world. Oat is a multifunctional crop nutritionally superior to many other unfortified cereals. It is commonly consumed as whole grains and known to provide healthy nutrients to humans. However, there are no biomarkers have been identified to re...
AGFD 130 Suppression of high-fat diet induced atherosclerosis by dietary oats avenanthramides Michael Thomas¹, Sharon Kim¹, F. William Collins², Mitchell Wise³, Mohsen Meydani¹, Mohsen.meydani@tufts.edu. (1) Jean Mayer HNRCA, Tufts Univ., Boston, Massachusetts (2) Agriculture and Agri-Food Canada, Eastern Cereal and Oilseed Research Center, Ottawa, Canada (3) USDA, ARS, Cereal Crops Research, Madison, Wisconsin. The consumption of oatmeal and oat bran has been shown to reduce total and low density lipoprotein (LDL) cholesterol levels in plasma, which are major risk factors for coronary heart disease. Oats, in addition to containing soluble fibers (β-glucan), are a good source of Avenanthramides (Avns), the unique soluble bioactive compounds present only in oats. We have previously reported that Avns suppressed endothelial expression of chemokines (MCP-1, IL-8), pro-inflammatory cytokines (IL-1, IL-6) through NF-kB, and several adhesion molecules in vitro, suggesting that oats are potentially anti-inflammatory and anti-atherogenic. Additionally, supplementing a high fat diet (HFD) of LDLr-/- mice with 27% or 40% oats significantly reduced lesion development. To elucidate the contribution of Avns to the inhibition of atherogenesis, we supplemented a HFD of LDLr-/- mice with regular oats (10 ppm Avn) or false-malted oats (FMO) (451 ppm Avn) for 16 weeks. Both oat-based diets (regular or false-malted) significantly reduced (p<0.05) HFD-induced atheromas in the aortic tricuspid valve, but no difference in the extent of lesions occurred between the two groups. However, LDLr-/- mice fed a HFD containing FMO with high levels of Avns had significantly lower numbers (p<0.05) of lesions in the descending aorta than mice fed a low fat diet, a HFD, or a HFD supplemented with regular oats. A non-significant trend toward the reduction of expression of VCAM-1 in the lesions of aortic valves of mice fed HFD containing FMO was observed. It is important to note that reduction of blood total cholesterol levels was the same in the two oat-supplemented groups; this suggests that FMO with their higher concentrations of Avns contributed more to the reduction of aortic lesions. These preliminary, in vivo data suggest the beneficial effects of consuming oats, especially FMO, on cardiovascular disease prevention. Supported by the U.S. Dept. of Agriculture – Agriculture Research Service (ARS), under Agreement No. 58-1950-0-014.

AGFD 131 Methylene donors in whole grains – potential mediators of a wide range of whole grain-related health benefits Alastair Ross¹, alastair.ross@chalmers.se, Mads V. Lind², (1) Biology and Biological Engineering, Chalmers Univ. of Tech., Gothenburg Sweden (2) Nutrition, Exercise and Sports, Univ. of Copenhagen, Denmark Over the past decade the high amount of the methyl donor glycine betaine in some whole grain cereals has come to the attention of researchers as potential explanation for some of the health benefits of diets rich in whole grains. Glycine betaine is of physiological importance as an osmolyte, biochemical importance as a methyl donor to convert homocysteine to methionine, and possibly of genetic importance as a source of methyl groups for DNA and histone methylation. Cereals provide around 60 % of glycine betaine in the Western diet and whole grain wheat and rye are among the best sources of this compound in the diet, though some less common foods such as quinoa have exceptionally high amounts. In addition to glycine betaine, whole grains are also an important source of the natural form of folate (5-methyltetrahydrofolate), also a methyl donor for the same reactions as glycine betaine in the series of pathways in what is known as one carbon metabolism, which also provides methyl groups for DNA methylation. The relatively high amount of these methyl donors in whole grains compared to refined grains may explain some of the possible health benefits of whole grains, including associations with reduction of homocysteine and blood lipids. They have also been hypothesised to reduce the risk of non-alcoholic fatty liver disease, a major emerging health concern. One area of concern is the low amount of folate and glycine betaine in gluten-free cereal foods, given the importance of cereal foods for the intake of these compounds. Many questions still remain about the role of glycine betaine and folate as mediators of health benefits of whole grains, in particular whether they could be important for epigenetic regulation via DNA methylation. Recent evidence also suggests a role for glycine betaine in the development of type 2 diabetes. The importance of these methyl donors in whole grains, and whole grain wheat in particular, is now emerging as a major area of research interest that may fill in many of the gaps in our understanding of whole grains beyond being a source of dietary fibre alone.

AGFD 132 Benzoxazinoids in cereals: Potential role for human health Inge S. Fomsgaard¹, inge.fomsgaard@agro.au.dk, Stine K. Steffensen¹, Khem B. Adhikari¹, Per L. Gregersen¹, Michael Borre², Søren Hayø², Lars K. Poulsen³, Bettina M. Jensen³, Claus H. Nielsen³. (1) Aarhus Univ., Slagelse, Denmark (2) Aarhus Univ. Hospital, Aarhus, Denmark (3) Copenhagen Univ. Hospital, Denmark In 2008 our group discovered that mature grains of rye, wheat, and maize contain secondary metabolites of the benzoxazinoid type (BXs). Until then literature repeatedly stated that "BXs are only present in young immature cereals". In our "BREAD AND BREAKFAST" project we have shown that the composition and quantity of BXs can be altered depending on the choice of food preparation process. We also now know that BXs are taken up, distributed and metabolized in the mammal body. We found that when bacteria induce the production of inflammatory cytokines in innate immune cells, a previous diet high in BXs enhances this production, indicating an immune-modulating effect of the BXs. We showed that BXs are synthesized during the development of the seed and accumulate in outer layers and in the embryo. During germination (malting) additional amounts of the compounds are formed. Our on-going project “RyeProC” was initiated on basis of a) clinical experiments showing that high amounts of rye whole grain and bran intake had shown beneficial effects on prostate cancer progression; b) in vitro studies showing suppressive effects of BXs on cancer cells, and c) our findings of BXs in rye bread. The first part of the study (method development) has now been finalized: The benzoxazinoid content was analyzed - using a method specifically developed for optimized sensitivity - in ten samples of prostate tissue from each of ten prostate cancer patients who participated in a one-week high-BX (rye-based) diet intervention prior to their prostatectomy. Six different BXs were quantified in the biopsies. HBOA-glc was the main analyte detected. These findings encourage further investigations. We thank our collaborators in Copenhagen and Aarhus Univ. Hospitals, Aarhus Univ. Dep. of Molecular Biology and Genetics, Aarhus Univ. Dep of Agroecology and the company Lantmännen.

AGFD 133 Chemical stability of citral Yu Wang¹, yy.wang@ufl.edu, Chi-Tang Ho¹. (1) Food Sci., Rutgers Univ., New Brunswick, New Jersey (2) Citrus Research and Education Center, Univ. of Florida, Lake Alfred Aroma is one of the most important aspects in food. The aroma quality depends on the aroma stability, environmental factors (such as light, atmospheric oxygen etc), and food matrix, among which aroma stability is the most important one. The functional groups of aroma such as carbonyl, hydroxyl, and thiol affect the chemical reactivity and stability. In this presentation, we will focus on the chemical stability of citral (3,7-dimethyl-2,6-octadienal) which is the major aroma compound in citrus oil. Citral can cyclize into monoterpenic alcohols such as P-mentha-1,5-dien-8-ol and P-mentha-1,2-dien-8-ol through acid catalysis. These monoterpenic alcohols go through the disproportionation and redox reactions to form more stable aromatic compounds
such as P-cymene, P-methylacetophenone, and P-cresol. However, P-methylacetophenone and P-cresol are the potent off-flavor notes. In order to stabilize citral, the antioxidants and emulsion system are used.

AGFD 134 Stability of the curry leaf aroma impact compound 1-phenylethanolthiol during traditional processing and use in the kitchen Martin Steinhaus, martin.steinhaus@lrz.tum.de. DFA Lebensmittelchemie, Freising, Germany Application of an aroma extract dilution analysis to curry leaves, a popular seasoning herb in south Asian cuisines with a pronounced sulfury and burnt odor revealed 23 odor-active compounds with flavor dilution (FD) factors ranging from 1 to 8192. High flavor dilution factors were determined for 1-phenylethanolthiol (8192), linalool (4096), a-pinene (2048), 1,8-cineole (1024), (3Z)-hex-3-en-1-ol (32), and (2E,6Z)-nona-2,6-dienal (32). Quantification of these potent odors followed by aroma reconstitution and omission experiments unequivocally revealed that 1-phenylethanolthiol is the impact compound of curry leaf aroma and responsible for the characteristic sulfury and burnt odor note. Then the stability of 1-phenylethanolthiol during traditional processing and use in the kitchen was studied. Experiments included the influence of chopping of the leaves, drying, as well as frying of fresh and dried leaves.

AGFD 135 Flavor and off-flavor in canned tuna fish Fei He1, YanPing L. Qian2, Michael C. Qian3, michael.qian@oregonstate.edu. (1) Oregon State Univ, Corvallis (2) Crop and Soil, Oregon State Univ., Corvallis (3) Food Sci. and Tech., Oregon State Univ., Corvallis Fish product is rich in long-chain n-3 polyunsaturated fatty acid (PUFA), and they are highly susceptible to oxidation and form secondary lipid oxidation compounds, which cause off-flavor and loss of nutritional value. Marine sources, processing and storage conditions can affect seafood flavor and quality and, therefore influence consumer’s preference of seafood. The objectives of this study are to study the off-odor compounds of canned tuna fish. Gas chromatography/olfactometry-mass spectrometry analysis showed that canned tuna odor was mainly contributed by aldehydes, ketones, sulfur compounds and fatty acids. The majority of the odor-active compounds were aldehydes such as hexanal, nonanal, (Z)-4-heptenal, (E,Z)-2,6-nonadienal, (E,Z)-2,4-decadienal, (E,E)-2,4-decadienal, ketone (1-octen-3-one) and acids including acetic, propanoic, butanoic, isovaleric, hexanoic and octanoic acids. Many of these compounds, especially those aldehydes, which contribute to fishy, oily off-flavor, are typically associated with unpleasant odor. Semi-quantitative analysis showed that the off-flavor compounds were dependent on fish species, fish origin, fish handling and process conditions.

AGFD 136 Unraveling the off-flavor formation of native cold-pressed rapeseed oil using the molecular sensory science concept Michael Granvogl, michael.granvogl@tum.de, Katrin Matheis. Tech Univ. of Munich, Freising Bavaria, Germany In the mid-1980s, the cultivation of the so-called “00-rape” has started resulting in a loss of bitterness of the rapeseed due to the low level of erucic acid and glucosinolates. Consequently, rapeseed oil gained more importance in human nutrition because of its positive physiological properties, which are correlated with their unsaturated fatty acids in the triglycerides. Additionally flavor attributes are one of the most important criteria for consumers to buy a food. Thus, more knowledge about the aroma composition and the possibility to avoid off-flavor development in rapeseed oils during processing or storage conditions can lead to a further increase of acceptance. By means of the Sensors approach, including aroma extract dilution analysis (AEDA), identification experiments, quantitation by stable isotope dilution assays (SIDAs), calculation of odour activity values (OAVs), and aroma recombination to validate the analytical data, native cold-pressed rapeseed with perfect sensory attributes (“Golden Standard”) was compared with rapeseed oil eliciting an “Off-flavor”. Eleven odorants with an OAV ≥ 1 were determined in the Golden Standard including 2-isopropyl-3-methoxy pyrazine (OAV = 330), dimethyl trisulfide (37), dimethyl sulfide (7), butanoic acid (7), 2-isobutyl-3-methoxy pyrazine (5), and 2-sec-butyl-3-methoxy pyrazine (3). Sixteen aroma-active compounds contributed to the overall aroma of the off-flavor rapeseed oil. Main differences between both rapeseed oils were obtained for compounds of microbial metabolism revealing a significant higher OAVs, e.g., dimethyl trisulfide (2900), 2-isobutyl-3-methoxy pyrazine (167), ethyl 2-methylbutanoate (95), 2-methoxyphenol (77), 2-sec-butyl-3-methoxy pyrazine (18), 3-methylbutanalan (10), 2-methylbutanal (11), 4-methylphenol (3), 2-methylbutanoic acid (3), and 3-methylbutanoic acid (2).

AGFD 137 NMR approaches to studying wine oxidation: Pathways of acetaldehyde Andrew L. Waterhouse, alwaterhouse@ucdavis.edu, Ana Peterson. Viticulture and Enology, Univ. of California, Davis As wine oxidizes, ethanol is converted to acetaldehyde, but its accumulation is not predictable, due to its reactions with alcohols, SO2, thiols, flavanols, and other wine compounds. Measurements of these specific products is stymied by multiple equilibria in the other forms during sample preparation. NMR spectra can be taken on intact samples and is thus ideal for measurement without disturbing these reactions. Equilibria of acetaldehyde with glycerol, (+)-catechin, and glutathione were studied separately in model wine solutions at pH 3-4 by 1H NMR and 2D (1H-1H) COSY spectra. All these reactions consumed only a fraction of the acetaldehyde present under wine-like conditions and equilibration took 3-10 days. The rate of equilibration was also studied. This data can be used to provide an accurate measure of total acetaldehyde, and consequently offer insight into wine oxidation.

AGFD 138 Preursors of H2S in wine – role of elemental sulfur degradation products Gavin L. Sacks1, gls9@cornell.edu, Jillian A. Jastrzembski2, Elle Friedberg2, Yi Chen2. (1) Food Sci., Cornell Univ., Ithaca, New York (2) Food Sci. and Tech., Cornell Univ., Ithaca, New York (3) tate Key Lab of Food Sci. and Tech., Nanchang Univ., Nanchang, China (4) Wellesley College, Wellesley, Massachusetts Hydrogen sulfide (H2S, “rotten egg”) is often detected in wines with sulfurous off- aromas. H2S can increase during bottle storage of certain wines, but the identity of latent H2S precursors is not fully established. Elemental sulfur (S) is widely employed in grapegrowing as a fungicide, and the role of S0 residues in producing H2S during fermentation is well established. We now demonstrate that S0 can form wine-soluble degradation products during fermentation capable of generating more H2S during storage. Grape juice was vinified in the presence of S0 (0-100 mg/L). The resulting wines were racked and sparged to remove free H2S before bottling and anaerobic storage. After 3 months of storage, free H2S increased proportionally to the original S0 concentration, corresponding to approximately 1% of the original S0 on a molar basis. Only small differences in formation of latent H2S precursors were observed across five yeast strains. For typical wines, our results indicate that S0 residues should be limited to <7 µg/g to avoid additional formation of latent H2S precursors. Addition of concentrated brine to S0 treated wines did not release additional H2S, indicating that the latent H2S form was not a metal sulfide complex. However, H2S could be released from treated wines by the reducing agent tris-(2-carboxyethyl) phosphate (TCEP). Following solvent fractionation, TCEP-releasable H2S was found only in the aqueous phase, suggesting polysulfides as likely intermediates.
AGFD 139 Stability of smoke taint during the aging of smoke-affected wine Lieke van der Hulst, lieke.vanderhulst@adelaide.edu.au, Renata Ristic, Kerry Wilkinson, kerry.wilkinson@adelaide.edu.au. The Univ. of Adelaide, Glen Osmond, South Australia Smoke taint is the term given to wines that exhibit objectionable ‘smoky’, ‘medicinal’, ‘ashy’ and ‘dirty’ characters that result from vineyard exposure to bushfire smoke. In the past decade, wine producing countries, such as Australia, North America, Canada and South Africa, have experienced warmer, drier growing seasons due to climate change, i.e. environmental conditions conducive to bushfires. Previous research has implicated volatile phenols, e.g. guaiacols, cresols and syringols, with the sensory attributes associated with smoke taint. Smoke-derived volatile phenols are taken up by grapevine leaves and fruit, but are quickly glycosylated following smoke exposure [3]. During fermentation, glycoconjugates are hydrolysed and the volatile phenols are released, but a significant portion of the glycoconjugate pool remains in the final wine. This study investigated changes in the composition and sensory properties of smoke-affected wines following 5-6 years of bottle aging. The concentration of volatile phenols and guaiacol glycoconjugates were measured by gas chromatography-mass spectrometry (GC-MS) and high performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS) respectively, in control and smoke-affected white and red wines after: (i) bottling (i.e. at t=0 years); and (ii) aging (i.e. at t=5 or 6 years). Sensory analysis was also performed to determine changes in sensory properties during aging. Results provide insight into the stability of smoke taint (of glycoconjugate precursors in particular) during aging of wine and have important implications for industry.

AGFD 140 Cellular and molecular mechanisms of salty taste: Implications for developing strategies to combat NaCl overconsumption Brian Lewandowski, blewandowski@monell.org. Monell Chemical Senses Center, Philadelphia, Pennsylvania Overconsumption of NaCl has been linked to increased morbidity from hypertension related diseases. Despite this, the highly appetitive quality of salty taste has caused recommendations from both government (e.g., the US Food and Drug Administration) and private (e.g., the American Heart Association) organizations to reduce dietary NaCl consumption to be met with limited success. Alternative strategies to reduce NaCl consumption, such as developing salt substitutes/enhancers that would enable a reduction in the NaCl content of foods without significantly impacting perceived saltiness, have been similarly unsuccessful. Part of this difficulty can be attributed to the complicated nature of salty taste at both the cellular and neural level. Unlike the other basic tastes, salty taste is mediated by two separate pathways each of which has its own mechanism for detecting salts. These two salt taste pathways also communicate information to the brain through different types of gustatory nerve fibers. Understanding how these two pathways interact to mediate the perception of salty taste is likely to be critical if dietary NaCl reduction is going to be accomplished through the development of a NaCl substitute. This talk will review our current understanding of the cellular and molecular basis of salty taste with a focus on how this knowledge can help researchers develop new strategies to reduce the NaCl content in food without affecting palatability.

AGFD 141 Aroma compounds to rescue the taste of healthy foods and beverages Thierry Thomas Danguin, Thierry.Thomas-Danguin@dijon.inra.fr, Christian Salles, Elisabeth Guichard. Center for Taste and Feeding Behaviour, CSGA, INRA, CNRS, Univ. of Bourgogne Franche-Comté, Dijon, France Health issues have led health organizations to endorse the decrease of fat, salt and sugar content in food. However, performing such reduction without changing consumer liking remains a major challenge because it usually alters products’ sensory characteristics. In order to maintain taste of low-fat/salt/sugar foods, we propose to use odorants to compensate for the loss in perception through the multi-sensory-integration mechanism underpinning flavor perception. In a series of studies relying on water solutions, model and real food products, we demonstrated that well-selected odorants can enhance taste perception through the odor-induced taste enhancement effect (OITE). Our results highlighted several features of OITE. First, for OITE to be observed, odorants need to be congruent with the target taste: only odorants with a salty dimension can enhance saltiness (Lawrence et al., 2009, 2011). Moreover, the OITE width is related to the actual taste intensity. Indeed, when salty taste intensity is too high, OITE is no more efficient while it can compensate for 25% salt reduction in water solutions at medium taste intensity (Nasri et al., 2011). We also ascertained the advantage of combining OITE with other strategies developed to maintain taste in low-salt foods (Nasri et al., 2013; Emorine et al., 2013). In model-cheeses varying in both salt and fat content, we reported that a mixture of odorants could increase salty taste in almost all tested products while fat perception was improved unevenly across products, which suggested a critical impact of food matrix composition and/or structure on OITE (Syarifuddin et al., 2016). Recently, we developed a method to screen for odorants associated to taste in real food (GC-OAT for Gas Chromatography-Olfactometry Associated Taste); and using an online odor recombination system we pointed out odorants which modulate sweetness perception of a real fruits juice odor. Overall, these findings demonstrate that cross-modal interaction can be an efficient strategy to compensate for salt/fat/sugar reduction, which should help to develop sustainable and healthy foods and beverages while maintaining a good acceptability for consumers. We acknowledge collaborators and students involved in this research and financial supports from Regional Council of Burgundy, European Regional Development Fund (FEDER), Unilever R&D, Marie S.A., Carnot Inst. Qualiment, AgreenSkills, EU Marie Sklodowska-Curie actions, EU TeRiFîQ project.

AGFD 142 Mechanisms of bitterness generation in whole wheat foods Qing Bin1, Devin G. Peterson1,2, dgp@umn.edu. (1) 225 FSCN, Univ Minnesota, Saint Paul, Minnesota (2) Food Sci. and Tech., The Ohio State Univ., Columbus Bitterness in whole grain foods is known to negatively impact consumer acceptability. This presentation will focus on the origin of bitter compounds in whole wheat bread crumbs. Based on sensory-guided fractionation techniques, the main bitter compounds were identified as L-tryptophan, apigenin-C-glycosides, and 9,12,13-trihydroxy-trans-10-octadeccenolic acid (pinellic acid). Sensory recombination analysis identified pinellic acid as the main contributor to the bitterness of whole wheat bread crumb. L-tryptophan and apigenin-C-glycosides were both reported to be endogenous to wheat flour and to degrade during the baking process, whereas pinellic acid was generated during bread manufacture. Stable isotope addition experiments (linoleic acid-13C18) indicated linoleic acid in the flour was the key precursor for the formation of pinellic acid. Two main mechanisms of pinellic acid generation were reported that included an enzymatic oxidation pathway that occurred during dough kneading and a non-enzymatic decomposition pathway of linoleic hydrogen peroxide (LOOH) that involved a free radical mechanism facilitated by transition metals during baking. In summary, these findings provide an improved understanding of bitterness development in wheat bread and a basis to develop flavor optimization strategies for whole wheat products.
AGFD 143 Effect of pressure and heat treatment on volatile profile in Chinese bayberry juice analysed by GC-MS during storage Suli Lin, ncsukinsuild@163.com, Yong Yu, Yi Lin, Songming Zhu. Institution of Agricultural Bio-Environmental Engineering, Hangzhou, China

Flavor is one of the most significant criteria for consumer’s acceptance of food products, and volatile compound is one of the most vital factors that affects the flavor quality of food products. The volatile profile of Chinese bayberry juice processed by high pressure processing and heat treatment were evaluated by the method of solid-phase micro-extraction combined with gas chromatography/mass spectrometry (SPME–GC/MS). 500 MPa, 10 min was used for high pressure processing and 55 °C, 5 min was selected for heat treatment according to the sterilization demand. The storage conditions were 4 °C for 0, 14, 25 days and 25 °C for 0, 4, 8 days. Processed samples were compared to the unprocessed samples. The results showed out that nearly one hundred volatile compounds had been identifed and (Z)-3-hexen-1-ol, 1-hexanol, linalool, cyclopetrasiloxane, octamethyl-, 1-cyclopentasiloxane, decamethyl-, carpyathylene, 2,4-Dimethylphenol, 1,3-cyclohexadiene, 1-methyl-4-(1-methylethyl)-, Temporin-4-ol and (Z)-3-nonene-1-ol were the primary components, accounting for roughly 72.60 %. Among the major compounds, 1-hexanol, carpyathylene and (Z)-3-hexen-1-ol had the highest content. During storage, both 1-hexanol and carpyathylene decreased with the increasing storage time, while (Z)-3-hexen-1-ol at 4 °C decreased at 14 days and then sharply increased at 25 days. The results still showed out that high pressure processing brought less changes than heat treatment, which indicated that high pressure processing might be an alternative Tech. for the preservation of volatile compounds of Chinese bayberry juice.

AGFD 144 Reducing astringency in persimmons through processing, an approach for increasing marketability Ivana J. Sedej¹, Rachelle D. Woods¹, Ana M. Vilches¹, Carl W. Olsen¹, John E. Preece², Rebecca R. Milczarek³, Andrew P. Breksa¹, andrew.breksa@ars.usda.gov. (1) HPFR, USDA, ARS, Albany, California (2) NCGR, USDA, ARS, Davis, California

Persimmons are an orange flesh fruit produced in temperate climates throughout the world. Varieties within the commercially most important species (Diospyros kaki) are divided into three astringency types- non-astringent, astringent, and pollination variant. In the U.S., California is the largest producer of persimmons and commercial production is predominately divided between astringent “Hachiya” and non-astringent “Fuyu” types, with limited production of pollination variant types by small-scale growers for specialty markets. The astringency in persimmons is due to the presence of low and high molecular weight soluble tannins. Astringency and a short shelf life are two characteristics that hamper consumer demand for persimmon fruit and persimmon containing products. Development of a product that overcomes these characteristics offers an opportunity to increase consumer demand. Two methods that show promise for reducing astringency are slow freezing, and drying. In order to determine effectiveness of these methods we selected non-astringent, astringent, and pollination variant types for evaluation. Samples were sourced from commercial growers and the National Clonal Germplasm Repository, Davis, CA. A total of 55 samples were evaluated. The fresh and treated samples were characterized for their organoleptic properties and tannin and polyphenol contents and evaluated for their sensory characteristics by a trained panel. Correlations between the chemical and sensory analyses will be presented, as well as identification of those varieties that responded best to the treatments.

AGFD 145 Mitigation strategies for toxicologically relevant styrene during the production of wheat beer Michael Granvogl¹, michael.granvogl@tum.de, Daniel Langos², Peter H. Schieberle³, (1) Tech Univ. of Munich, Freising Bavaria, Germany (2) Technical Univ of Munich, Freising, Germany (3) German Research Center for Food Chemistry, Freising, Germany

Styrene has recently been classified as “possibly carcinogenic to humans” by the International Agency for Research on Cancer (IARC). It can be formed from cinnamic acid either by thermally induced or enzymatically induced decarboxylation of the phenolic acid during wort processing and/or yeast fermentation. In parallel, 2-methoxy-4-vinylphenol, known as a degradation product of ferulic acid, and 4-vinylphenol, the degradation product of p-coumaric acid, have often been suggested as important aroma compounds of wheat beer. Therefore, the key aroma compounds of Bavarian wheat beers were identified and quantitated using the Sensomics approach. By combining all aroma compounds in the genuine concentration of the beers, aroma recombinates eliciting the typical aroma of wheat beer were obtained. While 2-methoxy-4-vinylphenol and 4-vinylphenol were proven to be important to the overall aroma, 2-methoxyphenol and styrene did not play a role. Besides clarifying the role of yeasts in the formation mechanism, possibilities to mitigate the formation of styrene, without influencing the typical beer flavor, by modifying the malting process will be discussed in the presentation. In addition, the choice of an appropriate malt, produced under specific conditions can reduce the undesired styrene precursor cinnamic acid in the malts and, thus, produce a "healthier" beer, but still eliciting the aroma well-known by the consumers.

AGFD 146 Phytochemicals in wheat bran for colon cancer prevention Shengmin Sang, ssang@ncat.edu, Yingdong Zhu, Junsheng Fu. Lab for Functional Foods and Human Health, Center for Excellence in Post-Harvest Technologies, North Carolina AT State Univ., Kannapolis

Many studies have found that dietary cereal fibers protect against colon cancer, however, not all cereal fibers are equally effective. Wheat bran is the only cereal bran that shows consistent protection against colon cancer in Lab animal models. It is still unclear whether the active components are phytochemicals or fibers. We and others have found that phytochemicals in wheat bran instead of fiber are the major active components for colon cancer prevention. The inhibitory effect of wheat bran extract on tumorigenesis was observed in our studies in the Apcmin/− mouse model. To identify the active phytochemicals in wheat bran, we conducted a systematic study on the chemical composition of wheat bran. We have purified and identified the major phytochemicals in wheat bran including alkylresorcinols, sphingolipids, and sterols. Using human colon cancer cells as the guiding assays, we identified alkylresorcinols as the major active components in wheat bran. The in vivo efficacy and the underlying molecular mechanism of alkylresorcinols will also be discussed in this presentation.

AGFD 147 Whole grain polyphenols in colon health: Positive interaction of complementary sorghum-legume flavonoids Joseph Awika¹, awika@tamu.edu, Shima Agah², Liyi Yang³, Susanne Talcott⁴, Clinton Alfred⁵, (1) Kellogg Company, Battle Creek, Michigan (2) Soil & Crop Science, Texas A&M Univ., College Station (3) Texas A&M Univ, College Station

Beneficial effect of whole grain consumption on colon health, e.g., colon cancer prevention, is well established. The polyphenols found in wholegrains, though generally present in low quantities, are important contributors to wholegrain health benefits. Evidence suggests that the overall contribution of grain polyphenols to health benefits is likely higher than presumed. Complementary structural features may enable the polyphenols to interact with different receptors or bind differently to the same receptors in ways that positively enhance their overall effect on target biomarkers. For example, our work with sorghum and legume flavonoids demonstrates that differences in substitution at position 3 of the heterocyclic ring,
and the C-2 – C-3 configuration are major determinants of their interactive effects on various markers targeting colon inflammation and cancer. We, for example, found that sorghum flavonoid mixtures of flavone and flavanone derivatives enhanced estrogen-b receptor activity in non-malignant colonocytes and reduced formation of premalignant lesions in ovariectomized mice more strongly (10-20 fold) than the individual flavonoid components. When 3-deoxyflavonoid derivatives from sorghum were combined with flavonoid 3-glycosides from pulses (derived from black-eyed peas in this study), significant enhanced action (10-50 fold higher) against various markers of inflammation in non-malignant colonocytes were apparent. Furthermore, the enhanced action of the complementary flavonoid mixtures was demonstrated to be partly due to their modulatory action on specific membrane transporter proteins (ABC transporters) in the colon. The evidence on strong enhanced action is practically interesting because cereals and legumes are traditionally consumed together in various parts of the world for their complementary protein nutritional profiles. Synergistic bioactivity of their polyphenols is likely to have important health implications to both developed and developing regions.

**AGFD 148 Phytochemicals in quinoa grains and their antioxidant and anti-inflammatory effects**

Rong Tsao¹, rong.cao@agr.gc.ca, Tang Yao², Ronghua Liu¹. (1) Agriculture & Agri-Food Canada, Guelph Food Research & Development Centre, Guelph, Canada (2) Tianjin Univ. of Science Technology, Tianjin, China Quinoa (Chenopodium quinoa Willd.) grains contain high quality macronutrients such as protein and polysaccharides, as well as micronutrients including polyphenols, betacyanins, carotenoids, vitamins and essential fatty acids. Lysine and isoleucine are especially higher in quinoa than common cereal grains, making it a complete protein source. The high nutritional quality and recent findings of additional health benefits by quinoa bioactives have triggered our study on the phytochemicals of quinoa and how they contribute to different health promoting effects. Bioaccessibility of the bioactives in cooked quinoa grains were assessed using in vitro gastrointestinal digestion system. Different forms of phenolic compounds i.e. free, conjugated and bound phenolics were characterized and their bioaccessible and bioactivities assessed. About 37-58% of these phenolics were lost after gastrointestinal digestion suggesting not all were bioaccessible. Our study examined the lipophilic and hydrophilic fractions of bioactive components, and assessed the antioxidant and anti-inflammatory effects using different chemical models such as ORAC, FRAP and DPPH assays, and cell-based antioxidant assay. The antioxidant activities of the lipophilic fraction were positively correlated with PUFA, total carotenoids and total tocopherols, while those of the hydrophilic fraction showed significantly positive correlation to the phenolic contents. Both phenolics and PUFA also significantly suppressed the formation of H₂O₂-induced oxidative injury in Caco-2 cells as measured by IL-8 secretion. In a Caco-2/TNFα cell model, both the hydrophilic and lipophilic fractions significantly inhibited the proinflammatory cytokines IL-6, IL-8, TNF-α, IL-1β and COX-2, and elevated expression of the anti-inflammatory cytokine IL-10. Further studies showed they reduced the activation of NF-κB and inhibited NF-κB signaling pathway. The activities were dose-dependent. This study provides basic information for further studies.

**AGFD 149 Buckwheat bioactive compounds, their derived metabolites and health benefits**

Juan Antonio Gimenez Bastida¹,²,³, juan.a.gimenez.bastida@vanderbilt.edu, Henryk Zielinski¹, Mariusz Piskula¹, Danuta Zielinska². (1) Inst. of Animal Reprod Food Rsch, Polish Academy of Sciences, Olsztyn, Poland (2) Univ Warmia Mazury Olsztyn, Olsztyn, Poland (3) Dept. of Clinical Pharmacology, Vanderbilt Univ., Nashville, Tennessee Whole grain consumption, including cereals and pseudocereals, may exert beneficial effects against chronic diseases. Buckwheat is a highly nutritious gluten-free pseudocereal that belongs to the Polygonaceae family. Common (Fagopyrum esculentum Moench) and tartary buckwheat (F. tataricum Gaertn), the main grown species, are widely consumed in numerous countries, such as Russia, China, the US, Canada and Europe. Recently, buckwheat has received increasing attention as a raw material for production of many different food products, including bread, noodles or tea. Consumption of buckwheat and buckwheat-enriched products consumption has been associated with a broad range of health benefits: antioxidant, anticancer, anti-inflammatory, anti-diabetic, hypocholesterolemic, hypotensive and neuroprotective. These beneficial effects have been partially related to the presence of a variety of bioactive compounds, including flavonoids, phenylpropanoids, and fagopyritols, among others. However, some of these compounds (i.e., the flavonoid rutin) are transformed in the gastrointestinal tract to derived metabolites and low-molecular-weight phenolic acids. Rutin (quercetin-rutinoside), the main buckwheat flavonoid, is hydrolyzed by the gut microbiota leading to the formation of its aglycone quercetin or its phenolic derivatives, such as 3-hydroxyphenylacetic acid (HPAA), 3,4-dihydroxyphenylacetic acid (DHPAA), and 4-hydroxy-3-methoxyphenylacetic acid (homovanillic acid, HVA). Hitherto, it is not clear what molecule(s) may be responsible of the benefits attributed to buckwheat. Thus, in order to shed some light about the compounds responsible for the effects observed after buckwheat consumption, in this study we investigated the biological activity (anti-inflammatory and antioxidant) of buckwheat bioactive compounds and their derived compounds.

**AGFD 150 Health-promoting lipids in corn kernels and corn oils**

Robert Moreau, robert.moreau@ars.usda.gov. Sustainable Biofuels and Coproducts, USDA, ARS, Wyndmoor, Pennsylvania Corn kernels contain about 4% oil and other lipids. Commercial corn oil is extracted from corn germ (embryo) and it is comprised of about 97% triacylglycerols, with linoleic acid the predominant fatty acid. In addition, commercial corn oil also contains higher levels of phytosterols (~1%) than most other edible plant oils, significant levels of tocopherols, and small amounts of carotenoids (~1% of the total carotenoids in the kernel). An experimental type of corn oil, corn fiber oil, can be obtained by extracting the pericarp and endosperm fiber of the corn kernel. Corn fiber oil is unique because it contains very high levels of phytosterols (10-15%), a major one of which is sitostanol-furulate, a phytosterol ester, which is similar in structure to oryzanol in rice. Most of the carotenoids in yellow corn are localized in the starch-rich endosperm portion of the kernel. Another experimental corn oil, corn kernel oil, is an oil that is exceptionally rich in lutein and zeaxanthin (oxygen-containing carotenoids that are valuable for eye health) and it can be obtained by extracting whole ground corn (including the endosperm) with a polar solvent such as ethanol. A new type of inedible corn oil, distillers corn oil, is now being produced commercially in the US by almost all of the 200 corn fuel ethanol plants. Approximately half of the distillers corn oil is being converted to biodiesel and half is been used an animal feed ingredient, mainly due to its high levels of lutein and zeaxanthin for laying hens.

**AGFD 151 Phytosterols and sterol conjugates in cereal grains**

Laura Nystroem, laura.nystroem@hest.ethz.ch. ETH Zurich, Zurich, Switzerland Phytosterols are health-promoting compounds found ubiquitously in plants. In addition to the sterol enriched functional foods, also high natural intakes of plant sterols are associated with lowered serum cholesterol levels, and thus reduction in the risk of cardiovascular diseases. Wholegrain products are amongst top three dietary sources of natural phytosterols. In grains phytosterols occur as free sterol alcohols (free OH-group in the C-3 position) or as various conjugates of fatty or phenolic acids, or sugars (which may further be esterified).
In addition to the cholesterol lowering activity, the phenolic acic esters and glycosylated conjugates of phytosterols are associated with additional health benefits, such as anticancer and antiinflammatory activities. Furthermore, differences in the biological activities between various molecular species of individual phytosterols have been reported. Cereal grains provide a great diversity of phytosterols and their conjugates, which are partially unique or strongly characteristic to individual grain species. For example, steryl phenolates are almost exclusively found in cereal grains, and the chemical composition of this class of sterols is significantly different in rice vs. corn vs. wheat. Furthermore, oats has an exceptionally high proportion of sterols in the glycosylated form, and also as conjugates of delta-5- and delta-7-avenasterols. The variability of phytosterols and sterol conjugates has been eluded to in the earlier literature, but only the most recent developments in the softer sample preparation techniques (enzymatic hydrolysis) and detailed analysis (accurate molecular masses and tandem-MS) have allowed for the differential characterization of cereal grains based on their sterol profiles. This, in combination with studies of bioactivity, will in the future bring us towards the detailed evaluation and optimization of various cereal grains (wheat, rye, oat, barley, rice, corn) as dietary sources of phytosterols and phytosterol conjugates as bioactive food constituents.

**AGFD 152 Genetic and environmental impacts bioactive components in cereals**
Peter R. Shewry, peter.shewry@rothamsted.ac.uk. Rothamsted Research, Harpenden, UK
Wheat and other cereals are rich sources of components that contribute to human health. These include components with well-established health benefits, such as B vitamins and dietary fibre, and a range of phytochemicals (notably phenolics and terpenoids) whose beneficial properties have been proposed but not conclusively established. These components vary in their location within the grain, being particularly concentrated in the bran and germ. Hence their levels in food products vary in inverse proportion to the extent to which the grain is refined during processing. The concentrations and compositions of bioactive components also vary widely between grain samples, including between different cereal species (such as barley, wheat and rye) and between genotypes and samples of the same species. It is therefore crucial to determine the basis for this variation. In particular, it is important to determine the extent to which the variation is determined by the genotype (heritability), environment or interactions between the genotype and environment (G x E). In this study, we evaluate the changes in composition among Armagnac and Cognac brandies and bourbon and Scotch whiskies using UHPLC/QTOF-MS.

**AGFD 153 Polyphenols in breakfast cereals and snacks; important contribution to beneficial health effects of whole grain consumption**
Jessica Goodman, jessica.goodman93@gmail.com, Joe A. Vinson, Szu-Yun Wang. Chemistry, Univ. of Scranton, Dalton, Pennsylvania
Whole grain consumption in the US has increased due to the introduction of whole grains in breakfast cereals and snacks. 2/3 of Americans now consume half their grains as whole (Oldways Whole Grain Council). Most people consider fiber as the health benefit of eating whole grains since this inhibits the absorption of fats and sugar in the GI tract. Polyphenols, the major antioxidants in the US diet, are primarily covalently bound to the fiber matrix of grains and are not bioavailable in this form. Our hypothesis is that polyphenols can be absorbed if there are free polyphenols in the food and/or hydrolysis of the bound polyphenols occurs during digestion. Systemic polyphenols and their metabolites can then make their way to cells, tissues and organs and exert their health effects throughout the body. We have used a Folin colorimetric method with catechin as the standard to measure methanol extractable compounds to measure free polyphenols in the samples. Total polyphenols (maximum) were analyzed after strongly basic hydrolysis. Maximum bioaccessible polyphenols were measured after in vitro hydrolysis simulating in vivo digestion. Breakfast cereals (n=34) were obtained from local supermarkets and done in duplicate. Free polyphenols averaged only 16% of the total polyphenols in the cereals. Total polyphenols ranged from 0.16 to 3.9 mg/g in regular cereals. Corn-based cereals had more total polyphenols than wheat but similar free polyphenols. Bran cereals had more total polyphenols than their whole grain counterparts. Specialty wheat cereals containing cocoa, chocolate and raisins had greater free and total polyphenols than wheat cereals. Snacks (n=34) had no detectable free polyphenols and the total ranged from 0.27 to 16.5 mg/g. A sprouted puffed pretzel had the highest total and digested polyphenol concentration. After digestion snack polyphenols averaged 63% of total polyphenols. This indicates polyphenol bioaccessibility is favorable after snack consumption.

**AGFD 154 Differences in the non-volatile composition of younger and older Armagnac and Cognac brandies and bourbon and Scotch whiskies using UHPLC/QTOF-MS**
Thomas S. Collins, tom.collins@wsu.edu. Viticulture and Enology Program, Washington State Univ., Richland
The non-volatile composition of distilled spirits evolves as the spirits age. Distilled spirits extract a range of phenolic compounds from the wooden casks in which they are stored, including lignin and ellagitannin degradation products arising from the charring or toasting of the interior surface of the barrel, as well intact ellagitannins and lignans from parts of the stave below the heat affected surface layers. Wood derived triterpenoids and their glycosides are also extracted from the wood. The concentrations of these extractives is dependent on a number of factors, including the length of time the spirit is aged in cask, the temperature and humidity in the storage facility, whether the cask may have been used previously for the aging of spirits, whether the cask was toasted or charred on the interior surface, as well as the species of oak used to make the cask. This study evaluates the changes in composition among Armagnac and Cognac brandies of varying ages as well as among bourbon and Scotch whiskies of varying ages. These spirits were selected to represent examples of the major contributing factors outlined above. Bourbon whiskies are aged in new charred casks made from American oak (primarily Quercus alba or similar), while the Scotch whiskies included in the study were aged in casks previously used for aging bourbon whiskey or in casks used previously aging Sherry; these casks are primarily made from Spanish oak (Quercus robur or others). Armagnac and Cognac brandies are typically aged in a combination of new and previously used casks produced from either local oak forests or from the nearby Limousin forest (Quercus robur or Quercus petraea); these casks are toasted rather than charred. The spirits included in this study ranged in age from 3 to 50 years. Analysis was conducted using an Agilent 1290 UHPLC/QTOF-6545 QTOF-MS system; MS data was collected in both MS scan and a data dependent automated MS/MS mode. The impact of aging conditions for the various spirits on their non-volatile composition will be presented.

**AGFD 155 Lichensin, a novel nonvolatile compound in Chinese distilled spirits reduced the headspace concentration of phenolic off-flavors via hydrogen-bond interaction**
Shuang Chen, chenshuang.hust@gmail.com, Yan Xu, Rong Zhang, Qun Wu. School of BioTech., Jiangnan Univ., Wuxi, Jiangsu, China
Nonvolatile components influence overall flavor volatility and perception in alcoholic beverages.
However, little information has been reported about the nonvolatile compounds in Chinese distilled spirits. For the first time, we isolated and identified a cyclic lipopeptide “lichenysin” as a novel nonvolatile compound in Chinese liquors, using preparative high performance liquid chromatography coupled with quadrupole-time-of-flight mass spectrometer and nuclear magnetic resonance. The concentrations of lichenysin were quantified in 14 main types of bottled Chinese liquors by using ultra performance liquid chromatography coupled with triple quadrupole mass spectrometer. The concentrations of lichenysin in Chinese liquor ranged from 0.01 to 111.74 µg/L, where the concentration was the highest in Dongjiu liquor. Furthermore, we found that lichenysin selectively affected aroma volatility in the Chinese liquor, using the headspace solid-phase microextraction coupled with gas chromatography-mass spectrometry. The headspace concentrations of 2-phenylethanol, phenol, and 4-methylphenol significantly decreased by respectively 58%, 76%, and 59% in 3 Chinese commercial liquors with an increase in lichenysin. It was found that lichenysin could selectively affect aroma volatility in strong-aroma type (Jiannanhu) liquor. Interaction of lichenysin and volatile phenolic compounds (off-odors in strong-aroma type liquor) was characterized using headspace solid-phase microextraction with gas chromatography–mass spectrometry (HS-SPME-GC-MS). HS-SPME results indicated that lichenysin very efficiently suppressed the volatility of phenolic compounds by 36–48% (P < 0.05). Thermodynamic analysis showed that the binding process was mainly mediated by hydrogen bonding. Furthermore, the mixture of lichenysin and 4-ethylguaiacol revealed intermolecular cross peaks between the aH (Val) of lichenysin and the 1H of 4-ethylguaiacol, by using nuclear Overhauser effect spectroscopy. These results indicated that lichenysin could be a novel nonvolatile compound that selectively affected aroma volatility in Chinese liquors with molecular interactions. Keywords: aroma volatility, Chinese liquor, HS-SPME-GC-MS, lichenysin, nonvolatile compound, NMR, UPLC-MS/MS, phenolic off-flavors, hydrogen-bond interaction

AGFD 156 Research on the aroma characteristics and impacts of the nonvolatile matrix composition on the aroma release of Vidal icewine based on multisensorics Ke Tang1, tandy81@126.com, Yan Xu2. (1) School of BioTech., Jiangnan Univ., Wuxi, Jiangnan, China (2) Mississippi Vegetable Fruit Improvement Center, Texas A and M Univ, College Station The key aroma compounds of Chinese Vidal icewine were characterized by means of gas chromatography–olfactometry (GC-O) coupled with mass spectrometry (MS) on polar and non-polar columns. Solvent-relative extraction (solid-phase extraction, SPE) and solvent-free extraction (stir bar sorptive extraction, SBESE) were used. The impacts of icewine non-volatile matrix on important aroma compounds were studied, further. By two extraction methods, a total of 61 odor-active aroma compounds were identified. 27 odorants were rated as important aroma compounds with the Osme value above 1.5, 26 of them were further quantitated. Among them, β-damascenone showed the highest Osme value in both extractions. Methional and furaneol were first observed as important odors in Vidal icewine. Aroma recombination experiments revealed a good similarity containing the 26 important aromas. Omission tests corroborated the significant contribution of β-damascenone and the entire group of esters. Besides, Furaneol and methional also had significant effect on icewine character, especially on apricot, cameral and tropical fruit characters. By instrumental analysis and sensory evaluation, the impacts of icewine non-volatile system on 4 kinds of important aroma compounds aroma were explored. The results showed that ethanol, fructose and (-)-epigallocatechin (EGC) had different impacts on headspace concentration and intensity of aroma compounds.

AGFD 157 Optimization of aroma compounds determination in Capsicum annuum cultivars using HS-SPME coupled with GC-MS Guddadarang Jayaprakasha, gkipg@tamu.edu, Kevin Crosby, Bhimu Patil. Vegetable Fruit Improvement Center, Texas A and M Univ, College Station Peppers (Capsicum annuum) are a good source of antioxidants, vitamins C, E, A and also rich in natural colors as well as aromatic compounds. Recently, aroma compounds are considered critical quality components for fresh produce. Certain distinct aroma compounds / odors from food have been reported to have antimicrobial activities, antioxidant and anticancer activities. The overall flavor of peppers, as perceived during consumption, is influenced by the composition of volatile and nonvolatile compounds, of which some (i.e., pungent principles) stimulate nonspecific or trigeminal neural responses. In the present study, aroma components of highly pungent peppers including Serrano, Cayenne, Poblano and Jalapeno were analyzed by HS-SPME coupled with GC-MS. Considering the low levels of volatiles in peppers, the method needs to be more optimized to understand volatile constituents present in various cultivars. Five SPME fiber coatings including 50/30µm divinylbenzene- carboxen- polydimethylsiloxane (DVB-CAR-PDMS), 65µm PDMS-DVB, 85µm CAR-PDMS, 85µm polyacrylate, and 85µm PDMS were tested for their volatiles adsorption efficiencies. In addition, volatiles were extracted by a conventional method using Likens-Nickerson apparatus for 4 h, to obtain them in a pentane layer, then analyzed by GC-MS. The volatiles were separated on polar and non-polar columns. A total 24 volatile compounds were identified in four varieties of peppers. Among the many complex volatiles, several compounds, particularly common to chili peppers including 9 hydrocarbons and 15 oxygenated hydrocarbons, were identified. The butyryl and green bean odor contributing compound, 2-pentylfuran was found to be major constituent in Cayenne and Poblano. β-Himachalene was found to be major in Serrano peppers. Linalool and nerolidol were found common in all four pepper varieties. The characteristic sesqui terpenes such as α-himachalene and β-himachalene of the chili peppers were found in all pepper varieties except poblano. The developed HS-SPME coupled to GC/MS technique is simple, rapid, sensitive, solvent free automated method for the routine analysis of many samples. This study was supported by US Dept. of Agriculture grant Designing Foods for Health through the Vegetable & Fruit Improvement Center 2010-34402-20875 and State funding 2013-12127 VFIC-TX state appropriation.

AGFD 158 Pterostilbene in blueberries and PPARG activation Agnes M. Rimando, agnes.rimando@ars.usda.gov. USDA ARS, Univ., Mississippi The discovery of pterostilbene in blueberries and that it acts a ligand for the peroxisome proliferator-activated receptor alpha isoform (PPARα) caused resurgence in interest on this compound. In our initial study, we demonstrated that pterostilbene produced greater induction of PPARα than ciglitazone, a known hypolipidemic drug, at 100 µM in H4IIEC3 cells. We have further demonstrated that pterostilbene significantly and dose-dependently (at 10, 20 and 50 µmol) increased PPARα gene expression in H4IIEC3 cells, and the effect at 10 µmol was greater than 100 and 200 µmol of fenofibrate. In a later study using age-accelerated mouse model, pterostilbene incorporated in the diet (120mg/kg of diet) was shown to positively modulate markers of cellular stress, inflammation, and Alzheimer’s disease pathology, and were associated with up-regulation of PPARα alpha expression in the hippocampus. In yet another feeding study, Syrian Golden hamsters fed diet fortified with blueberry peel ethanol extract (2% of diet), exhibited up-regulation of hepatic PPARα mRNA expression along with deceases in plasma LDL and total cholesterol. Whether the observed PPARα up-regulation is due to pterostilbene or other constituents (such as known anthocyanins in blueberry) will be discussed.
AGFD 159 Physiological effects of pterostilbene and blueberries in animal models of obesity Wallace H. Yokoyama, wally@nw.usda.gov, Dongyan Shao, Hyunsook Kim, Agnes M. Rimando. (1) Dept of Food and Nutrition, Hanyang Univ., Seoul, Korea (2) Northwest AF Univ., Yangling, China (3) USDA ARS, Univ., Mississippi (4) USDA Arsl Western Reg Rsch Lab, Berkeley, California Pterostilbene and resveratrol are two highly bioactive naturally occurring stilbenes. Their chemical structures are less complex yet share most of the important physical and physiological characteristics of complex flavonoids found in many fruits. They have low solubility in water and are not highly bioavailable yet have considerable physiological effects. In hamsters and mice on high fat diets supplementation with low levels of pterostilbene or resveratrol prevented increases in plasma cholesterol and body weight and other characteristics of obesity related metabolic dysfunction. Blueberry pomace also showed similar physiological response. The amount of pomace fed was much higher because the pomace contains large amounts of dietary fiber and flavonoids as well as resveratrol.

AGFD 160 Berry bioactives: the health benefits of color Britt Burton-Freeman, bburton@iit.edu. Inst. for Food Safety and Health, Bedford Park, Illinois Berry fruits provide a rich source of dietary anthocyanins to the human diet. Epidemiological evidence has identified dietary anthocyanins as specific flavonoids associated with lower cardiovascular risk and metabolic health. These data are consistent with in vitro and animal model findings. Human clinical trials are emerging to show how and in what amounts berry-rich anthocyanins need to be consumed to provide their benefits. This presentation will provide a brief overview of the berry and anthocyanin research to date focused on metabolic health and potential links to their benefits centrally.

AGFD 161 Effects of blueberries on cognition and neuroplasticity Amanda Carey, amanda.carey@simmons.edu, Abigail M. Rovnak, Kelsea R. Gildarie, Derek R. Fisher, Barbara Shukitt-Hale. (1) Psychology, Simmons College, Boston, Massachusetts (2) USDA, Boston, Massachusetts It has been demonstrated that consuming blueberries can prevent and even reverse the occurrence of neurochemical and behavioral changes associated with aging. Recent research suggests that consuming a high-fat diet (HFD) may result in behavioral deficits similar to those observed in aging animals. To determine if supplementation of a HFD with blueberries offers protection against behavioral declines, nine month old C57Bl/6 mice were fed low-fat diet (LFD) or HFD (60% calories from fat) with and without 4% freeze-dried blueberry (U.S. Highbush Blueberry Council) for 5 months. Novel object recognition memory was tested after 2, 3, and 4 months on the diets and the Morris water maze was used to assess spatial learning and memory after 5 months. Recognition memory was impaired in the HFD-fed mice at all time points, but mice fed HFD + blueberry showed a reversal of memory disruption after 4 months. Probe trial performance in the water maze was impaired in animals consuming the HFD, while animals on HFD + blueberry were not different from those on LFD. Brains of the mice were assessed for microglia activation, neuroplasticity by measuring brain-derived neurotrophic factor (BDNF), and neurogenesis by measuring doublecortin (DCX). There was significantly less microglia staining with Iba1 in mice fed HFD + blueberry. Moreover, BV-2 microglial cells treated with blood serum from mice fed HFD + blueberry produced less nitric oxide in response to stimulation with LPS compared to cells treated with serum from mice fed HFD. BDNF levels and the number of DCX positive cells were enhanced in the hippocampus of mice fed HFD + blueberry. Overall, this study demonstrated that supplementation of a HFD with blueberry was associated with reduced indices of microglia activation and increased neuroplasticity and neurogenesis; these changes may underlie the reduction of memory deficits observed in these animals.

AGFD 162 Phytochemicals against oxidative stress and inflammatory responses in microglial cells Grace Sun, sung@missouri.edu. Biochemistry, Univ. of Missouri, Columbia Microglia are the major immune active cells in the brain and known to play multiple functional roles, not only for scavenging cellular debris, but also ability to release pro-inflammatory and other factors that may affect neighboring cells. Activation of microglia has been implicated in a number of neurological diseases including traumatic brain injury and stroke. It is immensely important to keep microglia healthy in both young and old brain. Many dietary fruits and vegetables are known to contain phytochemicals with antioxidant properties. Our recent studies have identified compounds such as quercetin from berries that can effectively mitigate oxidative and inflammatory responses in activated microglial cells. Bacteria endotoxins (lipopolysaccharides, LPS) activate the Toll-like receptors in microglial cells leading to induction of the NF-κB transcriptional pathway and resulting in production of pro-inflammatory cytokines and nitric oxide. However, some of these phytochemicals not only are capable of inhibiting LPS-induced NF-κB pathway but also effective in stimulating the antioxidant pathway involving Nrf2 which mediates transcription activation of the Antioxidant Response Element (ARE) and synthesis of antioxidant enzymes such as heme oxygenase-1. There is evidence that phytochemicals that effectively inhibit the NF-κB pathway also are effective in stimulating the Nrf2 pathway. Our goals are focused on understanding mechanism mediating the cross-talk between these two signaling pathways and to identify novel phytochemicals effective in enabling healthy microglia to fight against neurological diseases.

AGFD 163 Quest for indirect modulators of the endocannabinoid system from natural products Abir El-Alfy, ael-alfy@csu.edu, Ehab A. Abourashed. Chicago State Univ., Illinois The endocannabinoid system has emerged as a popular pharmacologic target due to its diverse roles in physiological function. Anecdotal reports of nutmeg being used as a substitute for marijuana suggest its components may interact with the endocannabinoid system. The objective of this study was to utilize bioassay-guided fractionation to isolate pure nutmeg compounds and evaluate them for in vitro fatty acid amide hydrolase (FAAH) and monoacylglycerol lipase (MAGL) inhibition; key endocannabinoid degradation enzymes. Ten nutmeg fractions were screened for fatty acid amide hydrolase (FAAH) and monoacylglycerol lipase (MAGL) inhibition. All ten nutmeg fractions showed greater than 50% fatty acid amide hydrolase (FAAH) enzyme inhibition, with the enzyme recovering by 48 hours. From these, three active compounds, MF 30-7, MF 109-5 and MF 117-3, were isolated; showing an IC50 value of 7.02 μM ± 2.02, 4.57 μM ± 0.66 and 33.10 μM ± 5.35, respectively. Additionally, MF 30-7, MF 109-5 and MF 117-3 showed acetylcholinesterase (AChE) inhibitory activity, with percent inhibitions of 64.08 ± 7.88, 35.13 ± 1.89 and 71.80 ± 0.96. Of the three purified compounds, MF 109-5 possesses unique characteristics of highest potency and selectivity making it a viable candidate for in vivo testing in behavioral animal paradigms.

AGFD 164 Traditional plant breeding vs molecular plant breeding Wayne Parrott, wparrott@uga.edu. Crop and Soil Sciences, Univ. of Georgia, Athens The human food supply is contingent on modified plants. Modern crop varieties are partly the result of plants that have been modified by incorporating numerous desirable traits into one variety. At the advent of agriculture, plants were selected for various traits,
including better taste, storage ability, disease resistance, and yield. These initial efforts centered on selection of naturally occurring mutations that provided desired traits. Plants containing desirable mutations were crossed together, and the progeny were sorted through to identify the plants having the desired combination of traits; the great majority of the progeny would show undesired traits, and get discarded along the way. A limitation has been that since genes for traits are transferred as chromosomal segments rather than single genes, undesirable linked genes always get crossed in with the desirable one. Alternatively, when the needed traits are not present, attempts are made to create them via mutagenesis, or to resort to extraordinary measures to obtain them by crossing the crops with their distant relatives. Understanding the genetic changes that accompanied the selection of desired traits makes it possible to rationally design future changes. For such molecular breeding, the necessary genes for desired traits can be obtained from any other organism, and then get engineered into a crop variety. As opposed to conventional breeding that works with traits, molecular breeding works with the genes themselves, thus requiring an extensive upfront characterization of the gene and its function. With such knowledge in hand, hundreds of engineered plants are created and evaluated. Those that do not show the desired trait or that show undesired traits get discarded, and only one (the lead event) is subjected to extensive safety tests prior to commercialization.

AGFD 165 BioTech. innovations and solutions for sustainable agriculture Deryck J. Williams, jeremy.williams@monsanto.com, WE4A, Monsanto Company, Saint Louis, Missouri BioTech. has proven to be versatile tool to combat many of the challenges farmers face. It enables growers to sustainably improve the opportunity for yields while protecting biodiversity. Insect control traits provide an improved way for controlling pests above and below ground, and have led to a reduction in the amount of insecticide used. Below-ground insect control traits have also indirectly helped plants better withstand water stress. Integrating bioTech. with other key advancements such as those in molecular breeding, crop protection technologies, digital agriculture, microbials and other technologies will be key as we look to feed our growing world population. Monsanto’s SmartStax® PRO, currently in phase 4 of the R&D Pipeline, demonstrates the ability to help improve crops with Bt combined with RNAi. Companies across the industry are leveraging RNAi to develop products, like the genetically modified Apple® and J.R. Simplot Company’s Potato, which bring additional benefits like reduced food waste, to farmers and society. Through an integrated solutions approach, the agriculture industry can bring farmers more options for sustainably managing on-farm challenges.

AGFD 166 Herbicide-resistant crops: Past, present and future Stephen O. Duke, sduke@olemiss.edu. NPURU, USDA/ARS, Oxford, Mississippi Glufosinate- and bromoxynil-resistant crops were introduced in 1995, but had little impact. In 1996, the first glyphosate-resistant (GR) crops (soybean and canola) were introduced, and these and later GR crops (cotton, maize, sugar beet, and alfalfa) had a huge impact on weed management, with more than 90% adoption where they were available. GR crops have been the most commonly used transgenic crops, and, as a result, glyphosate became the most used herbicide globally. The strong selection pressure from the almost exclusive use of glyphosate in GR crops led to the evolution of many GR weed species. This is leading to greater adoption of glufosinate-resistant crops and crops made resistant to auxinic herbicides (2,4-D and dicamba), with other herbicide-resistant crops on the way. In most cases, the GR trait is included with the genes for these additional herbicide resistance traits. So, farmers are still using large amounts of glyphosate to kill non-GR weeds in GR crops. Some scientists have indicated that glyphosate alters the mineral composition of GR crops, but most studies have not found this to be true. Additionally, there have been claims that glyphosate makes GR crops more susceptible to plant pathogens, but this has not been substantiated, and there is better evidence that glyphosate reduces infection by some plant pathogens in GR crops. Glyphosate and its degradation product, aminomethylphosphonic acid, are found in the harvested seed of GR soybeans treated with glyphosate, but in the few published studies, the levels found have been below what is allowed by the US FDA. Other weed management technologies are under develop that will probably reduce glyphosate use in the future.

AGFD 167 Challenges for the production and acceptance on transgenic wheat Peter R. Shewry, peter.shewry@rothamsted.ac.uk. Rothamsted Research, Harpenden, UK Transgenic crops have been grown in many countries for many years, including maize for food, feed and industrial use. However, although transgenic wheat has been produced as a research tool for over 20 years, it has not led to any commercial varieties. This is surprising as wheat is the most widely grown staple crop and the dominant crop in temperate zones, accounting for up to 70% of the calories in some developing countries. I will therefore discuss progress in developing transgenic wheat as a commercial crop in the context of wheat production and utilisation. This will incude attitudes to the acceptability and safety of transgenic wheat, and the importance of focusing on improving traits which are of value to consumers due to benefits for health and quality of life.

AGFD 168 How basic research can lead to development of improved cereal crops: But where are they? Peggy G. Lemaux, lemauxpg@berkeley.edu. Univ. of California, Berkeley Thioredoxin (Trx), a small molecular weight protein, catalyzes reactions via a dithiol-disulfide exchange mechanism involving redox-active cysteine residues. The Trx redox center, with its disulfide (S-S) bridges, interacts with specific target proteins, facilitating changes in their structure and activity. Trxs are present in all living organisms, including large, complex families in plants. Work, primarily in cereals, established the role of one family member, Trx h, as a central regulatory protein in seeds, due its reductive effects on seed storage proteins, enzymes and enzyme inhibitors. The Trx h expression in potato bodies or the cytosol of cereal grain endosperm. In barley, embryo germination was accelerated and starch-degrading enzymes were enhanced when Trx h5 was overexpressed, important traits for the malting and brewing industry. Trx h5 was also overexpressed in wheat endosperm, leading to increased solubility of disulfide proteins and decreased allergenicity. Using an antisense Trx h9 construct, underexpression of Trx h9 was achieved in wheat, resulting in the engineered grain germinating slower with a dramatic delay in preharvest sprouting, which causes costly losses in grain yield. But where are these improved cereals? Regulatory costs for introducing genetically engineered foods into the market is outside the financial resources of academic scientists and small companies. And the regulatory pathway to commercialization is not always clear. And once in the market concern and possible backlash by consumers raises concerns with food marketers. Will use of genome editing to improve crops and foods lead to a different scenario?

AGFD 169 Prebiotic-like properties of feruloylated arabinoxylan-oligosaccharides generated from rice bran arabinoxylan Sun-Ok Lee1, suneok@uark.edu, Tung Pham1, Brett J. Savary1, Ming-Hsuan Chen2, 1 (1) Arkansas Biosciences Inst., Arkansas State Univ., Jonesboro (2) USDA ARS, Stuttgart, Arkansas (3) Dept. of Food Sci., Univ. of Arkansas, Fayetteville Rice bran is a rich source of functional biopolymers that may promote gastrointestinal health by differentially stimulating beneficial gut microbiota. Arabinoxylan (AX) is the major
functional biopolymer in cereal dietary fiber, and feruloylated arabinoxylan oligosaccharides (FAXOs) derived from it, have been implicated for having prebiotic-like activities because of their ability to pass through the upper gastrointestinal tract to the colon undigested where they are hydrolyzed and subsequently fermented by gut microbiota. The fermentation products, short-chain fatty acids (SCFAs), play important roles in regards to the host’s colon health. However, there is limited information available on colon health promoting activities of biopolymers from rice bran. In order to understand the prebiotic-like properties of functional biopolymers in rice bran, we determined the fermentation patterns of FAXOs and their impact on the composition of human gut microbial populations. For these studies, fresh fecal samples collected from healthy adults (n = 10) with no signs or symptoms of bowel diseases or conditions were diluted and cultured with anaerobic medium. SCFA concentrations were measured quantitatively using gas chromatography. Microbial populations were analyzed by 16S rRNA gene profiles via the Illumina MiSeq sequencing platform and QIIME (Quantitative Insights Into Microbial Ecology) software for microbial community analysis. Results showed that SCFA production was significantly increased with FAXOs and was comparable to fermentation with the well-established prebiotic fructo-oligosaccharides. Changes in microbiota population profiles in vitro indicate that FAXOs may function to modulate microbiota profiles in vivo. Thus increasing the bioavailability of FAXOs from rice bran products can potentially promote colon health through a prebiotic function.

AGFD 170 Transition metal-mediated oxidation reactions of sulfidic compounds in wine Gal Y. Kreitman1, John C. Danilewicz2, David W. Jeffrey3, Ryan J. Elias3, elias@psu.edu. (1) The Pennsylvania State Univ., Univ. Park (2) 44 Sandwich Road, Canterbury, UK (3) School of Agriculture, Food and Wine, Waite Research Inst., Adelaide, South Australia Copper fining is a common method for removing fermentation-derived sulfidic off-odors in wine, such as hydrogen sulfide (H2S) and various low molecular weight thiols. The popular view surrounding this mechanism is that exogenous copper, typically added as Cu(II) sulfate, reacts preferentially with H2S and thiols to yield a sulfide precipitate that can be easily removed from wine. Unfortunately, the mechanism underlying this copper fining remains poorly understood, and appears to result in increased Cu concentrations that can lead to deleterious reactions in finished wine. Moreover, it is now clear that other transition metals (e.g., Fe, Mn) found as endogenous components in wine also affect the rate and/or course of copper-H2S/thiol reactions. The present study describes a mechanistic investigation of transition metal-mediated reactions of H2S, cysteine, 3-sulfanylhexan-1-ol, and 6-sulfanylhexan-1-ol with oxygen. The concentrations of H2S, thiols, oxygen, and acetaldehyde were monitored over time, and it was found that Cu(II) was rapidly reduced by both H2S and thiols to Cu(I). The addition of Fe(III) in combination with Cu resulted in the rapid reduction of Fe(III) by Cu(I) and the resulting Fe(II) then redox cycled by reacting with oxygen. Furthermore, the presence of Fe and thiols prevented the removal of H2S by precipitation as insoluble CuS, and promoted H2S oxidation and polysulfide formation, thus effectively keeping both metals and sulfide species in solution after the addition of copper. These results strongly suggest that the general practice of copper fining in winemaking needs to be re-evaluated.

AGFD 171 Identification of antimicrobial peptide fragments from soy protein Ning Xiang1, Yuan Lyu1, Xiao Zhu2, Arun K. Bhunia3, Ganesan Narasimhan1, narsimha@purdue.edu. (1) Dept of Agric Biological Eng, Purdue Univ., West Lafayette, Indiana (2) Research Computing, Purdue Univ., West Lafayette, Indiana (3) Food Sci., Purdue Univ., West Lafayette, Indiana Antimicrobial peptides (AMPs) inactivate microbial cells through pore formation in cell membrane. Because of their different mode of action compared to antibiotics, AMPs can be used to replace antibiotics in human health and animal feed and immobilized on food packaging films. We developed a methodology based on mechanistic evaluation of peptide-lipid bilayer interaction to identify AMPs from a protein which was applied to soy protein. Initial screening of peptide segments from soy glycinin and β-conglycinin subunits was based on their hydrophobicity, hydrophobic moment and net charge. Out of several candidates chosen from the initial screening, two peptides satisfied the criteria for antimicrobial activity, viz. (i) lipid-peptide binding in surface state and (ii) pore formation in transmembrane state of the aggregate, as evaluated by all-atoms molecular dynamics (MD) simulation. Their antimicrobial activities against Listeria monocytogenes F4244 and E.coli O157:H7 EDL933 were confirmed by bioassay.

AGFD 172 Enhancement of natural antimicrobial efficacy via biomimetic iron chelating active packaging Paul Castrale1, pcasatrele@gmail.com, Maxine Roman1, Eric A. Decker2, Julie M. Goddard1. (1) Food Sci., Univ. of Massachusetts Amherst (2) King Abdulaziz Univ., Jeddah, Saudi Arabia Chelation of trace metal ions represents a common strategy to inhibit degradative processes in foods. Metal chelators have also exhibited a synergistic antimicrobial effect when used in combination with some natural antimicrobials. Chelating additives such as Ethylenediaminetetraacetic acid (EDTA) are effective, yet there is a significant consumer demand to remove such synthetic food additives from packaged foods. Our group has explored active packaging to perform the function of some synthetic additives including metal chelators. Chelating ligands covalently bound onto the food contact surface of packaging films, such as poly(hydroxamic acid) grafted from polypropylene (PP-g-HPHA) or poly(acetic acid) grafted from polypolypropylene (PP-g-PPA), have demonstrated iron chelating capacities of approximately 52.7 ± 13.4 nmol/cm² and 53.7 ± 9.8 nmol/cm², respectively. The antimicrobial activity of lysozyme against Listeria monocytogenes was enhanced in the presence of PP-g-PPA film, reducing the minimum inhibitory concentration from 2000 µg/mL to 1000 µg/mL. Through the binding of soluble iron, active packaging films are capable of influencing both the chemical stability and antimicrobial efficacy of a food system. As such, iron chelating films represent value added opportunities in cleaner label food applications.

AGFD 173 Solid/oil/water emulsions as novel approaches of encapsulating probiotic bacteria Yun Zhang, Qin Xin Zhong, qzhong@utk.edu. Univ. of Tennessee, Knoxville, Tennessee Probiotic bacteria are recommended for fortification of foods but can be easily deactivated during processing, storage, and digestion. Encapsulation is a well-established principle to protect probiotics against environmental stresses. However, common approaches using water-in-oil-in-water emulsions and alginate beads have drawbacks such as instability and potential sandy texture due to the big bead dimension. In this paper, recent advances of encapsulating probiotics in solid/oil/water emulsions will be presented. Spray-dried probiotics are suspended in oil before emulsification as the solid core in emulsion droplets smaller than 10 micrometers. Droplet surface can be fabricated with double layers of protein and citrus pectin or single-layered sugar beet pectin, which can be further strengthened by calcium cross-linking. Emulsions as fabricated can improve the stability of probiotics against dehydration, thermal processing, storage, and simulated gastric and intestinal digestions. These characteristics are critical for incorporation of probiotics in foods to receive the health benefits in vivo.
AGFD 174 Gut microbiome research and influence on warfighter performance Jason W. Soares¹, jason.soares@us.army.mil, James P. Karl¹, Lauret A. Doherty¹, Steven Arcidiacono¹, Kenneth Rациcot¹. (1) US Army Natick Soldier Research, Development, & Engineering Center, Natick, Massachusetts (2) US Army Research Inst. of Environmental Medicine, Natick, Massachusetts The gut microbiome is a malleable factor playing a pivotal role in human health and performance. As such, there is growing recognition within the Dept. of Defense (DoD) that research towards supporting a healthy and resilient gut microbiome will be critical to optimizing the health and performance of future Warfighters. The joint efforts of our internal Warfighter Gut Microbiome Working Group (WGMWG) includes a multi-faceted research effort seeking to characterize and understand how specific military-relevant stressors influence the delicate balance within a healthy gut microbiome. Additionally, the work seeks to identify nutritional interventions that build resiliency to these stressors by targeting the gut microbiome. Current clinical studies are investigating the effects of environmental and physiologic perturbations on the gut microbiome. Samples obtained from these efforts will be used in in vitro fermentation studies coupled with in vitro cell culture techniques aiming to understand the impact of these perturbations on gut metabolism and biological function, including gut permeability, inflammation and innate immunity. Additionally, in vitro fermentation will be employed to screen dietary input factors that could restore microbiome homeostasis and build resiliency toward stressor-induced dysbiosis. Military relevant stressors currently under study include sudden changes in diet, extreme physical exertion with undernutrition, and extended exposure to altitude (i.e. hypoxia), with cognitive and heat stress under consideration for future studies. Ancillary to our research efforts, the WGMWG is also actively developing a research roadmap to align complementary programs within this emerging DoD research area. Toward this end, a gut microbiome informational meeting was recently held with representatives from all services within the DoD. As part of the discussion, several key strategic research and capability gaps were identified that will need to be addressed in order to effectively meet the future potential of the gut microbiome as a tool for managing Warfighter performance. The talk will highlight the outcomes of the informational meeting as well as provide recent data from the ongoing clinical trials and in vitro studies.

AGFD 175 Microencapsulation of tributyrin to improve sensory qualities and intestinal delivery Youngsoo Lee, lees@illinois.edu, Wan-Yuan Kuo. Food Sci. and Human Nutrition, Univ. of Illinois, Urbana-Champaign Butyrate, a short chain fatty acid, is well known for improving gastrointestinal health. However, putrid aroma of butyrate has limited its incorporation into foods. Tributyrin, which is converted to butyrate in GI tract, is an alternative to butyrate, but tributyrin elicits extreme bitter taste and negative aroma as well. Gamma-cyclodextrin complexation of tributyrin may provide a solution to mask the bitterness. Gamma-cyclodextrin can add additional benefits, as it is fermented to butyrate in the colon, while the tributyrin released from complexation is converted to butyrate in the small intestine. The overall objectives of this study were to: 1) Measure the impact of gamma-cyclodextrin on the retention of microencapsulated tributyrin; 2) Determine the site of intestinal delivery and release of butyrate from microencapsulated tributyrin; 3) Assess sensory properties of microencapsulated tributyrin in an infant formula system. Tributyrin was complexed with gamma-cyclodextrin using a shearing mixing method followed by either spray or oven drying. Tributyrin was also encapsulated in whey-protein-based walls using a spray drying. The use of gamma-cyclodextrin resulted in the higher tributyrin retention (95%) when oven dried than when spray dried (62%). During in-vitro digestion test, all samples containing tributyrin showed limited butyrate release (~5%) during oral and gastric stages. In the small intestine stage, tributyrin microcapsules released approximately 75% of their total butyrate content with no significant differences (p>0.05) between the samples. During fermentation (large intestine), the gamma-cyclodextrin microcapsule produced significantly more butyrate (p<0.001) than the whey-based microcapsules. The oven dried gamma-cyclodextrin was able to deliver butyrate to the small and large intestine effectively. In an infant formula, the microencapsulation of tributyrin using oven dried gamma-cyclodextrin (GCT OD) produced a microcapsule that was able to reduce the sensory perception of tributyrin to a level that it was indistinguishable from a control formula containing no tributyrin as indicated by R-Index. Overall, findings from this study can be used to guide the production and application of microencapsulated tributyrin for use in food products for the potential improvement of intestinal health or disease states.

AGFD 176 Characterization and biocidal efficacy of cationic and N-Halalnine based antimicrobial coatings Yu-Ting Hung, yutinghung@umass.edu, Luis J. Bastarachea, Julie M. Goddard. Food Sci., Univ. of Massachusetts Amherst Surface modification with N-halalnine enables the development of antimicrobial materials for food handling with regenerative activities. Alternating layers of branched polyethyleneimine (PEI) and different molecular weights of styrene maleic anhydride (SMA) were applied onto the surface of polypropylene. Changes in surface chemistry was analyzed by ATR-FTIR which confirmed the cross-linking between PEI and SMA. Modified materials were further characterized using contact angles, and colorimetric assays for amine and chlorine quantification. The resulting coating was challenged against Listeria monocytogenes and Escherichia coli O157:H7 in both its unchlorinated and chlorinated form with varied contact times. Coatings exhibited antimicrobial character even with only 1 hour contact, and enabled more than 5 logarithmic cycles reduction against L. monocytogenes after 2 hours. In its chlorinated form, the coating also inactivated Escherichia coli O157:H7 by more than 5 logarithmic cycles. The antimicrobial coating exhibits dual antimicrobial nature by the presence of both N-halalnine and cationic moieties, and represents a promising approach for cross-contamination in the food industry.

AGFD 177 How to eat a plant-phytochemical detoxification in bees vs butterflies May R. Berenbaum, maybe@illinois.edu. Dept. of Entomology, Univ. of Illinois, Urbana-Champaign In 1961, H.T. Gordon postulated that the propensity of herbivorous insects to develop resistance to pesticides is "the result of selection for endurance of prolonged biochemical stresses" associated with dietary phytochemicals. Thirty years later, at the 202nd national meeting of the American Chemical Society, Rene Feyerisen and his colleagues presented their findings on patterns of expression of CYP6A1 in the house fly Musca domestica -- the first cytochrome P450 associated with insecticide resistance. A year later, the first P450 involved in phytochemical detoxification, CYP6B1, which detoxifies furanocoumarins in Papilio polyxenes, was characterized. In 2016, the 25th anniversary of the characterization of the first xenobiotic-metabolizing cytochrome P450, entire CYPomes are available from insects with a broad diversity of diets and a substantial literature suggests that plant-feeding insects vary enormously in how they detoxify the phytochemicals in their food. The structural, functional, and regulatory diversification of cytochrome P450s in herbivorous insects is reviewed in the context of the Gordon's remarkable insight.

AGFD 178 Dietary pterostilbene is a novel chemopreventive and therapeutic agent in prostate cancer: Pre-clinical studies Anait Levenson, anait.levenson@liu.edu. Long Island Univ., Arnold & Marie Schwartz College of Pharmacy and Health Sciences, Brooklyn, New
A potential strategy for chemoprevention and cancer therapy is to discover/develop new plant-derived bioactive molecules with anti-inflammatory and anticancer activities. Studies in our lab have shown that dietary stilbenes such as resveratrol and its analogs inhibit oncogene and epigenetic modifier metastasis-associate protein 1 (MTA1) expression in prostate cancer cell lines and xenografts. Pterostilbene, a dimethoxy analog of resveratrol that is found in grapes and blueberries, showed the highest MTA1 and MTA1-signaling inhibitory activity in prostate cancer cells compared to resveratrol and other analogs. The purpose of this study was to determine the MTA1-targeted chemopreventive and therapeutic efficacy of pterostilbene in Pten-loss pre-clinical model of prostate cancer that have elevated MTA1 levels compared to wild type animals. Prostate-specific Pten heterozygous (Pten−/+ ) and Pten knockout (Pten−/−) mice, which represent chemoprevention and intervention scenarios, respectively, were utilized. We found that pterostilbene both as a dietary supplementation and interventional daily injections, through targeting MTA1 and MTA1-dependent oncogenic network, inhibited inflammation, proliferation and angiogenesis and induced apoptosis in prostate tissues. These effects resulted in reduction of prostatic intraepithelial neoplasia (PIN) lesions and adenocarcinomas in precancerous Pten−/+ and cancer-prone Pten−/− models, respectively. We believe that pterostilbene is a novel MTA1-targeted chemopreventive and therapeutic agent that may have potential clinical applications in prostate cancer management.

AGFD 179 Topical pterostilbene prevents UV-B-mediated skin damage
Ryan Dellinger, ryand@chromadex.com. ChromaDex inc., Irvine, California
Skin is the human body’s first and best defense against environmental exposures including solar ultraviolet (UV) radiation. Exposure to UV light is a key factor in the development of many skin disorders. Skin cancer is the most prevalent type of cancer in the US, affecting an estimated one out of every seven Americans. UV radiation is one of the most powerful (and common) environmental factors that can cause a wide range of cellular disorders by inducing mutagenic and cytotoxic DNA lesions. Resveratrol, a natural polyphenol found in grapes, berries and other plants, has been proposed as an ideal chemopreventive agent due to its putative plethora of health promoting activities. However, despite its promise as a cancer prevention agent its success in human clinical trials has been limited, in part due to its poor bioavailability. Thus, interest in other natural polyphenols is intensifying including the naturally occurring dimethylated analog of resveratrol, pterostilbene, which has been proposed to have better bioavailability in humans. In this study, a SKH-1 (hairless) mouse model was used to examine if pterostilbene, like resveratrol, was effective in preventing UV-mediated skin damage. Mice were exposed to 180 mj/cm² UV-B radiation every other day for two weeks or left unexposed as a control. Thirty minutes prior to each exposure, topical pterostilbene, resveratrol, or vehicle was applied to the back of each mouse. We clearly show that pterostilbene prevented UV-B-induced damage in mouse skin. Visually, pterostilbene prevented redness on back skin and associated nicely with the prevention (or reduction) of hyperplasia, skin thickening and transepidermal water loss as compared to vehicle + UV-B treated mice. Furthermore, pterostilbene prevented UV-B mediated DNA damage (both cyclobutane pyrimidine dimer formation and 64-pp) in the skin of mice as compared to vehicle + UV-B. Interestingly, pterostilbene was more effective than resveratrol in all of our experiments.

AGFD 180 Health benefits of natural tocopherol mixtures
Nanjoo Suh, nsuh@pharmacy.rutgers.edu. Chemical Biology, Rutgers Univ., Piscataway, New Jersey
Tocopherols, members of the vitamin E family, are lipophilic antioxidants present in vegetable oils, such as cottonseed, corn and soybean. The tocopherols consist of four forms, designated as α, β, γ, and δ variants. Recently, γ-tocopherol, the most common form of vitamin E in the diet in the US, has shown anti-inflammatory and anti-cancer activities in experimental animal models. We have found that dietary administration of natural tocopherol mixtures (high in γ and δ forms) suppresses mammary tumor growth and tumor multiplicity in Sprague Dawley rats treated with N-methyl-N-nitrosourea, inhibits MCF-7 estrogen dependent xenograft tumor growth and reduces estrogen-induced mammary carcinogenesis in ACI rats. In our studies, treatment with natural tocopherol mixtures increases the expression of p21, p27, caspase-3 and peroxisome proliferator activated receptor-γ (PPAR-γ), while inhibits estrogen signaling in mammary tumors. In ACI rats implanted with slow release estrogen, natural tocopherol mixtures have also shown anti-estrogenic action and anti-tumorigenic activities. Our mechanistic study suggests that tocopherols activate PPAR-γ and Nrf2, while antagonize estrogen action in animal models of mammary tumorigenesis. Overall, natural tocopherol mixtures high in γ and δ-tocopherols may be potentially beneficial agents in the prevention of breast cancer.

AGFD 181 Chemistry, safety and calorific value of partially hydrolyzed guar gum
John W. Finley, jfinley@agcenter.lsu.edu. Louisiana State Univ., Baton Rouge
Partially hydrolyzed guar gum (PHGG) is obtained by partial hydrolysis of guar gum which comes form the Indian cluster bean (Cyanopsis tetragonolopus). PHGG is composed of galactomannan polymers with a molecular weight ranging from 200 to 300 kDa. The intact and partially hydrolyzed forms have multiple food applications. Guar gum can form gels or be used as a thickening agent in foods. The intact material can be used to control the viscosity, stability, and texture of foods. PHGG is highly soluble and has little physical impact on foods. Both forms are indigestible but are excellent sources of fermentable dietary fiber. The calorific value of intact guar gum is accepted as 2.0 kcal/g. This paper will review the chemistry, safety, in vivo effects, and calorific value of PHGG.

AGFD 182 Fifty years of smelling sulfur: From the chemistry of garlic to the molecular basis for olfaction
Eric Block, EBLOCK@ALBANY.EDU. Univ at Albany SUNY, Dept. of Chemistry, Albany, New York
Smell is one of five senses through which we perceive the world. By one estimate, humans can sense more than one trillion olfactory stimuli. My talk will focus on strong-smelling sulfur-containing odorants, whose chemistry I have been studying for more than 50 years, with a major focus being on sulfur compounds from garlic, onions and related species (“Allium chemistry”), particularly newly discovered thiolane derivatives. Humans and animals have an exquisitely sensitive sense of smell toward low-valent, volatile sulfur compounds. In 1887, Emil Fischer wrote that concentrations of ethanethiol as low as 0.05 ppb are “clearly perceptible to the sense of smell”. In 2005 we identified (methylthio)methanethiol (MeSCH₂SH; MTMT) as a garlic-smelling social-signalizing compound found in mouse urine. We subsequently identified the mouse odorant receptor (OR), MOR244-3, responding robustly to MTMT, finding that it employs Cu as a cofactor. Extending this research, I will describe the identification of a Cu-requiring human OR, responding robustly to 2-methyl-2-propanethiol, the odorant in natural gas, and related thiols. Taking a broader look at the sense of smell, I will discuss the vibrational theory of olfaction, focusing on musk odorants and their human ORs. Our collaborative OR studies use QM/MM modeling and site-directed mutagenesis to understand the molecular basis for olfactory detection of strong-smelling compounds.
AGFD 183 Rancidity development in roasted almonds (Prunus dulcis): Relationships between chemical changes and sensory descriptive analysis Lily Franklin, Dawn Chapman, Ellie King, Guangwei Huang, Alyson E. Mitchell, aemitchell@ucdavis.edu. (Food Sci. Tech., UC Davis, Davis, California) Almond Board of California, Modesto, California Sensory Science, The National Foods Lab, LLC, Livermore, California. Almond quality is dependent upon many factors including the development of rancidity. To date, little is known regarding correlations between chemical markers of rancidity and consumer acceptance/perception of roasted almonds. Raw almonds (cv. Nonpareil) were roasted for 60 min at 115 C to give a light roast, and 20 min at 157 C to give a dark roast. Markers of oxidative stress including: peroxide value (PV), free fatty acids (FFA), vitamin E, and volatile profiles were measured in roasted almonds stored at 39 ± 2 C and relative humidity of 15 ± 3% over 12 months. Marked changes in volatiles related to lipid oxidation (e.g. hexanal, octanal, nonanal, (E)-2-octenal, 1-heptanal, 1-octanol, etc.,) were noted by 3 months of storage. PV values did not exceed 5 millieq until 4.5 months. Levels of FFA did not change significantly during the 12 months of storage. Sensory descriptive analysis indicate that degree of difference vs. control, total oxidized flavor, cardboard flavor, painty/solvent flavor, soapy flavor, bitter taste, pungent/irritation/burning mouthfeel and astrigent mouthfeel increase with storage whereas clean nutty aroma and flavor, and clean roasted flavor decrease. Significant sensorial changes were notable by 6 months of storage and correlated with markers of oxidation.

AGFD 184 Chemical mechanisms for 3-MCPD ester formation Liangli L. Yu, lyu5@umd.edu. Univ of Maryland, College Park, Maryland 3-MCPD fatty acid esters are a group of processing-induced food toxicants. The free radical mediated chemical mechanisms for 3-MCPD ester fromation from triglyceride, diglyceride, and monoglyceride were investigated. ESR determination demonstrated a free radical mediated mechanism for 3-MCPD ester formation, whereas FT-IR examination suggested the involvement of a carbonyl group during the reaction(s). Possible mechanisms and radical intermediates were investigated and will be discussed. In addition, the possible catalytic role of Fe in 3-MCPD ester formation and thermal decomposition were studied and will be discussed.

AGFD 185 GMO crops may contribute to decline of monarch butterfly populations James N. Seiber, jnseiber@ucdavis.edu. Dept of Environmental Toxicology, Univ of California Davis, Recent trends indicate a significant decline in the monarch butterfly populations that migrate from summer breeding stocks to overwintering sites in Mexico and the California coast. Contributing to the ‘disappearing monarchs’ are habitat alteration, including deforestation, loss of milkweed flora which serves as a larval host for the monarchs, as well as drought and altered agricultural practices. The use/overuse of herbicides that are active against perennials, such as milkweeds, can be a factor for the decline as monarchs depend on this plant for vital components of their life cycle including egg laying and larval food. Planting of crops that have been genetically modified for resistance to Roundup (glyphosate) herbicide has facilitated the decline of weeds. This presentation will focus on factors that might come into play to reduce Monarch populations as a result of this GMO-inspired Tech. and changes in farming practice. The populations of milkweeds in the U.S. had declined significantly during the same period when Monarch populations declined and the use of GMO crops expanded (roughly from the 1990s to the present). Milkweeds harbor cardiac glycoside poisons that can poison livestock, causing the plants to be undesirable for ranchers, leading to use of Roundup and other herbicides. Glyphosate is also effective against invasive weeds—whose populations have also increased during the same time period and Senecio spp. Loss of milkweeds and Senecio to herbicide treated acreage, as well as overlying drought, results in fewer plants to serve as hosts for monarch larvae, thus reducing the availability of cardiac glycoside poison for sequestration, which defend monarchs from predators during the reproduction, feeding, metamorphosis, and migration cycles. A compelling scenario can be postulated that links herbicide use, drought effects, and changing agricultural/forestry practice to monarch decline. Various solutions to counter these threats to Monarch populations are under discussion.

AGFD 186 Impressive progress, opportunities, and obstacles in the use of genetically engineered trees Steven H. Strauss, steve.strauss@oregonstate.edu. Forest Ecosystems and Society, Oregon State Univ., Corvallis Genetic engineering (GE) provides options for circumventing some of the considerable difficulties of breeding trees, including their delayed onset of reproduction, limited capacity for hybridization/introgression, and intolerance of inbreeding. The capabilities provided by GE are likely to become increasingly important in a world characterized by rapid environmental change, climatic stress, and associated shifts in tree pests. I will review the scientific progress in creating and studying GE trees, including new opportunities provided by RNA interference and gene editing advances. I will also review the case for market and regulatory reforms, which are badly needed if the potential benefits of GE to society are to be realized.

AGFD 187 Progress on transgenic approaches to solving citrus greening disease Manjul Dutt, Jude W. Grosser, jgrosser@ufl.edu. Citrus Research and Education Center, Univ of. Florida, Lake Alfred, Florida Huanglongbing (HLB) has become the dominant disease threatening the Florida citrus industry. HLB affects all cultivated citrus varieties and causes a rapid decline of trees and produces unmarketable fruit. This disease is caused by a phloem limited noninigenous bacterial pathogen and causes substantial economic losses to every commercial citrus cultivar. Incorporation of gene(s) via genetic engineering can potentially confer resistance in susceptible cultivars, while maintaining the varietal fidelity. Several antimicrobial peptide gene constructs (AMPs) and the SAR inducing genes NPR1 and SABP2 have been tested in commercial sweet orange cultivars with varying degrees of success. Field trials in an HLB endemic environment as well as greenhouse based insect vector transmission trials have identified a few genes that can potentially confer tolerance to HLB. Initially, the AMP genes looked promising, but the tolerance response faded over time. The most successful genes to date are the SAR induction genes NPR1 and SABP2, driven either by a constitutive d35S promoter or a phloem specific Arabidopsis SUC2 promoter. Independent transgenic lines with these genes continue to show tolerance to HLB after four years in the field at a challenging field site. We will also discuss our current citrus improvement strategies to develop more consumer-friendly transgenic plants by the utilization of plant based genetic constructs. We have developed a transformation system to generate reporter gene expression free citrus by coupling a visual citrus derived anthocyanin producing transcriptional factor gene with an embryo specific promoter to regenerate genetically modified plants that have the marker gene switched off. In addition, we are also evaluating a large number of citrus derived genes, promoters, genes and terminators to create an all citrus transformation vector. These constructs are also being incorporated using our protoplast transformation system, which allows the incorporation of linear DNA pieces into the citrus genome. HLB-resistant transgenic citrus containing all plant DNA should have quicker regulatory approval as well as improved public acceptance.
AGFD 188 American chestnut research and restoration project William A. Powell, wapowell@esf.edu, Andy Newhouse, Charles K. Maynard, Lihnda McGuigan, Allison D. Oaks, Kristen R. Stewart, Tyler Desmarais, Dakota Mathews, Yoks Bathula, Vernon Coffey. SUNY College of Environmental Science & Forestry, Syracuse, New York The American chestnut (Castanea dentata) and chestnut blight is the classic example of what happens when our forests succumb to exotic pests and pathogens. Because of its environmental, economic, and social importance, many tools have been brought to bear on the chestnut blight problem. We have focused on enhancing blight resistance by adding only a couple genes to the approximately 40,000 gene pairs in the chestnut genome using the tools of genetic engineering. Although we have eight candidate genes that putatively enhance blight resistance slightly, one stands out among the rest. The most promising gene to date encodes an oxalate-detoxifying enzyme, called oxalate oxidase (OxO). This gene comes from bread wheat (Triticum aestivum), but is also a common defense gene found in many plants including all grain crops as well as bananas, strawberries, peanut, and other familiar produce. The OxO is not a pesticide, not an allergen, and is not a gluten protein. According to chestnut leaf and small stem assays that predict the level of blight resistance, this OxO has raised resistance levels in American chestnut at least as high as those found in the blight-resistant Chinese chestnut (C. mollissima). This will be the first time an ecosystem restoration program will use the tools of genetic engineering. The next step is to have the trees reviewed by three federal regulatory agencies, the USDA, EPA, and FDA. Once approved, these blight resistant American chestnut trees can be used to rescue the genetic diversity and local adaptation in the remnant, surviving population of American chestnut and be an additional tool for the restoration of this important keystone tree.

AGFD 189 Transgenic and gene edited animals for use in agriculture: Where are we now? J. D. Murray, jdmurray@ucdavis.edu. Dept. of Animal Science; Dept. of Population Health and Reproduction, Univ. of California-Davis There have been many developments in Tech. to create transgenic since the early 1980s, including somatic cell nuclear transfer-based cloning, effective use of PGCs in chickens, lentiviral vectors, and among others. The development of gene editing methodologies has improved our ability to precisely alter the genome of animals and, with the large number of sequenced genomes, we have unprecedented access to sequence information, including, control regions, coding regions, and known allelic variants. We now can create new transgenes that will express when and where we want and can target precisely in the genome where we want to make a change or insert a transgene. However, to date we have only one GE animal approved for use as food anywhere in the world, the AquAdvantage Salmon. World-wide there has been a failure of the regulatory processes to effectively move forward. Estimates are that we will need to increase our current food production by 70 to 100% by 2050; that is we will have to produce the total amount of food each year that has been consumed by mankind over the past 500 years. The combined use of transgenic animal Tech. and gene editing will become increasingly more important tools to help feed the world. However, the practical benefits of these technologies have not yet reached consumers in any country and in the absence of predictable, science-based regulatory programs it is unlikely that the benefits will be realized in the short to medium term.

AGFD 190 Microalgae derived ingredients, oils and the future of foods Walter G. Rakitsky, wrakitsky@gmail.com. TerraVia, South San Francisco, California At TerraVia, we are redefining the future of food. By harnessing the power of algae, our Tech. brings better, next generation, plant-based nutrition to people along with economic and environmental stability for the planet. Microalgae, the mother of all higher plants and the earth’s first triglyceride oil producers, have evolved over hundreds of millions of years to very efficiently convert light and/or simple sugars into biomass and oils; often in very inhospitable parts of our planet, making algae the earth’s original superfood. Algae are poised to play a growing role in the world’s food supply. Microalgae are extremophiles and can be found thriving in environments such as polar and high alpine regions, thermal vents and hot springs, soda lakes as well as natural salt lakes. Provided adequate energy and nitrogen sources are available microalgae direct their efforts to reproduce; thereby, driving biomass production. In the presence of an energy source but the absence of nitrogen, microalgae respond by producing triglyceride oils that are stored inside the cells for future use. Carbohydrates, vitamins and pigments critical for human and animal nutrition are also routinely produced by microalgae. In this presentation, we will explore how TerraVia has harnessed the robustness, efficiency and productivity of heterotrophic microalgae to develop Tech. platforms that vastly expand the functionality of microalgae ingredients to create healthy, nutritious and appealing foods, improving the lives of people and the planet. In particular, we will discuss utilizing native microalgae to produce protein rich and lipid rich whole microalgae ingredients as well as oils and the composition, properties and usefulness in foods of oils and butters from tailored microalgae. We’ll also take a closer look at how algae-based platforms offer a superior sustainability profile as well.

AGFD 191 Supramolecular design of coordination bonding architecture on zein nanoparticles for pH-responsive drug deliver and the cellular uptake mechanism Hongshan Liang, lianghongshantz@163.com. (1) Rutgers Univ., New Brunswick, New Jersey (2) Food Sci., Huazhong Agriculture Univ., Wu Han, Hu Bei, China A pH-responsive system by constructing a designable coordination a bonding-based metal-tannic acid (TA) architecture on zein nanoparticles (NPs) has been investigated. The prepared metal-TA coated zein NPs demonstrated good stability in cell culture medium. Because of the pH-responsive coordination bonding between TA and metal ions, the functional property of the metal-TA NPs was tailored for drug delivery. In vitro viability studies revealed that the zein-TA/metal NPs showed no significant cytotoxicity against HepG2 cells for 24 h. Biocompatible AuNPs were produced using zein-TA/metal NPs as reducing and stabilizing agents which were promising in the photothermal therapy of cancers and other diseases. In order to form more controllable release profile, we implied the complex NPs prepared with the combination of zein and HTCC. The cleavage of either the “NH2-metal” or the “metal-TA” coordination bond, in response to pH variations, gave rise to a significant release of guest molecules under designated pH conditions. EuIII was used to chelate with ligand named 2-thionyltrifluoroacetone (TTA) to intense fluorescence intensities of EuIII-TA films so as to develop pH-responsive zein/HTCC-TA/metal NPs for anticancer drug delivery as well as cell imaging. We further study the effect of coatings on cellular uptake of zein NPs. Because of the hydrophobicity of zein NPs, they can be easily recognized by immune cell which reduce the uptake of targeted cells. In our study, metal/T-A coatings would reduce the phagocytosis of macrophages. Moreover, the increase in the thickness of the coatings illustrated different uptake efficiency. The coated NPs showed different mechanism of endocytosis.

AGFD 192 Preparation, characterization, in vitro lipolysis and cell study on antioxidant and anti-inflammatory activities of carnosic acid nanoemulsion Huijuan Zheng, huijuanzheng87@gmail.com, Qingrong Huang. (1) Food Sci., Rutgers Univ, New Brunswick, New Jersey (2) Food Sci., Rutgers Univ., New Brunswick, New Jersey Carnosic acid has great biological and pharmacological benefits, including antioxidative, anticarcinogenic, anti-inflammatory properties and so on. However, the oral use of carnosic acid is limited due to its high
hypodermicity, low water-solubility and poor bioaccessibility. In the present work, carnosic acid nanoemulsion (NE-CA), as potential active ingredients for liquid food, was prepared with GRAS components by high pressure homogenization, followed by wide physicochemical characterization including size and size distribution, zeta potential, rheology, stability and so on. In vitro lipolysis showed that nanoemulsion delivered carnosic acid was digested considerably faster and more bioaccessible than unformulated suspension. The cellular antioxidant assay and cellular uptake by HepG2 cells showed that compared with free carnosic acid, NE-CA had slightly lower cellular antioxidant activity, which is mainly attributed to its slow cellular uptake as detected by fluorescence microscopy. NE-CA showed greatly improved anti-inflammatory activity than pure carnosic acid by studies on lipopolysaccharide activated RAW 264.7 macrophage cells, which may be explained by the synergistic anti-inflammatory effect of carnosic acid with medium-chain tracyglycerol and phosphatidylcholine in the lecithin. The present study suggests that nanoemulsion is effective to deliver carnosic acid, to increase the bioaccessibility and the ability to suppress inflammation and provides theoretical and practical guides for the further application of carnosic acid nanoemulsion.

AGFD 193 Evaluation of postharvest washing on Ag NPs removal from spinach leaves Zhiyun Zhang¹, zhiyunzhang@foodsci.umass.edu, Lili He², (1) Food Sci., Univ. of Massachusetts Amherst (2) Food Sci., Univ. of Massachusetts-Amherst There is an increasing tendency to apply silver nanoparticles (Ag NPs) as pesticides for fruits and vegetables due to their unique antimicrobial and insecticidal properties. However, the residue of Ag NPs in these fresh produce may transfer through food chains and pose a potential risk to public health. The objective of this study is to determine whether postharvest washing can remove Ag NPs that accumulated on fresh produce. Commerically available 40 nm citrate coated Ag NPs (4×10⁴ mg) were applied to contaminate the spinach leaves, followed by washing with deionized water, Tsunami 100 (80 mg L⁻¹) and Clorox® bleach (200 mg L⁻¹) respectively. Then, the removal efficacy of these three treatments on Ag NPs that attached on spinach leaves was evaluated by a combination of techniques, including surface enhanced Raman spectroscopy (SERS), scanning electron microscopy (SEM)-energy dispersive spectrometer (EDS), and inductively coupled plasma mass spectrometry (ICP-MS). As for the total amount of silver element, ICP-MS showed that no significant difference in deionized water treated group while Tsunami 100 and Clorox® bleach treatment resulted in a 21% and 10% decrease (P < 0.05), which indicated the Ag NPs dissolution and Ag⁺ release upon contact with the oxidizing agents, for example, peroxycetic acid and hydrogen peroxide in Tsunami 100, and sodium hypochlorite in Clorox® bleach. According to SERS results, no significant difference in Ag NPs amounts on spinach was observed following the deionized water and Tsunami 100 treated group, whereas for Clorox® bleach, the amount of Ag NPs decreased over 90% (P < 0.05). SEM-EDS images revealed the formation of large silver chloride (AgCl) (over 100 nm) under Clorox® bleach treatment. This study demonstrates that the low removal efficacy of postharvest washing on Ag NPs and the necessity to develop a highly efficient washing method for removing Ag NPs residues from fresh produce surfaces in the future.

AGFD 194 Influence of food matrix on the fate of titanium dioxide (TiO₂) nanoparticles in gastrointestinal tract Xiaqing Cao¹, Xiaqingcao.cao@gmail.com, Hang Xiao², David McClements¹, (1) UMASS Dept of Food Sci., Amherst, Massachusetts (2) Food Sci., Univ. of Massachusetts, Amherst TiO₂ nanoparticles are commonly added to food products as part of food additives, and they have been associated with potential adverse effects on human health. TiO₂ nanoparticles have specific surface reactivities and can interact with cellular proteins forming a protein corona that imparts their biological activities. However, the most of toxicity studies have been focused on the TiO₂ nanoparticles per se without considering the effects of food matrices where TiO₂ exist. Detailed understanding on the fate of TiO₂ nanoparticles at the presence of food in gastrointestinal tract will facilitate the safety assessment of TiO₂ nanoparticles in food. In this study, the fate of TiO₂ nanoparticles was characterized during the simulated digestion of milk. TiO₂ nanoparticles were isolated after gastric and intestinal digestion by ultracentrifugation. The particles size and protein corona composition were characterized. Interaction between TiO₂ nanoparticles and intestinal epithelium was studied using an intestinal monolayer model. TiO₂ nanoparticles isolated from gastric and intestinal phases of digestion showed difference in surface charge, size and protein corona composition. Trans-enterocyte uptake of TiO₂ nanoparticles was altered by the milk protein/TiO₂ nanoparticle interaction. Overall, our results demonstrated that the fate of TiO₂ nanoparticles was significantly influenced by food matrices in the gastrointestinal tract, which may have significant impact on the potential toxicity of TiO₂ nanoparticles.

AGFD 195 Application of new nanomaterials as signal probes in immunoassay Gaoshuang Hu, huaohu@163.com, Shuo Wang, Wei Sheng, Yan Zhang. Tianjin Univ. of Science and Tech., Tianjin, China Immunoassay has been successfully commercialized and applied in practice to detect contaminants and foodborne toxicants in food and environment. These methods offer practical advantages and can be employed effectively in both Lab and field settings, and which have contributed to wide use of immunoassay as necessary testing tools in food safety supervision. In order to improve the performance of immunoassays and related commercial products, development and application of new signal probes become an issue of great concern recently. Besides the classic signal probes, such as HRP enzyme and colloidal gold, new signal probes, which showed different special properties and admirable characters, have been employed in quantitative analytical methods with different assay formats. Based on our challenging research work, case studies referring to the use of multiple signal probes in immunoassays will be introduced, including application of up-conversion nanoparticles, quantum dots, colloidal carbon and nanogold-polyaniline-nanogold microspheres. We have developed a series of novel fluorescence immunoassays for the detection of sulfaquinoxaline, norfloxacin and nitenpyram by the use of up-conversion nanoparticles as labels. Besides, we have developed a series of immunochromatographic assays for the detection of enrofloxacin, salbutamol, flumequine and plasticizer by the use of up-conversion nanoparticles, quantum dots, carbon black and nanogold-polyaniline-nanogold microspheres. The obtained results demonstrates that the application of new signal probes make the immunoassays and immunochromatographic assays show improved performance with pleasing characters, such as fast-response, high sensitivity, less matrix effects, etc., and which indicates the prospective future of new signal probes applied in immunoassays.

AGFD 196 Assemblies, properties and food applications of kafirin nanoparticles based Pickering emulsions Jie Xiao¹, xiaojieacademicic@gmail.com, Qingrong Huang¹. (1) Food Sci., Rutgers Univ, New Brunswick, New Jersey (2) Food Sci., 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 fulfilling its application potentials were scarce. In the present study, kafirin protein was fabricated into spherical nanoparticle via anti-solvent precipitation method, and the as-prepared kafirin nanoparticles were...
capable of stabilizing oil in water type of Pickering emulsions (KPE). We then reported for the first time the interface microstructure as well as rheological properties of KPE and elucidated their responses to operation parameters. KPE was then utilized as a novel delivery vehicle for oil soluble nutraceutical and its storage stability and oral digestion profile were then fully investigated. Furthermore, we proved the feasibility of employing kafirin nanoparticles as outer stabilizer of double emulsion (KDE) and characterized their structural and digestion properties. To address the observed poor storage stability and premature release of oil phase after oral intake in both KPE and KDE, we immobilized the kafirin stabilized Pickering emulsion within an alginate based hydrogel matrix to deliver readily applicable Pickering emulsion formulation with ease of preparation, improved processing stability and sequential digestion profile.

AGFD 197 Real-time and in situ monitoring of pesticide penetration in edible leaves by surface-enhanced Raman scattering mapping

Tianxi Yang, tianxiyang@umass.edu, Lili He, Food Sci., Univ. of Massachusetts Amherst. Understanding of the penetration behaviors of pesticides in fresh produce is of great significance for effectively applying pesticides and minimizing pesticide residues in food. There is lack, however, of an effective method that can measure pesticide penetration. Herein, we developed a novel method for real-time and in situ monitoring of pesticide penetration behaviors in spinach leaves based on surface-enhanced Raman scattering (SERS) mapping. Taking advantage of penetrative gold nanoparticles (AuNPs) as probes to enhance the internalized pesticide signals in situ, we have successfully obtained the internal signals from thiabendazole, a systemic pesticide, following its penetration into spinach leaves after removing surface pesticide residues. Comparatively, ferbam, a non-systemic pesticide, did not show internal signals after removing surface pesticide residues, demonstrating its non-systemic behavior. In both cases, if the surface pesticides were not removed, co-penetration of both AuNPs and pesticides was observed. These results demonstrate a successful application of SERS as an effective method for measuring pesticides penetration in fresh produce in situ. The information obtained could provide useful guidance for effective and safe applications of pesticides on plants.

AGFD 198 Development of a neuroprotective index for ayurvedic medicinal plants

Weixi Liu\(^1\), weixi_liu@my.uri.edu, Hang Ma\(^1\), Lu Zhang\(^1\), Chunpeng Wan\(^1\), Joel A. Dain\(^2\), Navindra P. Seeram\(^1\). (1) Biomedical and Pharmaceutical Sciences, College of Pharmacy, Univ. of Rhode Island, Kingston (2) Chemistry Dept., Univ. of Rhode Island, Kingston. Twenty-six chemically-characterized Ayurvedic (Indian traditional system of medicine) medicinal plant extracts were evaluated using a panel of bioassays to establish a Neuroprotective Potential Index (NPI) for these natural products. Bioassays were selected based on established links between Alzheimer’s disease (AD) and oxidative stress, glycation, and amyloid \(\beta_{1-42}\) protein aggregation. Thus, the extracts were evaluated for: 1) total polyphenol content (Folin-Ciocalteu assay), 2) free radical scavenging capacity (DPPH assay), 3) reactive carbonyl species scavenging capacity [methylglyoxal (MGO) trapping assay], 4) anti-glycative effects (BSA-fructose and BSA-MGO assays) and, 5) anti-amyloid beta (\(\beta_{1-42}\)) fibrillation effects (thioglycinn-T assay). Among the extracts, pomegranate (Punica granatum), contained the highest polyphenol content, showed the most potent free radical scavenging, reactive carbonyl species scavenging, and anti-glycation properties, and inhibited \(\beta_{1-42}\) fibrillation. The data provided by the NPI, established in the current study, correlates with published studies supporting the anti-AD effects of several of these medicinal plants, including pomegranate.

AGFD 199 Effects of brewing conditions and re-infusion on the antioxidant activity of twenty-four varietal green teas

Erica M. Sharpe\(^1\), ericashrp@gmail.com, Fang Hua\(^1\), Stephanie Schuckers\(^1\), Silvana Andreescu\(^1\), Ryan Bradley\(^1\). (1) Clarkson Univ., Potsdam, New York (2) SUNY Canton, Canton, New York (3) National Univ. of Natural Medicine (NUNM), Portland, Oregon. The effect of brewing conditions and re-infusion on the antioxidant capacity of twenty-four commercial green teas has been measured using two antioxidant assays. The first method was a high-throughput adaptation of our paper-based NanoCerac antioxidant assay (Sharpe, Frasco, Andreescu, & Bradely, 2012). The second assay, used as a comparative measure, was the popular oxygen radical absorbance capacity (ORAC) assay, frequently applied to complex foods and beverages. We utilized these assays monitor a novel antioxidant parameter: sustained antioxidant capacity, or the total inherent antioxidant capacity (TI-NanoCerac and TI-ORAC). This value was measured by infusing each tea six times. Both NanoCerac and ORAC assays correlated moderately with respect to single and multiple infusions (R2 0.80 ± 0.19). The average first-brew NanoCerac, TI-NanoCerac, first-brew ORAC and TI-ORAC were: 0.73 ± 0.1 GAE/g tea; 2.4 ± 0.70 mmol GAE/g tea; 1.0 ± 0.3 mmol TE/g tea and 2.1 ± 0.71 mmol TE/g tea respectively. Effects of brewing conditions (temperature, brew time, etc.) were assessed using one popular tea as a standard. Brewing conditions including water temperature and infusion time significantly affected antioxidant capacity. The high-throughput adaptation of the original NanoCerac assay tested here offered excellent advantages over ORAC, including portability and rapid analysis.

AGFD 200 Comparative study of performance of regular pyrolysis oil and TGRP oil for catalytic cracking with HZSM-5

Yongsuck Choi, kurz.john@gmail.com, Yaseen Elkasabi, Paul Tarves, Charles A. Mullen, Akwasi Boateng. Eastern Regional Research Center, USDA-ARS, Wyndmoor, Pennsylvania. Bio-oil from fast pyrolysis of biomass has the potential to be processed into value-added chemicals and transportation fuels. However, the composition of bio-oils differs significantly from that of petroleum fuels and contains high oxygen and water content. Therefore, bio-oil needs to be upgraded before it can replace fossil fuels. Currently, there are two main routes for upgrading of bio-oil. Bio-oil may be upgraded via catalytic hydrodeoxygenation (HDO), in which it is hydrotreated with high pressure \(H_2\) (30-140 bar) in the presence of a catalyst. However, the HDO process is costly due to the large consumption of \(H_2\). In contrast, catalytic cracking of bio-oil with solid acid catalysts (typically zeolites) occurs under atmospheric pressure without the addition of \(H_2\), which makes the process more economical. In the present study, catalytic cracking of two different bio-oil feedstocks, one a regular bio-oil from a conventional pyrolysis process and the other, a partially deoxygenated bio-oil from the tail-gas reactive pyrolysis process (TGRP), was performed using HZSM-5. We further investigated the effects of these bio-oil feedstocks on the yield and selectivity of monoaromatic and polyaromatic compounds. Additionally, the selectivity was studied at different temperatures and the stability of HZSM-5 was assessed by reusing the catalyst without regeneration.

AGFD 201 Novel promising biocomposite derived from calcined eggshells for mitigating soil antibiotic resistance bacteria/gene dissemination and accumulation in bell pepper

Ye Mao\(^1\), yemao@issas.ac.cn, Sun Mingming\(^2,3\), Xu Li\(^3\), Arthur Paul Schwab\(^4\), Xin Jiang\(^1\). (1) Soil Chemistry and Environmental Protection, Inst. of Soil Sciences,Chinese Academy of Sciences, Nanjing, Jiangsu, China (2) Soil
Ecology Lab, Nanjing Agricultural Univ., Nanjing, Jiangsu, China (3) Civil Engineering Dept., Univ. of Nebraska, Lincoln (4) Dept. of Soil and Crop Sciences, Texas A&M Univ., College Station The accumulation of antibiotics, heavy metals, antibiotic resistance bacteria (ARB) genes (ARGs) in vegetables have become a new threat to human health. This is the first study to investigate the feasibility of calcined eggshells modified by aluminum sulphate as novel agricultural biocomposites to impede mixed contaminants from transferring to bell pepper. In this work, eggshell amendment significantly enhanced the dissipation of soil tetracycline, sulfadiazine, roxithromycin, and chloramphenicol; and decreased the water-soluble fractions of antibiotics and exchangeable Cd, which further impeded the accumulation of pollutants to bell pepper; and declined the diversity and abundance of ARB/ARGs inside the vegetable. Furthermore, ARGs levels in the bell pepper fruits were significantly decreased to 10^{12} copies/16S copies, indicating limited transferring risk of ARGs along the food chain. Meanwhile, the restoration of soil microbial biological functioning further suggested the calcined eggshells are environmentally-friendly biocomposites to control the dissemination of soil ARB/ARGs in the soil-vegetable system.

AGFD 202 Stability of anthocyanin pigments in purple wheat bran and powder isolates Elsayed M. Abdelaal1, elsayed.abdelaal@agr.gc.ca, Pierre Huc2. (1) Guelph Research and Development Centre, Agriculture and Agri-Food Canada, Guelph, Canada (2) Crop Development Centre, Univ. of Saskatchewan, Saskatoon, Canada Anthocyanins are naturally-occurring pigments found in fruits, vegetables and grains which can be used in the food and healthcare industries as natural colorants, antioxidants and/or dietary supplements. In the current study anthocyanins in purple wheat were concentrated in the bran fraction with dry milling and further processed into anthocyanin powder with ethanol extraction and column purification. The two products represent two different matrix structures, i.e. bran in buffer suspension and anthocyanin powder solubilized in buffer. Effects of pH (1, 3 and 5), temperature (35, 60 and 90 °C) and time (60, 90 and 120 min) on anthocyanin stability were investigated using a factorial experimental design. Purple wheat pigments either in the bran matrix or isolated form were more stable at pH 1 and their content decreased substantially at pH 3 and 5. Anthocyanins in the bran showed an increase in total anthocyanin content with increasing temperature. In contrast, the anthocyanins in the powder significantly degraded with increasing temperature. The increase of total anthocyanin content in the case of bran possibly was due to continued extraction of anthocyanin pigments from the bran matrix, while anthocyanins in isolates were soluble in solution and thus exposed to thermal degradation. The effect of time was significant either in the purple wheat bran or isolate but it was not as strong as the pH or temperature effects. In addition, the interactions between pH, temperature and time showed significant effects on anthocyanin stability in most cases. In conclusion, the stability of anthocyanins appears to be dependent on their physical state in addition to the processing conditions.

AGFD 203 Ascorbic acid-catalyzed degradation of cyanidin- and malvidin-3-O-β-glucoside: Proposed mechanism and identification of novel hydroxylated products Nate B. Stebbins3, nbstebbi@uark.edu, Luke Howard1, Ronald L. Prior1, Cindi Brownmiller4, Rohana Liyanage5, Jackson O. Lay5, Xiaoyu Yang5, Steven Qian5 (1) Univ of Arkansas, Fayetteville (2) Dept of Chemistry, Univ of Arkansas, Fayetteville (3) Food Sci., Univ of Arkansas, Fayetteville (4) Pharmaceutical Science, North Dakota State Univ., Fargo Anthocyanins in the presence of ascorbic acid are readily degraded, which adversely affects color and health benefits of anthocyanin-rich beverages. The project involved searching for novel pigmented compounds in a simple model system composed of cyanidin-3-O-β-glucoside and ascorbic acid, and a second model system consisting of blackberry extract supplemented with ascorbic acid. Degradation products were identified by HPLC-PDA and HPLC-MS and hydroxyl radical formation was monitored by ESR. Over 72 hours at 23°C, 67% of cyanidin-3-O-β-glucoside was lost in the model system during which time an unknown pigmented compound was formed. The unknown compound was also identified in a more complex model system consisting of blackberry extract and ascorbic acid. The unknown compound was identified as 6-hydroxy-cyanidin-3-O-β-glucoside. The mechanism was validated with a mixture of malvidin-3-O-β-glucoside and ascorbic acid, which produced a hydroxylated malvidin-3-O-β-glucoside. Production of hydroxyl radical in the base and blackberry model systems was confirmed by ESR.

AGFD 204 Analysis of changes in anthocyanin and volatile compounds of Fuji apple under different sizes and storage conditions Hae Won Jang1, hwjkti@kfri.re.kr, Moon-Cheol Jeong2. (1) Food Analysis Center, Korea Food Research Inst., Seongnam, Korea (2) Korea Food Research Inst., Seongnam, Korea Apple is one of the most widely consumed fruits in worldwide. Recently, the content of chlorophyll and anthocyanin as color pigment and volatile compounds in apple have received much attention because those compounds contribute to the overall sensory quality from different varieties and storage conditions during ripening. The objective of the present study was to investigate anthocyanin in ‘Fuji’ apples sorted based on five different sizes under different storage conditions (air, controlled atmosphere and 1-methylcyclopropene). As a result, there was no significant amount of anthocyanin in the apples. However, the significant difference was observed among the apples under the different storage conditions. From our sensory test of the apples, the results demonstrate that the colors and flavor of the apples play important role for consumers. Therefore, the changes of volatile profile in the apples were analyzed to assess the quality of apples by headspace solid-phase microextraction (HS-SPME) coupled with gas chromatography-mass spectrometry (GC-MS). There was also difference in ester types as the major compounds from the apples according to the above mentioned conditions. The results suggest that anthocyanin and volatile compounds could be used as the potential indicators as quality assessment in apples.

AGFD 205 Measuring color in turbid beer and wort samples Roger Barth, rbarth@wcupa.edu. Chemistry, West Chester Univ., West Chester, Pennsylvania Finished beer and beer in process generally has at least some turbidity, called “haze” in brewing jargon. Before spectroscopic determination of the depth of color can be accomplished, time-consuming clarification procedures must be applied. For moderately turbid beer and wort, it is possible to correlate 850 nm light scattered at 90 degrees from the source with the transmittance at 430 nm to produce a corrected transmittance free of the effect of turbidity. Simultaneous measurement of transmittance at 430 nm and 90 degree scatter at 850 nm can be processed to give a color measurement without elaborate sample work-up. This method has the potential to improve productivity and lower cost in brewing and malting laboratories.

AGFD 206 Investigation of monoterpen enantiomers in Pinot gris wine and sensory perception of these compounds on matrix interactions Mei Song, songme@oregonstate.edu, Elizabet Tomasino. Oregon State Univ., Corvalli Monoterpenes are aromatic compounds that contribute to the characteristic aromas of white wines. Chiral monoterpen profiles were chosen based concentration and combination of the different compounds quantified in 50 Pinot gris wines. The majority of the concentrations of these compounds were found to be below
known perception thresholds. Such low levels of aroma compounds have been found to impact aroma perception. Therefore it was of interest to determine the impact of the measured chiral monoterpenes to sensory perception of Pinot gris wine. Additionally the effect of the matrix was investigated, as the composition of the matrix has been found to impact aroma perception as well [3]. Nine different chiral monoterpenes were chosen. The effect of these profiles was measured in three different “matrices”: (1) 14% ethanol, pH 3.2, (2) deamortized Pinot gris wine and (3) commercial Pinot gris wines with low levels of chiral terpenes. Matrix 1 was chosen to determine if the chiral monoterpenes could influence aroma by themselves. Matrix 2 was chosen to show any nonvolatile matrix effects to chiral monoterpenes perception and matrix 3 was chosen to determine any volatile aroma compound interactions with the chiral monoterpenes. Regular white wine drinkers participated in triangle tests across 10 different tasting sessions for each wine matrix. The chiral monoterpenes were not found to significantly impact aroma when in Matrix 1 or 2 was used, suggesting that the chiral terpene content did not affect aroma perception by themselves (matrix 1) and that there were no or little interactions with nonvolatile components to effect perception. However sensory perception did change when chiral monoterpenes were in matrix 3, showing that in combination with other aromatic compounds, the chiral monoterpenes altered sensory perception. These results suggest that aroma perception of some wine compounds are due to interactions even at concentrations below their perception threshold.

AGFD 207 Safer salads and grilled meats: Clean and green approaches Sadhana Ravishankar, sadhravi@email.arizona.edu. School of Animal & Comparative Biomedical Sciences, Univ. of Arizona, Tucson. Foodborne illness outbreaks occurring due to the consumption of contaminated food products have been increasing over the last few decades. It is estimated that there are 48 million illnesses, 128,000 hospitalizations, and 3,000 deaths each year due to foodborne causes in the US. The major foodborne pathogenic bacteria involved in foodborne outbreaks include Salmonella enterica, Escherichia coli O157:H7 and Listeria monocytogenes. Current consumers are becoming more aware of the health risks due to the use of chemical preservatives in food products and prefer natural ingredients and processes in food production. Research is needed to devise appropriate intervention strategies that employ natural ingredients and processes in food production. Antimicrobials derived from plant sources have been found effective in inactivating foodborne pathogenic bacteria as well as spoilage microorganisms. Phyto-antimicrobials could also help enhance the flavor of foods and may provide health benefits such as reduction in blood sugar levels and cholesterol as well as anticarcinogenic effects. These include essential oils, their active components, plant extracts, spices and plant powders. Their effectiveness against foodborne pathogenic bacteria in vitro and on/in foods has been investigated. The effectiveness of phyto-antimicrobials against foodborne pathogenic bacteria in vitro will be discussed. Their applications in the wash water for produce decontamination will be discussed. The use of antimicrobial edible films on meats/poultry and in salad bags will also be discussed. The use of phyto-antimicrobials in improving the safety of grilled meats by reducing not only Escherichia coli O157:H7 but also the potentially carcinogenic heterocyclic amines that can be formed at high grilling temperatures will be discussed. Phyto-antimicrobials have the potential to improve the microbiological safety of foods.

AGFD 208 Organic acids as food antimicrobials Joshua Gurtler, joshua.gurtler@ars.usda.gov. Food Safety and Intervention Technologies, USDA, Agricultural Research Service, Wyndmoor, Pennsylvania. Hundreds of fruits and vegetables eaten around the world, in addition to thousands of processed foods, contain organic acids, often serving as intentional or incidental antimicrobials. Organic acids’ preservative properties and use in foods is historically and anthropologically dated to several thousand years B.C. Some common foods containing organic acids are juices, sports drinks, sauces, luncheon meats, pickled and fermented food products, fruit spreads, yogurt and diverse fermented dairy products, dressings, canned vegetables, mayonnaise, pickles, pickled eggs, pickled meats and sausages, kimchi, sauerkraut, salsa, desserts, etc. Major acids naturally occurring in fruits include citric, quinic, malic, tartaric, and ascorbic acids, although 17 more acids have been identified. Processed and/or fermented foods are known to frequently contain acetic, lactic, citric, malic, benzoic, propionic, sorbic, tartaric, ascorbic, adipic and fumaric acids, or their salts. Ways in which acids act as preservatives include weakening microorganisms to make them more heat-sensitive, thus reducing the requisite thermal cooking intensity (such as is applied in industrial vegetable canning). Some acids and/or their resultant reduced pH levels prevent outgrowth of spoilage or pathogenic bacterial spores. Certain organic acids (e.g., benzoic, sorbic, propionic) act more strongly on yeast and molds and are added to bread and drink products to extend shelf life and prevent food spoilage. Undissociated carboxylic acids are commonly used as preservatives against bacteria, because they are able to cross the cell membrane barrier and shed acidiﬁying protons, either killing the microorganism or preventing multiplication. In recent years, perorganic acids, such as peroxyacetic acid, have become more popular for washing meats and fresh produce, while acetates and lactates are added to ready-to-eat meat products. One example is a USDA, ARS-patented mixed perorganic acid produce wash that was developed with an industry partner and has FDA approval. Novel applications of organic acids include combining with surfactants, which weakens the cell membrane, allowing the acid to more easily enter the cell and acidify the cytoplasm. One example of this is a patented combination of levulinic acid and sodium dodecyl sulfate, which has a synergistic effect and inactivates microorganisms at a much lower concentration than if either of the compounds had been added separately.

AGFD 209 Natural and value-added antimicrobials for pathogen control Byron Brehm-Stecher, byron@iastate.edu. Food Sci. and Human Nutrition, Iowa State Univ., Ames There is a critical need for control of human pathogens in foods and in food-processing or related environments. Chemical sanitizers such as chlorine and hydrogen peroxide are widely used in foods such as produce, but industry and consumer interest in "greener" or more "natural" interventions is at an all-time high. This talk will focus on our recent work on development of natural antimicrobial systems for control of E. coli O157:H7 and Salmonella spp. in produce and on collaborative work with materials scientists focused on development of value-added antimicrobial coatings generated from soy, castor and other plant oils. Natural antimicrobial systems capable of inactivating bacterial pathogens in organically complex matrices would provide attractive clean-label solutions for enhancing produce safety. Inexpensive and environmentally friendly plant oil-based coatings may find applications in controlling human pathogens in food processing or storage environments or in allied fields, such as in healthcare, where their use may significantly impact the problem of multidrug-resistant microorganisms.

AGFD 210 Effectiveness of food grade antimicrobials for controlling Listeria monocytogenes in/on ready-to-eat meat and poultry products Anna C. Porto-Fett, anna.portofett@ars.usda.gov, John B. Luchansky. US Dept. of Agriculture, Wyndmoor, Pennsylvania Listeria monocytogenes is a foodborne pathogen of particular concern due to its ubiquity and ability to grow/survive in products that are stored at
refrigeration temperature and consumed without further cooking, such as ready-to-eat (RTE) meats. Thus, further research is warranted to evaluate the effectiveness of selected food grade antimicrobials to better manage *L. monocytogenes* presence, levels, and/or persistence during manufacture and extended storage of high risk/high volume RTE meats. Our group has conducted inoculated package challenge studies to determine the viability of *L. monocytogenes* on a variety of commercially-prepared RTE meats, such as deli-style ham, sliced turkey breast, frankfurters, and roast beef. Products were formulated with food grade antimicrobials, such as potassium lactate, sodium diacetate, potassium acetate, potassium propionate, potassium levulinate, or buffered vinegar, alone or in combination, at regulatory allowable concentrations varying from 0.1 to 3.0%. Each individual package/slice was surface inoculated with a five-strain cocktail of *L. monocytogenes* to achieve a target level of ca. 3.0 to 4.0 log CFU and then surface treated or not treated with lauric arginate. Next, packages were vacuum sealed and stored for up to 180 days at 4°C in a temperature-controlled incubator. Regardless of the product, in the absence of any added antimicrobials, *L. monocytogenes* numbers increased by ca. 4.0 to 6.0 log CFU during extended refrigerated storage. However, depending on the product and antimicrobial type and concentration, we observed reductions of about 0.5 to 2.0 log CFU and/or in some instances pathogen outgrowth was prevented during the extended refrigerated storage. Collectively, these studies validated that inclusion of food grade organic acids as an ingredient would effectively control *L. monocytogenes* on RTE meats, and as a result, lessen the occurrence, risk, and severity of listeriosis associated with consumption of contaminated RTE meats in an event of post process contamination.

**AGFD 211 Improve microbial food safety of fresh fruits and vegetables with aqueous and vapoorous essential oils** Xuetong Fan1, xuetong.fan@ars.usda.gov, Changqing Wu2,3. (1) ARS, USDA, Wyndmoor, Pennsylvania (2) Dept. of Animal and Food Sci.s, Univ. of Delaware, Newark (3) Center for Food Safety and Security Systems, UMD, College Park, Maryland (UMD), College Park (2) Center for Food Safety and Security Systems, UMD, College Park, The phenolic extract of blueberry pomace (byproducts), a natural antibacterial component, is uniquely capable of complete elimination of several bacterial pathogens including *Salmonella enterica*, *Campylobacter jejuni*, *Listeria monocytogenes*, and meticillin resistant *Staphylococcus aureus* (MRSA) and their biofilm. In addition, this natural antibacterial phenolic blueberry pomace extracts (PBPE) can restore the antibacterial activity of several inactive antibiotics including meticillin and erythromycin. The major reason of the inability of current available antibiotics to kill MRSA and other biofilm forming bacteria is failure of target bacterial cells within a biofilm. Researchers reported that biofilms contain heterogeneous bacterial cell populations of multiple phases, slow or no growing and persistent cells with rigid cell wall, which are highly tolerant to kill by traditional antibiotics. Many bactericidal antibiotics require penetrating cell wall to be corrupted in order to kill. Biofilm forming bacterial pathogens are protected from the traditional antibiotics due the failure of penetrating cell wall. The PBPE can increase the hydrophobicity and auto-aggregation of several bacterial pathogens. Further, PBPE is anti-oxidogenic and anti-inflammatory. In this presentation, the possible application of PBPE in pre- and post-harvest food production and its benefits will be narrated.

**AGFD 212 Berry pomace extracts in enhancing microbial food safety** Debabrata Biswas1,2, dbiswas@umd.edu. (1) ANSC, Univ. of Maryland (UMD), College Park (2) Center for Food Safety and Security Systems, UMD, College Park, The phenolic extract of blueberry pomace (byproducts), a natural antibacterial component, is uniquely capable of complete elimination of several bacterial pathogens including *Salmonella enterica*, *Campylobacter jejuni*, *Listeria monocytogenes*, and meticillin resistant *Staphylococcus aureus* (MRSA) and their biofilm. In addition, this natural antibacterial phenolic blueberry pomace extracts (PBPE) can restore the antibacterial activity of several inactive antibiotics including meticillin and erythromycin. The major reason of the inability of current available antibiotics to kill MRSA and other biofilm forming bacteria is failure of target bacterial cells within a biofilm. Researchers reported that biofilms contain heterogeneous bacterial cell populations of multiple phases, slow or no growing and persistent cells with rigid cell wall, which are highly tolerant to kill by traditional antibiotics. Many bactericidal antibiotics require penetrating cell wall to be corrupted in order to kill. Biofilm forming bacterial pathogens are protected from the traditional antibiotics due the failure of penetrating cell wall. The PBPE can increase the hydrophobicity and auto-aggregation of several bacterial pathogens. Further, PBPE is anti-oxidogenic and anti-inflammatory. In this presentation, the possible application of PBPE in pre- and post-harvest food production and its benefits will be narrated.

**AGFD 213 Olive leaf extract inhibits growth and biofilm formation in *L. monocytogenes*** Yanhong Liu, yanhong.liu@ars.usda.gov, Lindsay McKeever, Nasir Malik. Molecular Characterization of Foodborne Pathogens Research Unit, ERRC-ARS-USDA, Wyndmoor, Pennsylvania Olive extract has been used as a traditional herbal supplement since it contains polyphenolic compounds with a wide range of beneficial properties ranging from promoting increased energy and healthy blood pressure, supporting the cardiovascular system and the immune system. In addition to the beneficial effects, olive extract also has antimicrobial effects. The aim of this work was to investigate the antimicrobial effect of olive extract against *Listeria monocytogenes*, which is a major foodborne pathogen. Our results demonstrated that olive extract inhibited the growth of *Listeria monocytogenes*. The effects of olive extract against biofilm formation of *L. monocytogenes* were measured using a crystal violet assay. Our results showed that the olive extract inhibited biofilm formation and reduced the swimming motility of *L. monocytogenes*. Since biofilm formation is a serious problem for the food industry, olive extract, as a natural product, has the potential to be used as a food additive to control *L. monocytogenes* in food.

**AGFD 214 Chemical synthesis of optically pure rhizopines: Steps towards engineering a synthetic symbiosis between bacteria and crops** Amelie M. Joffrin1, ameliejoffrin@live.co.uk, Barney Geddes1, Hitesh Sangane1, Vikki Fleming1, Philip Poole2, Stuart J. Conway2. (1) SASS9 Mereside, AstraZeneca, Cheshire, UK (2) Dept. of Chemistry, Univ. of Oxford, UK (3) Plant Science Dept., Univ. of Oxford, UK In agriculture addressing crop productivity while ensuring sustainability has become crucial. Despite this, with nitrogen as the major limiting nutrients for efficient crop growth, unsustainable nitrogen fertilisers are still being extensively used. Leguminous plants form a symbiotic association with diazotrophs called Rhizobia. Rhizobia resides in legume root nodules, and converts atmospheric nitrogen into its biologically accessible form. Therefore, engineering a synthetic nitrogen-fixing symbiosis between Rhizobia and crops, such as corn and wheat, would lead to more sustainable agriculture. One major challenge is ensuring that symbiotic bacteria are able to efficiently colonize crop roots. In addition, Rhizobia should acquire sufficient carbon to energise nitrogen fixation. Rhizopines (+)-5, (−)-5 and 6, are uniquely able to mediate the growth of Rhizobia, facilitating the formation of a symbiotic relationship. Engineering rhizopine synthesis in crops therefore represents an exciting target for enhancing productivity and sustainability. We aim to characterise the biosynthetic and catabolic pathways of rhizopines. This can only be achieved using synthetic rhizopines (+)-5, (−)-5 and 6. We have thus completed the first enantioselective synthesis of (+)-5 and (−)-5, starting from myo-inositol 1. Both enantiomers were synthesised, in 13 steps via racemic triol (+)-2, using a novel diastereoisomeric protection-resolution strategy. This route was also applied to the synthesis of 6. Chemically
synthesised rizopines (+)-5 and 6 were used as standards in GC–MS studies to gain further insight into the biosynthetic pathway towards 5. A new biosynthetic pathway was therefore proposed. In addition, synthetic SI 6 was shown to serve as a sole carbon and nitrogen source for Rhizobia. Finally, using the enantiomerically pure Rhizopines synthesised, the natural enantiomer of 5 will be identified.

AGFD 215 Engineering a bypass of 1-deoxyxylulose-5-phosphate synthase in *Escherichia coli* for the conversion of pentose sugars to isoprenoid chemicals and biofuels Jason R. King, abmiramor@gmail.com, Benjamin M. Woolston, Gregory Stephanopoulos. Chemical Engineering, Massachusetts Inst. of Tech., Cambridge Despite significant advances in the microbial conversion of plant biomass to simple alcohol biofuels via microbial engineering, several challenges remain in the industrial conversion of lignocellulose to bio-based chemicals and drop-in replacements of gasoline for transportation energy. With regards to lignocellulosic feedstocks, the co-utilization of pentose and hexose sugars in plant hydrolysate to sustain growth and chemical production in genetically tractable microbes is a major challenge to the field. Likewise, the sufficient capture of this energy into valuable chemicals and so-called advanced biofuels at high productivity and titer remains elusive. Here we engineered the metabolism of *Escherichia coli* K12 strain MG1655 to produce 1-deoxyxylulose-5-phosphate (DXP) from D-arabinose while bypassing the native enzyme DXP synthase (or DXS). A *de novo* bypass of DXS for DXP synthesis has, to our knowledge, not been reported and promises to allow increased carbon flux into the isoprenoid pathways of the cell, which in turn allows for production of mid-sized alcohols (C5-C10) or hydrocarbon biofuels and high-value isoprenoids common in fragrances and medicines.

AGFD 216 Genetically programmed functional bacterial biofilms Ebuzzer Kalyoncu1,2, ebuzzer.kalyoncu@bilkent.edu.tr, Tolga T. Olmez1,2, URARTU SEKER1,2. (1) Bilkent Univ., ANKARA, Turkey (2) UNAM, Ankara, Turkey Biofilm engineering is an emerging field of synthetic biology for the design of functional bionano-interfaces. *Escherichia coli*, Bacillus subtilis and Pseudomonas aeroginosa are among the bacteria that attach to surfaces and form biofilms through the expression of curli-related proteins. E. coli produces curli proteins with two structural components, the major subunit csgA and minor subunit csgB proteins. The csgB subunit helps the csgA subunit to stack on top of each other and form fibrous superstructures. We aimed to control the morphology, mechanical properties and electrical properties of the amyloid nanofibers to be utilized as new generation of protein based materials. We used native and functionalized curli subunits to produce electrodynamically curli fibers in bacteria. Anhydrotetracycline-inducible riboswitches were used to control the expression of curli subunits, allowing the on-demand synthesis of protein-based bio-nanomaterials at the biotic/abiotic interface with desired functionalities such as controlled electrical conductivity and controlled mechanical properties. We also built AND, A NIMPLOY B, B NIMPLOY A and NOR logic gates to control the expression of curli subunits and the morphology of curli nanofibers. Initial studies with aromatic acid functionalized scaffold peptides guided us for the modified versions with aromatic amino-acid insertions of curli nanofibers for bio-conductive structures. Following the selection of the most conductive aromatic aminoacid residues we achieved peptide insertions into the curli nanofiber monomeric protein CsgA inspired by conductive Geobacter metallidurans PilA protein. We kindly thank to TUBITAK 115Z217 and 114M163 for its support and funding.

AGFD 217 Novel combination of megaTAL nuclease-driven genome engineering with a drug selection cassette increases efficiency of HIV gene therapy Biswajit Paul1, bish@uw.edu, Hans-Peter Kiem2. (1) Univ. of Washington, Seattle, Washington (2) Fred Hutch Cancer Consortium, Seattle, Washington Human Immunodeficiency Virus (HIV) infection remains a substantial health problem worldwide. The human C-C chemokine receptor 5 (CCR5) gene, which encodes a co-receptor required for HIV entry into CD4+ T cells, is a promising alternative therapeutic target. Early clinical trials using CCR5-disrupting nucleases in patients are promising, with the exception of two limitations: (a) a need for higher levels of CCR5-disruption and (b) preferential selection of gene modified cells. The CCR5-targeting megaTAL is a nuclease architecture that combines a LAgLIDAGD homing endonuclease scaffold with an eleven repeat transcription activator-like (TAL) effector array to achieve efficient site-specific cleavage. We are coupling megaTAL nuclease treatment with drug selection in order to disrupt the CCR5 locus and select modified CD4+ T-cells. The mutant human dihydrofolate reductase (DHFR) construct renders cells resistant to lymphotoxic concentrations of the drug methotrexate (MTX) at 0.02 µM. For optimal cell viability we deliver nucleases via mRNA and selection-constructs via adeno-associated virus (AAV). Electroporation with megaTAL mRNA demonstrated robust CCR5 disruption: 95% in *GHOST* null modified cells and 70-90% in human CD4+ T-cells. Gene-modified human T-cells were transplanted into NOD/SCID/γc-null ‘humanized’ mice and subsequently challenged with HIV-1 infection. CCR5-null modified cells preferentially survived during active HIV infection in vivo (100-fold increase). Initially, the HIV plasma viremia was significantly lower in the nucleus-treated mice. However, the virus levels rebounded over time. We hope to address this by selectively transplanting cells that have been CCR5 disrupted to achieve therapeutically relevant levels of HIV-protected cells. In our preliminary experiments, primary T-cells lentivirally transduced with a Tyr-22-DHFR cassette at 15% efficiency showed an enrichment of >90% over 7 days in 0.02 µM methotrexate. More recently, we have demonstrated AAV-mediated targeted gene insertion followed by chemoselection and reached >50% enriched populations of human CD4 T-cells. The CCR5-megaTAL nuclease platform produces very high levels of gene-modified CD4+ T-cells and protects these cells from subsequent HIV infection in vivo. We are able to knock-in a selection cassette at the CCR5 disruption-site and specifically enrich for gene-modified cells.

AGFD 218 Analysis of the everninomicin gene cluster and dichlorosoeverninic acid biosynthesis in *Micromonaspora carbonacea* var. *aurantiaca* in pursuit of novel everninomicin analogs Audrey Ynigez-Gutierrez, Audrey.ynigez@vanderbilt.edu, Emilianne M. Limbrick, Brian O. Bachmann. Dept. of Chemistry, Vanderbilt Univ., Nashville, Tennessee The rapid emergence of antibiotic resistant illnesses is a growing threat to human health that could eventually lead to a post-antibiotic era. Currently, there is a renewed interest in not only discovering new antibiotics but also revitalizing previously described scaffolds. One such class of molecules is the everninomicins, complex polysaccharides produced by *Micromonaspora carbonacea* var. *aurantiaca*. They contain a number of unique structural features, such as orthoester linkages, a methylenedioxy bridge, a dichlorosoeverninic acid moiety, and a nitro sugar. During previous development, the everninomicins showed strong activity against antibiotic resistant strains of bacteria via inhibition of protein translation. However, the everninomicins’ development was hindered by an inability to access analogs via total synthesis or semi-synthetic methods. We propose to derivatize the everninomicins using the natural biosynthetic machinery via genome editing to develop novel analogs with increased antibacterial potency. All natural everninomicin analogs contain at least one iterative type I polyketide synthase (PKS)-derived dichlorosoeverninic acid (DCE) moiety. This conserved functionality’s biosynthesis and role in activity are poorly understood. In order to
elucidate everninomicin biosynthesis, the four genes associated with DCE biosynthesis will be deleted using methods specifically designed to avoid disruption of the overall everninomicin gene cluster. The enzymes will also be biochemically characterized and their substrate specificity explored to evaluate the incorporation of non-natural substrates. Genomic editing and incorporation of non-natural substrates will allow for investigations into the ability of M. carbonacea var. aurantiaca to produce everninomicin analogs with diversified everninomic acid moieties containing bulkier alkyl groups or non-chlorine halogens. Analogos properly designed with useful synthetic handles could eventually be utilized for coupling reactions to increase everninomicin potency and study ribosomal inhibition. The proposed genetic manipulations and enzymatic studies will elucidate the biosynthesis of everninomcins and provide novel analogs in an attempt to revitalize this potent class of antibiotics.

AGFD 219 It is about safety Vic C. Knauf, vic.knauf@arcadiabio.com. Arcadia Biosciences, Seattle, Washington In general, the first set of questions relating the chemistry and safety of a GMO-derived crop are whether the GMO food or feed source has the equivalent chemical composition of the original crop source, other than the intended effect of the genetic change. The second set of questions focuses on any unintended consequences directly or indirectly resulting from the novel and intended change made in a GMO crop plant. A third aspect meant to relate the chemistry with the safety of a GMO food can rely on a precautionary principle that one cannot predict all of the long-term consequences that might happen with a GMO crop source of food or feed. Application of the precautionary principle effectively has reduced the number of GMO crops commercialized by adding significant cost and time requirements that are only met by a small number of applicants. Whether these approaches have increased food safety; whether these methods have ever failed to protect the consumer; and whether these approaches have unfortunately resulted in stifling a safe and sufficient global food supply are subjects for discussion.

AGFD 220 Synergism between sulforaphane and luteolin in anti-inflammation Kanyasiri Rakarityatham, krakarity@foodsci.umass.edu, Xian Wu, Hang Xiao. UMass, Amherst The interaction between different bioactive food components may play important roles in the health effects of whole foods when different bioactive components are consumed together. Sulforaphane and luteolin have been shown to have anti-inflammatory property. Herein, we determined the combination effects of sulforaphane and luteolin in inhibiting inflammation in lipopolysaccharide (LPS)-stimulated RAW 264.7 macrophages. Both sulforaphane and luteolin showed dose-dependent inhibition on LPS-induced production of nitric oxide (NO) in the macrophages. The combined treatments with sulforaphane and luteolin led to stronger inhibition on NO production in comparison with the singular treatments with sulforaphane and luteolin. Isobologram analysis confirmed that the combined treatments produced synergy between sulforaphane and luteolin. Western blotting showed that the combined treatment reduced the expression levels of pro-inflammatory proteins such as inducible nitric oxide synthase, phosphorylated-IkB, and cyclooxygenase 2 in LPS-treated macrophages. ELISA results demonstrated that sulforaphane and luteolin combination caused significant reduction of inflammatory cytokines, interleukin-1 and interleukin-6. Moreover, the combination treatments reduced reactive oxygen species in cells and increased the expression level of heme oxygenase-1, an antioxidative protein. In conclusion, our findings support the notion that certain bioactive food components may act synergistically to produce enhanced health effects such as anti-inflammation. (This work was partly supported by funds from USDA).

AGFD 221 3-MCPD 1-palmitate induced tubular cell apoptosis via JNK/P53 pathways Guoren Huang1, huangguoren@sjtu.edu.cn, Man Liu1, Weiying Lu1, Xiangjun Sun1, Liangli Y. Yu2. (1) Inst. of Food and Nutraceutical Science, School of Agriculture and Biology, Shanghai Jiao Tong Univ., Shanghai, China (2) Univ of Maryland, College Park 3-MCPD esters are a group of processing-induced food contaminants with nephrotoxicity, but the molecular mechanism remains unclear. This study investigated the role of JNK/p53 pathway in 3-MCPD 1-palmitate (MPE)-induced nephrotoxicity in Sprague-Dawley rats. Microarray analysis of the kidney from the Sprague-Dawley rats treated with MPE using Gene Ontology categories and KEGG pathways, revealed that MPE altered mRNA expressions of the genes involved in the MAPK (JNK and ERK), p53 and apoptotic signal transduction pathways. The changes in the mRNA expressions were confirmed by qRT-PCR and western blot analyses, and were consistent with the induction of tubular cell apoptosis as determined by histopathological, TUNEL and immunohistochemistry analyses. Additionally, p53 knockout attenuated the apoptosis, and the apoptosis-related protein bax expression and cleaved caspase-3 activation induced by MPE in the p53 knockout C57BL/6 mice, whereas JNK inhibitor SP600125 inhibited MPE-induced apoptosis while ERK inhibitor U0126 did not function. Furthermore, the knockdown of p53, JNK1, JNK2, or JNK3 via shRNA transfection in NRK-52E cell significantly decreased the protein levels of caspase 3 and bax/bcl2 ratio, indicating the important role of p53 and JNK in the MPE induced apoptosis. In conclusion, the present study provided evidences that MPE may induce apoptosis via activation of JNK/p53 pathway. The results from this study may advance our understanding of the molecular mechanisms involved in the nephrotoxicity induced by 3-MCPD fatty acid esters and lay foundation for safety evaluation of 3-MCPD fatty acid esters.

AGFD 222 Functional analyses on antioxidant and anti-inflammatory effects of polyphenols extracted from a chinese bitter tea (Ilex latifolia thunb) Tiqiantian Zhang1, ttzhang89@hotmail.com. (1) Food Sci., Rutgers Univ., New Brunswick, New Jersey (2) Food Sci. and Tech., South China Univ. of Tech., Guangzhou, Guangdong, China Consumption of plant foods has been negatively associated with the risk of developing chronic diseases, which is partly attributed to their rich and diverse phytochemicals. To promote the rational and effective application of Ilex latifolia Thunb., a Chinese bitter tea widely consumed as a health beverage, polyphenols were extracted from its leaves and their cellular antioxidant activity (CAA) and anti-inflammatory effect against mouse macrophage RAW 264.7 cells were analyzed. Polyphenols from I. latifolia were mainly caffeyloquinic acid derivatives, including chlorogenic acid; 3,4-di-caffeoylquinic acid; 3,4-di-O-caffeoylquinic acid methyl ester; 3,5-di-O-caffeoylquinic acid methyl ester. Results showed that the antioxidant capacity of polyphenols was high, and their CAA values in PBS wash and no PBS wash protocols were 6871.42 ± 85.56 and 25161.61 ± 583.55 μmol QE (quercetin equivalents) /100 g phenolic extracts, respectively. In addition, polyphenols from I. latifolia displayed strong inhibition on LPS-induced NO-production in RAW 264.7 cells. Polyphenols treatment inhibited the release of pro-inflammatory cytokines (TNF-α, IL-1β and IL-6) induced by LPS in a dose-dependent manner by ELISA and mRNA expression analysis. Western blot results showed that the anti-inflammatory activity of polyphenols from I. latifolia might be exerted through inhibiting the activation of MAPKs (ERK and JNK) and NF-κB to decrease NO, and pro-inflammatory cytokines production. Thus, the polyphenols enriched extracts from I. latifolia are good source of natural antioxidants with a beneficial effect against inflammation, and they may be applied as food supplement and/or functional ingredient.
AGFD 223 Role of cell walls in controlling the release and bioaccessibility of polyphenols from raw compared to processed apples
Dongjie Liu1, djiu0827@gmail.com, Michael J. Gidley2, Patricia Lopez-Sánchez1, (1) QAAFI, the Univ. of Queensland, Brisbane, Australia
(2) Food Sci., Swedish Univ. of Agricultural Sciences, Uppsala, Sweden. Apples are rich in phenolic compounds with potential roles in health promotion and disease prevention. To exert their bioactivity, they must first be released from apple cells through mechanical forces or processing and transported to the target sites for potential uptake. This bioaccessibility is a useful prediction tool to assess the nutritional efficiency. Plant cell walls have been identified as a critical factor in influencing polyphenol bioaccessibility by interactions. However, studies of polyphenol bioaccessibility have been limited to either fresh fruits or vegetables or processed food. The aims of this study are to identify the process conditions i.e. temperature, pH, time required for polyphenol release from cells and the role of cell walls in re-distribution of polyphenols, as well as the subsequent interactions between polyphenols and cell walls that can affect the bioaccessibility of polyphenols. To investigate the release of polyphenols in apples, the cell wall and membrane of apples subjected to different processing conditions were fluorescently labelled, and together with auto-fluorescent polyphenols were observed using a confocal laser scanning microscope. The results revealed that processing led to the release of polyphenols from cells and the released polyphenols accumulated primarily on cell walls subsequently. The interactions between polyphenols and cell wall polysaccharides were confirmed by using bacterial cellulose as a plant cell wall model. The associations were slightly decreased by hydrothermal processing, but strongly reduced by dehydration processing. This result highlighted the importance of water in maintaining an open and swollen network favoring polyphenol adsorption. Plant cell walls act as physical barriers at the beginning of polyphenol digestion and modulate their release from plant tissues under digestive tract conditions. Processing (mechanical, thermal, pH) initially promotes the release of polyphenols from intracellular compartments, thus increasing the contact with cell walls. Typical food processing conditions, particularly dehydration, caused changes in the structure and properties of cellulose and cell walls that regulated their interactions with polyphenols.

AGFD 224 Redox active antioxidants increase chemical stability and biological function of curcumin
Weicang Wang, weicangwang@umass.edu. Food Sci., Univ. of Massachusetts-Amherst. Curcumin, a major bioactive polyphenol from turmeric, has received increasing attention as a dietary supplement in anti-cancer therapy. However, poor chemical stability of curcumin limits its clinical application. Here, we show redox active antioxidants increase the chemical stability of curcumin, which contributes to enhanced anti-cancer effect of curcumin. In colorimetric assay, a series of redox active antioxidants, including ascorbate, tert-butyldihydroquinone (TBHQ), gallic acid, rosmarinic acid, and Trolox, greatly increase the stability of curcumin in phosphate buffer at physiological pH. In particular, co-addition of ascorbate leads to a >200-fold increase in half-life of curcumin from ~10 minutes to 48 hours. Moreover, converting the radical-initiating phenolic group to methoxy group significantly increases curcumin stability, supporting a redox-dependent phenolic radical mechanism in curcumin degradation. In MC38 colon cancer cells, co-addition of ascorbate or Trolox enhances the anti-proliferation effect of curcumin, from 20% to 40-80% growth-inhibition, due to increased stability of curcumin in serum-free medium. Finally, co-administration of TBHQ leads to 6-fold increase in the circulating level of curcumin in mice, suggesting redox active antioxidant increases stability of curcumin in vivo. Together, our results demonstrate redox active antioxidants increase the chemical stability and biological function of curcumin in vitro and in vivo, which provides a practical strategy to develop more effective curcumin-based therapeutics.

AGFD 225 Enhancing bioavailability of lipophilic nutraceuticals in natural food: Excipient emulsion design
Ruojie Zhang1, ruojiezhang.umass@gmail.com, David McClements1, David McClements1 (1) UMASS Dept of Food Sci, Amherst (2) Food Sci., Univ. of Massachusetts Amherst. The oral bioavailability of many lipophilic nutraceuticals from natural food products is limited due to various physicochemical and physiological processes: poor release from food matrices; low solubility in gastrointestinal fluids; metabolism or chemical transformation within the gastrointestinal tract; low epithelium cell permeability. The excipient emulsions were specifically designed to enhance the bioavailability of these lipophilic nutraceuticals by controlling their release, solubilization, transport, metabolism, and absorption within the gastrointestinal tract. The purpose of this research is to highlight the major factors that limit the oral bioavailability of hydrophobic bioactive agents from fruits and vegetables, and then to describe how excipient emulsions can be developed to overcome these hurdles. This knowledge could be used to develop a new range of excipient food products specifically designed to increase the bioavailability of bioactive agents from natural products (such as fruits, vegetables, cereals, meats, or fish), e.g., excipient sauces, dressings, dips, creams, or beverages.

AGFD 226 Impact of harvest time and switchgrass cultivar on conversion to sugars and pyrolysis oils using biochemical and thermochemical routes
Michelle Serapiglia1, michelle.serapiglia@ars.usda.gov, Charles A. Mullen1, Akwasi Boateng1, Bruce S. Dietz1, Michael Casler2, (1) Sustainable Biofuels and CoProducts, USDA – Agricultural Research Service - Eastern Regional Research Center, Lansdale, Pennsylvania (2) US Dairy Forage Research Center, USDA-ARS, Madison, Wisconsin. Switchgrass (Panicum virgatum L.), a perennial grass native to much of North America, is undergoing development as a dedicated energy crop. The nutritional, environmental and harvest time and switchgrass cultivars, replicated trials across three sites (Arlington, WI, Marshfield, WI, and Urbana, IL) were established in 2009. The switchgrass cultivars were harvested once annually at upland peak, after killing frost, or post-winter in the spring for each growing season. Samples were processed using the biochemical or thermochemical routes for conversion to sugars and bio-oils, respectively. Near-infrared reflectance spectroscopy models were developed and utilized to characterize biomass traits and conversion potential among the cultivars. Mineral content was found to be highest in the biomass harvested at upland peak and decreased as harvest was delayed. Relative cell wall polymer content (i.e., hemicellulose, cellulose, and lignin) increased for the biomass as harvest was delayed. Changes in biomass yield and composition and their impacts on enzymatic sugar and potential ethanol yields and fast pyrolysis product yield will be presented and discussed.

AGFD 227 Impact of selected phenolics on the quality and health aspect of cookie
Yuanning Ou, u3003343@connect.hku.hk, Mingfu Wang. The Univ. of Hong Kong. Phenolic compounds have the reputation to promote our health and inhibit the formation of food toxincants. They are often used as food ingredients and incorporated into food. However, limited study reported the chemical and bioactivity changes of
phenolics in food processing. Maillard reaction is one of the most important chemical reactions occurring under thermal conditions, which can help to produce desirable color, taste, and aroma while also produce hazardous substances. Our previous study has confirmed that some phenolics such as naringenin can participate in the Maillard reaction and give rise to some human beneficial adducts. In this study, rosmarinic acid and resveratrol, two kinds of phenolics possessing high antioxidant, antibacterial and anticancer activity, were incorporated into the cookie dough and their impact on the quality of cookies and antioxidant activity were analyzed. The results indicated that after the addition of phenolics, the cookie color is darker and the fragility is decreased. In the meantime, they degraded at different level, rosmarinic acid was much more stable than resveratrol under thermal treatment. The antioxidant activity in the cookies with the addition of these two antioxidants increased compared to phenolics with or without heating, possibly due to the formation of new chemicals through different chemical reactions during the baking process. Besides, we also discovered that they showed anti-glycation effect against the formation of fluorescence AGEs. Further detailed investigations about the chemical and bioactivity changes are still ongoing.

AGFD 228 Effect of cluster sunlight exposure on rotundone concentration in Noiret grapes and wine

Lauraj A. Homich1, laura.homich@gmail.com, Ryan J. Elias2, Michela Centinari2, Justine Vandenh Heuvel3. (1) Dept. of Food Sci., The Pennsylvania State Univ., Univ. Park (2) Dept. of Plant Science, The Pennsylvania State Univ., Univ. Park (3) Dept. of Plant Science, Cornell Univ., Ithaca, New York. It is generally recognized that wine quality begins in the vineyard; therefore, it is important to understand how the vineyard environment and management techniques impact the development of specific compounds which contribute to, or detract from, perceived wine quality. The aroma impact compound rotundone was recently identified as the main contributor to the spicy, black pepper aroma in many grapes, wines, herbs, and spices. While the mechanism of rotundone development remains unknown, it has been observed that mesoclimate plays an important role. In addition, studies have suggested that viticultural practices, such as leaf removal, may be a useful tool for manipulating rotundone concentrations and therefore black pepper character in wines. This study aims to: 1) determine if and how the timing and duration of cluster sunlight exposure affect rotundone concentration and 2) understand how these treatments impact perceived black pepper aroma intensity in the resulting wines. The effect of leaf pulling treatments on rotundone concentration was monitored through vine canopy density and fruit microclimate measurements. Rotundone content and the dynamics of its development in the fruit were assessed using SIDA SPE-SPME-GCMS. Rotundone concentrations in wine were plotted against the perceived black pepper aroma intensities by sensory descriptive analysis to determine if a correlation exists. The 2014 vintage showed no differences in fruit rotundone concentrations at harvest with non-detectable concentrations prior to veraison. These observations may have resulted from insufficient leaf pulling to allow for differences in light intensity reaching the fruiting zone. The light and canopy density measurements showed more pronounced differences for the 2015 vintage. This resulted in significantly different (p < 0.10) rotundone concentrations in the sun exposure treatments with greater concentrations arising when sun exposure was maintained throughout the fruit ripening period.

AGFD 229 Antimicrobial and antioxidant activities of lignin from corn stover residue

Mingming Guo1, mingguo@udel.edu, Changqing Wu2, Tony Jin1, Nhuon Nghiem1, Xuetong Fan1, Phoebe X. Qi3, Chan Ho Jang3, Lingxiao Shao1. (1) USDA-ARS-ERRC, Wyndmoor, Pennsylvania (2) Dairy and Functional Foods, USDA-ARS-ERRC, Wyndmoor, Pennsylvania (3) Animal and Food Sci.s, Univ. of Delaware, Newark. Introduction: Corn stover is a good source for biomass-to-ethanol production. However, the process also produces lignin, which has traditionally been burned as fuel to produce energy. To improve the economic viability of biofuel production from biomass, the improvement in lignin quality is a current priority. Purpose: The objective of this study was to investigate the antimicrobial and antioxidant activities of the lignin extracted from corn stover residue. The extraction was conducted using low moisture anhydrous ammonia in alkaline pretreatment condition, followed by enzymatic hydrolysis to remove residual carbohydrates. Method: Corn stover residue were extracted using low moisture anhydrous ammonia (LMAA) pretreatment process, followed by enzymatic hydrolysis. The extracted lignin was prepared using alkaline extraction at various temperatures (20°C, 50°C), extraction time (60, 120 min) and residue/solvent ratios (1/4, 1/8). The optimal extraction conditions that favored high lignin yield, while preserving its antimicrobial and antioxidant activities were determined. The estrogenic property of lignin extracts was also evaluated. All lignin extracts were characterized using FTIR to determine the relationship of lignin structure and its antioxidant/antimicrobial activity. Results: Lignin extracted exhibited strong antioxidant and antimicrobial activities against Listeria innocua. The optimum extraction condition, which resulted in the highest antimicrobial and antioxidant activities of lignin, was determined to be at 50°C, 120 min, and 1/8 residue to solvent ratio using 4% sodium hydroxide. At this extraction condition, 33.92 g lignin was obtained from 100 g of corn stover residue. All lignin extracts had minimal estrogenic impacts when tested using MCF-7 cell proliferation assay, as shown by the results that 10 µg/mL extracts having similar effects as 100 fM of 17β-estradiol. Moreover, the antimicrobial and antioxidant activities of lignin extracts were consistent to the lignin structure, as determined using FTIR analysis. Significance: This study provides an innovative approach to develop antimicrobial and antioxidant applications of lignin from corn stover residue, which can increase the economic outlook of the biomass-to-ethanol process.

AGFD 230 Restoring herbicide control in multiple herbicide resistant black grass (Alopecurus myosuroides)

Maria C. Schwarz1, maria.schwarz@durham.ac.uk, Patrick G. Steel1, Ehmke Pohl2, Glynn Mitchell2. (1) Durham Univ., Durham, UK (2) Syngenta, Bracknell, UK. Over the last 40 years there has been a dramatic increase in the frequency and diversity of herbicide resistant weed biotypes, which poses a substantial threat to the sustainability of agriculture both locally and globally and, with the growth in global population leading to increasing demands for food production, to food security. Modern agriculture couples the management of invasive weed species with enhancing crop yields through the intensive use of herbicides. Many of the most problematic weeds including black grass, one of the most damaging weeds of winter cereals, have now evolved multiple herbicide resistance (MHR), which is associated with an enhanced ability to detoxify xenobiotics, enabling the weed to survive herbicide application irrespective of the mode of action. Black-grass populations showing MHR, exhibit an upregulation in the expression of a specific phi-class glutathione transferase (AmGSTF1), which is thought to have a direct regulatory control on metabolism. The importance of AmGSTF1 in MHR has been confirmed both genetically by transgene experiments and chemically through inhibition experiments (Figure 1). This offers the opportunity to develop potential herbicide synergists, which are active towards AmGSTF1 and restore herbicide control in multiple herbicide resistant black grass. Recently a new class of AmGSTF1 inhibitors, derived from flavonoids, could be identified. Considering the rapid spread of MHR in grass weeds and the limited development of new herbicides, synergists offer an important alternative strategy in counteracting resistance in the field.
AGFD 213 - Withdrawn

AGFD 232 Multi-year ambient air monitoring network to measure multiple pesticides in various California agricultural communities: 2011-2015 sampling results Atac Tuli, Edgar Vidrio, Edgar.Vidrio@cdpr.ca.gov, Pamela Wofford, Randy Segawa. California Dept. of Pesticide Regulation, Sacramento, California In February 2011, the California Dept. of Pesticide Regulation (DPR) implemented a multi year statewide Air Monitoring Network (AMN) to measure pesticides in various agricultural communities. This AMN is the first multi year air monitoring study conducted by DPR and to our knowledge, the first air monitoring network designed to continuously measure for 30+ pesticides for multiple years. The goals of the AMN are to provide data that assists in assessing potential health risks, developing measures to mitigate risks, and measuring the effectiveness of regulatory requirements. As part of the AMN, DPR monitors a total of 37 chemicals (32 pesticides and 5 pesticide breakdown products) in three agricultural communities. Pesticides monitored in the AMN were selected based primarily on potential risk to human health. Higher risk pesticides were prioritized and targeted for monitoring. Higher risk pesticides were identified and prioritized based on higher use, higher volatility, and higher toxicity. DPR evaluated 226 California communities and selected Salinas, Shafter, and Ripon for inclusion in the AMN. No state or federal agency has established health standards for pesticides in air. Therefore, DPR developed health screening levels and regulatory target concentrations for the monitored pesticides to place the results in a health based context. Health screening levels are based on a preliminary assessment of possible health effects, and are used as triggers for DPR to conduct a more detailed evaluation. Regulatory target concentrations are levels that DPR’s legal requirements are designed to stay below and are established after a complete assessment of possible health risks. DPR calculated 24-hour, 4-week, 1 year, and overall average concentrations for all pesticides in the AMN and compared detected concentrations to health screening levels or regulatory target concentrations. Air monitoring results show that most of the pesticides monitored were below levels of health concern. Highest chlorpyrifos and diazinon concentrations were 47% and 74% of screening levels, respectively. Highest concentration for other non-fumigant pesticides was <2% of screening levels. Highest concentrations for the four fumigants included in the AMN (MITC, Chloropicrin, Methyl Bromide, and 1,3-Dichloropropene) were 23% – 175% of screening levels or regulatory targets.

AGFD 233 Hg speciation by different biological processes generation at UV-B and UV-C wavelengths Guoying Chen1, guoying.chen@ars.usda.gov, Buhong Lai2, Ni Mei1, Jixin Liu4, Xuefei Mao1. (1) Eastern Regional Research Center, USDA ARS, Wyndmoor, Pennsylvania (2) Eastern Regional Research Center, USDA, ARS, Wyndmoor, Pennsylvania (3) Shanghai Inst. for Food and Drug Control, Shanghai, China (4) Beijing Titan Instruments, Beijing, China (5) Chinese Academy of Agricultural Sciences, Beijing, China Mercury speciation was accomplished by different photochemical reduction at two UV wavelengths; the resulting Hg0 vapor was quantified by atomic fluorescence spectrometry. After microwave digestion and centrifugation, analyte solutions were mixed with 20% (v/v) formic acid in a reactor coil, and exposed sequentially to narrow-band UV-B fluorescence lamps and a low-pressure UV-C Hg discharge lamp. The signal intensity under each wavelength was linked to Hg0 concentration. This was followed by vacuum or aerobic packaging and storage (4 or 7.2°C, 35 or 20 days). Samples were taken periodically during storage to check for pH, color changes and analyze the microbial populations. Sensory evaluations were performed on ham slices and frankfurters treated with 0.05–0.23% HSA solutions, followed by vacuum packaging and aerobic storage (4.0 or 7.0°C, 30-35 days). HSA could induce maximum reductions of 1.2–1.5 log10CFU/cm2 (P<0.05) in unstressed- and ASA-L. monocytogenes populations on ham slices and frankfurters. During storage, the unstressed-L. monocytogenes populations on HSA-treated ham and frankfurters were 0.5–2.0 log10CFU/cm2 lower (P<0.05) than control samples and those dipped in DI water. The lag-phase of the unstressed-L. monocytogenes population was extended from 3.396–7.125 days (control) to 7.194–10.920 days in the HSA-treated ham and frankfurters. However, the ASA-L. monocytogenes population showed resistance to HSA. Dipping in HSA solution did not adversely affect the color or sensory attributes of ham and frankfurters. These results are useful for helping ready-to-eat meat processors develop operational procedures for applying HSA on ready-to-eat meat products.

AGFD 235 Natural antimicrobials for acid and acidified foods ChangHo Chung1, Howard Haley2, Robert Price3, Fred Breidt3, Fred.Breidt@ars.usda.gov. (1) Dept. of Culinary Science and Food Service Management, Sejong Univ., Seoul, Korea (2) Kalsec Inc., Kalamazoo, Michigan (3) ARS, USDA, Raleigh, North Carolina Sodium benzoate has been widely used as a preservative in fermented and acidified vegetable products. Recently, consumer demand has driven a search for alternatives to benzoate in acid and acidified foods and beverages. We examined commercially available plant extracts, including hop iso-alpha acids, cassia oil, clove oil and garlic oil extracts, singly and with selected combinations, to determine efficacy in preventing spoilage of refrigerated cucumber pickle products by lactic acid bacteria (Lactobacillus plantarum) and yeasts (Zygosaccharomyces globiformis). Our objective was to find extract concentrations that prevented growth of spoilage microorganisms, but had little or no adverse flavor impact for refrigerated pickles. Growth rate data in a cucumber juice medium (pH 6.5) with 0 to 1,000 ppm of selected extracts indicated a hop extract effectively inhibited the growth of a Lactobacillus plantarum strain, while the garlic oil inhibited a Zygosaccharomyces globiformis strain. Acidified cucumber pickles were prepared with 100 mM acetic acid (pH 3.5), using a typical commercial brine formulation in 1.36 L (46 oz) jars. Brines with and without plant extracts or sodium benzoate were inoculated with Lactobacillus plantarum and 5 Zygosaccharomyces globiformis strains at 10^6
CFU/ml (each) and incubated 4C. A hop (5 ppm)-garlic (150 ppm) extract had no evidence of growth (including sugar utilization or acid production) of the microorganisms for up to 2 months, comparable to sodium benzoate treatment, while either ingredient alone (hop or garlic extract) had evidence of growth and turbidity after 1 week. Preliminary data indicates no adverse flavor impact of the hop – garlic extract combination. These data indicate that combined plant extracts may offer an effective means of preservation for pickled vegetable products without the use of sodium benzoate.

AGFD 236 Use of plant-based antimicrobials for enhanced pressure destruction of pathogens in juices Aubrey Mendonca, aubreymen5@gmail.com. Food Sci. and Human Nutrition, Iowa State Univ., Ames Negative consumer perceptions of synthetic preservatives are driving food manufacturers to investigate the use of natural alternatives in microbial food safety and shelf-life applications. To meet the rapidly growing consumer demand for safe, minimally processed foods with “fresh-like” characteristics, several food companies are exploring the effectiveness of natural antimicrobials and “clean technologies” such as high pressure to enhance food safety. This presentation will focus on recent research findings related to: i) the antibacterial effects of two plant-based extracts namely, cinnamaldehyde and geraniol, against Escherichia coli O157:H7 and Salmonella enterica in refrigerated fruit juices such as carrot juice and blackberry juice, and ii) the judicious choice of fruit beverages with naturally strong flavors to mask those of the added antimicrobials. It will also highlight the efficacy of low concentrations of these antimicrobials for increasing the sensitivity of E. coli O157:H7 and S. enterica to high pressure thus permitting the use of far lower pressures to achieve microbial food safety of juices. Additionally, the economic benefits of using those plant-based antimicrobials for meeting consumer expectations of “clean label” foods, increasing industry cost savings from use of lower pressures, lowering equipment maintenance costs, and extending the life of high pressure equipment, will be discussed. Low concentrations of natural antimicrobials combined with high pressure Tech. may have much broader food applications for destroying foodborne pathogenic and spoilage microorganisms while meeting consumer expectations for safe, fresh-like, wholesome food products with no added synthetic preservatives.

AGFD 237 Use of natural antimicrobials with combined non-thermal treatments to control Listeria monocytogenes and Clostridium sporogenes in food systems Monique Lacroix, monique.lacroix@iaf.inrs.ca. Inrs Armand-Frappier/Crma-Cic, Laval, Canada Essential oils and nisin are natural antimicrobial compounds that could be used in food system to reduce or to eliminate the use of synthetic additives. However, these natural antimicrobials are not stable during storage or in contact with food system. The development of microencapsulation methods using alginate or modified alginate have permitted to protect the antimicrobial during storage, to improve the antimicrobial potential of formulations developed and to assure a control release of the active compounds during time. The use of the bioactive coating in combination with three non-thermal treatments (ozone, UV-C and γ-rays) in combination showed that the coating and ozonation showed a high antilisterial effect on broccoli florets for 3 days of storage but the use of the coating and γ-rays ensured microbial safety during the whole storage with a reduction of 2.5 log CFU/g of L. monocytogenes after 13 days of storage. Microencapsulation using alginate in presence of nanocrystalline cellulose (CNC) and γ-irradiation showed a synergistic antimicrobial effect against L. monocytogenes in ready to eat meat (ham). The use of alginate-CNC matrix is an innovative approach to stabilize the emulsion and to protect the active compounds during storage. The use of CNC has permitted the improvement of the physico-chemical properties of the alginate-based-beads and a significant improvement of the bacterial radio sensitization. Microencapsulation with oregano and cinnamon essential oil in combination with nisin showed the highest bacterial radio sensitization by 2.89 and 5 times respectively in ready to eat meat (ham). A formulation based on nisin, nitrite, and organic acids and mixed essential oils has been developed using modeling to eliminate Clostridium sporogenes in sausage. The increase of the concentration of essential oils and organic acids has permitted the reduction of 50% of nitrite and assured an anti-clostridial activity in sausage during storage. However, the use of γ-irradiation in combination was found to be less effective as compared to formulations alone.

AGFD 238 Modeling the impact of the natural antimicrobial citral and high pressure processing on the survival of Escherichia coli O157:H7 and uropathogenic E. coli in ground beef Shih-Yung Chien³, Shioουshu Sheen³, shioουshu.sheeν@ars.usda.gov, Christopher Sommers³, Lee-Yan Sheen³. (1) ARS, USDA, Wyndmoor, Pennsylvania (2) USDA-ARS, Wyndmoor, Pennsylvania (3) Inst. of Food Sci. and Tech., National Taiwan Univ., Taipei Shiga toxin-producing Escherichia coli (O157:H7) and uropathogenic E. coli (UPEC) are common contaminants in meat and poultry and cause disease in humans. To reduce and/or eliminate the risk of E. coli O157:H7 and UPEC, the combined lethal effect of high pressure processing (HPP) and an antimicrobial (e.g. citral) were studied. Ground beef was inoculated with E. coli O157:H7 and UPEC and treated at different HPP (250-350 MPa; 10-20 min) and citral (0.75-1.25 %) conditions using a central composite design. Bacterial inactivation was assessed in terms of logarithmic reductions of E. coli O157:H7 or UPEC. Quadratic equations were developed to describe and predict the reductions of E. coli O157:H7 (R² = 0.93, p<0.001) and UPEC (R² = 0.92, p<0.001). In addition, dimensionless nonlinear models consisting of three impact factors were also developed and compared with the linear models. These models were experimentally validated. Citral enhanced the HPP lethal effect, which may reduce the high pressure level necessary to inactivate pathogenic E. coli in meat, and alleviate the negative effects of high pressure on meat quality. The models may provide the food industry and regulatory agencies a better means to assess the risk associated with E. coli O157:H7 and UPEC in ground meat.

AGFD 239 Development of delivery systems for essential oils and applications for foods and biofilm removal Lynne McLandborough, lm@foodsci.umass.edu. Food Sci., Univ. of Massachusetts, Amherst Essential oils are mixtures of natural plant based antimicrobials with the ability to inhibit growth of a wide range of microbes and at high enough concentrations can destroy pathogens. These compounds also have potential as agents for biofilm remediation, but they are insoluble and non-dispersible in aqueous solution. Therefore, delivery systems are needed for these antimicrobials, which require both high physical stability and antimicrobial efficiency. This talk will focus on a variety of antimicrobial delivery systems including antimicrobial emulsions, micelles and nano-complexes and strategies that can be used to generate stable antimicrobial systems for use in foods and against biofilms in the food processing environment.

AGFD 240 Novel uses of lauric arginate for food preservation: Physical and antimicrobial properties Qiumin Ma, Qixin Zhong, qzhong@utk.edu. Food Sci. and Tech., Univ. of Tennessee, Knoxville Lauric arginate (LAE) is an effective, generally-recognized-as-safe preservative approved for certain food products. Antimicrobial properties of LAE in meat, dairy, and produce products will be briefly
reviewed. Recent studies combining LAE with other food antimicrobials and chelating agents aiming to improve the antimicrobial efficacy will be discussed. The antimicrobial combinations may result in synergistic, additive, or antagonistic activities depending on molecular structures of antimicrobials and cellular structures of bacteria. The last group of studies will be presented for essential oil emulsions prepared with LAE for application in aqueous matrices. Approaches of preparing stable emulsions include the blending of essential oils with non-volatile lipids and the adoption of multiple surfactants. Strategies of stabilizing emulsions can impact antimicrobial properties in microbial growth media and food matrices. Understanding physical and antimicrobial properties of these systems will facilitate the application of LAE to improve the microbiological safety of food products.

AGFD 241 Methods to deliver natural antimicrobials to food Tony Jin, tony.jin@ars.usda.gov. USDA-ARS-ERRC, Wyndmoor, Pennsylvania In recent years, there has been a growing interest in the use of natural or bio-based antimicrobials or preservatives to reduce spoilage microorganisms and foodborne pathogens in food. However, technical challenges exist in incorporating these antimicrobials into food, as there are many different types of food, each has different shape, size, surface characteristics (such as smooth/roughness, hydrophilic/hydrophobic, etc.), and other physicochemical properties (liquid or solid, pH, compositions, etc.), which could significantly influence the effectiveness of an antimicrobial in food. In other words, the same antimicrobial with same dosage that may work on food A may not work on food B. Therefore, developing a method to effectively deliver an antimicrobial to a target food is necessary and important. Nisin is a bacteriocin isolated from Lactococcus lactis and ally Isothiocyanate (AIT) is a major essential oil component of cruciferous plants. This presentation will use nisin as a model for solid antimicrobials and AIT as a model for liquid antimicrobials, and discuss the methods how to deliver them to different types of food and play their antimicrobial roles effectively in extending shelf life and enhancing safety of various foods. Minimizing the loss of their antimicrobial activities during applications will be addressed. Furthermore, advantages and disadvantages of the use of solid or liquid form of antimicrobials will also be compared. Through the case studies in this presentation, some of the key factors that control the effectiveness of antimicrobials will be introduced and discussed.

AGFD 242 Unintended effects associated with GM crops are both expected and low risk Rod Herman, raherman@ dow.com, Wayne Parrott’. (1) Dow AgroSciences LLC, Indianapolis, Indiana (2) Crop and Soil Sciences, Univ. of Georgia, Athens One concern often raised for GM crops is the occurrence of unintended effects. Such unintended effects may result from random DNA modification or might be a direct or indirect consequence of the intended trait. In reality, unintended effects are most often attributable to plant breeding itself, and not specific to GM crops. Conventional breeding has always been accompanied by unintended effects, and plant breeders must always select plant lines without adverse agronomic or anti-nutritional characteristics. GM crops are not immune to these biological realities, although a better knowledge of the mechanisms that underlie GM traits reduces unexpected effects compared with less comprehensively characterized traits selected based on phenotype from non-GM variants or mutants. Extensive experience with unintended effects from both non-GM and GM traits, including pest resistance and herbicide tolerance, suggest low food, feed, and environmental risk.

AGFD 243 Assessing the risks of resistance evolution for transgenic crops for insect control: Capitalizing on successes and learning from mistakes Blair Siegfried, bsiegfried1@ufll.edu. Entomology and Nematology, Univ. of Florida, Gainesville Transgenic plants for insect pest control have become an important component of a number of crop production systems. Resistance management has been and continues to be an important consideration in the registration of transgenic plants expressing protein toxins from Bacillus thuringiensis. In some instances, target pests have remained susceptible to these technologies and even resulted in area wide population suppression. However, instances of field-evolved resistance to Bt crops has increased substantially in recent years and has become a major obstacle to continued success of this technology. Examining the factors that have resulted in both successful and unsuccessful resistance management should provide insight into sustainable approaches to using the technology.

AGFD 244 FDA’s safety evaluation of foods from genetically engineered plants Robert I. Merker, robert.merker@fda.hhs.gov. Office of Food Additive Safety, Food and Drug Administration, College Park, Maryland Developers of new plant varieties have a rich history of introducing new traits into plant varieties using various techniques. By law, food producers are responsible for ensuring that they produce food that is safe and nutritious. The development of bioTech. posed new challenges for government based on the ease of introducing traits from different species into other organisms. In 1992, as part of its response to the Office of Science and Tech. Policy’s Coordinated Framework for the Regulation of BioTech., FDA published a policy that describes the responsibilities of developers of new plant varieties and FDA’s encouragement for them to consult with the agency to ensure the safety and regulatory compliance of their products. Since 1994, FDA has consulted with developers on over 150 varieties. The varieties encompass many vegetables and some fruits, primarily soybeans, corn, cotton, canola, and potatoes, with various traits, predominantly herbicide tolerance and insect resistance. The specific applications of food law to the challenges of genetic engineering are discussed, as well as the types of products, regulatory and scientific challenges, and specific examples from completed consultations.

AGFD 245 Intellectual property issues of GMO food crops Andrew Coates, coatesa@unlv.nevada.edu. Univ. of Nevada, HendersoN Genetically-modified organisms have brought intellectual property (IP) rights into the focus of the agricultural industry. All commercialization hinges on IP rights, and this is no different for transgenic food crops. Research dollars must be recovered with profits in the marketplace. If you cannot assert legal ownership of your crops, then you cannot commercialize your product. IP rights are key to the success – or failure – of genetically-modified agriculture. However, GMO-related IP issues are not just about making a profit, there is also the question of farmers’ rights to their own crops. This paper will provide a brief overview of legislation governing genetically-modified food crops, followed by a survey of legal controversies pertaining to GMOs and IP rights. The necessity (or possible lack thereof) of GMO labeling will also be included.

AGFD 246 Communication of GMO issues to non-technical audiences John Finley, JFinle5@bsu.edu. Louisiana State Univ., Baton Rouge, Louisiana One of the major short comings of the scientific community has been effectively communication of the Tech. and risks associated with GMO foods. Transgenic proteins for drug therapy are well accepted but there remains fear and resistance to GMO foods. Advocacy groups have effectively raised public concern about the dangers of GMOs. As a scientific community we have to find ways to
communicate what GMOs are, why they are produced, the safety and environmental concerns and risks to human health. We need to establish clear language that explains the Tech. in clear non-technical terms while providing assurance about the safety, environmental concerns and health risk issues. The long term benefits to the consumer need to be explained. Comparison to conventional plant breeding, weed control and insect resistance should be carefully described. The reduced use of chemicals and direct gene insertion or blocking can be compared to conventional techniques.

AGFD 247 Filter based approach to rapid and sensitive SERS detection of ferbam in environmental water Siuye Gao¹, siuyeagao@umass.edu, Lili He². (1) Food Sci., Univ. of Massachusetts Amherst, (2) Food Sci., Univ. of Massachusetts-Amherst Surface enhanced Raman spectroscopy (SERS) has been widely applied for rapid and sensitive detection of various chemical and biological targets. Here, we incorporated a syringe filter system into the SERS method to detect pesticide ferbam in water. Silver nanoparticles (Ag NPs) were aggregated by sodium chloride (NaCl) to form nanoclusters that could be trapped in the pores of the filter membrane to from the SERS-active membrane. Then samples were filtered through the membrane. After capturing the target, the membrane was taken out and air dried before measuring by a Raman instrument. After optimization of various parameters, the developed filter SERS method was able to detect the fungicide ferbam as low as 2.5 ppb and had a good quantitative capability. The developed method was successfully applied in three water samples, including double distilled water, tap water, and pond water. The test has also been carried out on site using a portable Raman instrument. This study shows the filter based SERS method improve the detection capability in water samples, including the sensitivity and porability, and could be applied in the detection of various toxins in real world water samples.

AGFD 248 Development of immunoassays for detecting oxyfluorfen residue in agricultural products Enze Sheng, Xiude Hua, Minghua Wang, shengenze@sina.com. Nanjing Agriculture Univ., Nanjing, China Oxyfluorfen [2-chloro-alpha, alpha, alpha-trifluoro-p-tolyl-3-ethoxy-4-nitrophenyl] belongs to a diphenyl ethers herbicide, which has been widely applied to rice, vegetables and orchard crops variety of season broadleaf weed and gramineous weeds, and high toxic to aquatic animals. The carry-over of oxyfluorfen to agricultural products can occur and increase human exposure. The Currently, immunoassays have emerged as fast, simple, and economic detection methods. In this study, two immunoassays based on monoclonal antibodies (McAbs for oxyfluorfen) are described: enzyme-linked immunosorbent assay (ELISA) and time resolved fluorescence immunoassay (TRFIA). Oxyfluorfen hapten was synthesized and conjugated to bovine serum albumin (BSA) and ovalbumin (OVA) to produce immunogen and coating antigen. Antioxyfluorfen McAbs were obtained from immunized Balb/c mouse (six weeks old). Under optimal conditions, the half-maximal inhibition concentration (IC₅₀) and the limit of detection (LOD, IC₁₀) of oxyfluorfen were 20.1 and 2.86 ng/mL for the ELISA, 2.03 and 0.022 ng/mL for the TRFIA, respectively. There were no obvious cross-reactivities of the antibodies with its analogues except for fluoroglycofen and acifluorifene. The results of immunoassays for spiked and authentic samples were largely consistent with gas chromatography. Therefore, the proposed immunoassays ELISA and TRFIA could be two feasible quantitative/screening methods for oxyfluorfen in agricultural products due to their high sensitivity, rapidity, lower expenses, and high sample throughput.

AGFD 249 Rapid electrochemical detection of Salmonella in agricultural water based on redox cycling Danhui Wang³, danhuiwang@foodsci.umass.edu, Ziyuan Wang¹, Juhong Chen¹, Sam R. Nugen². (1) Room 118, UMass Amherst (2) 246 Chenoweth Lab, Univ. of Massachusetts, Amherst (3) Food Sci., Univ. of Massachusetts Amherst A redox cycling-based electrochemical method combined with immunomagnetic separation and pre-concentration was developed for rapid and sensitive detection of Salmonella in agricultural water. The level of pathogenic bacteria in agricultural water has a significant influence on the safety of fresh produce, especially for the leafy greens which are consumed raw. Electrochemical methods for the detection of bacteria offer the advantages of instant quantification with minimal equipment. Unfortunately, the limits of detection are often poor compare to other transduction methods such as fluorescence and chemiluminescence. We demonstrated an electrochemical method which is both rapid and has a low limit of detection. A two-step strategy, which included immunomagnetic pre-concentration and redox cycling was used to amplify the signal. Magnetic beads modified with anti-Salmonella antibodies were used for separation and pre-concentration of Salmonella from agricultural water. Then anti-Salmonella antibodies conjugated with alkaline phosphatase (ALP) were employed for labeling the Salmonella which had been captured by magnetic beads. Alkaline phosphatase catalyzed the substrate L-ascorbic acid 2-phosphate (AAP) to electroactive species L-ascorbic acid (AA) while tris(2-carboxyethyl)phosphine (TCEP) facilitated the regeneration of AA on the gold electrode to form redox cycling resulting in an amplified signal. Under the optimal conditions, the Salmonella in PBS buffer as well as in agricultural water were detected. The limit of detection of this approach was approximately 7.6 × 10⁵ CFU/mL and 6.0 × 10⁵ CFU/mL in PBS buffer and agricultural water, respectively, without pre-enrichment in 3 hours.

AGFD 250 Detection of Escherichia coli (E. coli) and sensing of antibiotic drugs using engineered enzymatic bacteriophage Juhong Chen¹, juhong@foodsci.umass.edu, Samuel D. Alcaine⁵, Vincent M. Rotello⁴, Sam R. Nugen². (1) Room 118, UMass Amherst (2) Univ of Massachusetts, Amherst, (3) Univ. of Massachusetts, Amherst (4) Food Sci., Univ. of Massachusetts, Amherst A T7 bacteriophage (phage) has been genetically engineered to carry the reporter gene to enable the overexpression of reporter enzyme during phage infection for enzymatic detection of Escherichia coli (E. coli) cells. During the phage infection cycle, phages can specifically recognize target E. coli cells and express reporter enzyme, which can be used to design enzyme-based colorimetric, fluorescent, and electrochemical transduction. The obtained transduce signals can reflect and represent the concentration of E. coli cells. In my degree research, three different reporter genes were inserted into T7 phage genome to express reporter enzymes, detecting E. coli cells and sensing antibiotic drugs. Firstly, T₇phoA phages, which can express alkaline phosphatase during phage infection, have been demonstrated to detect E. coli cells and test the antibiotic susceptibility of E. coli strain. Next, in order to improve the detection limit, engineered phage carrying lacZ gene was built to force overexpression of beta-galactosidase to detect E. coli cells and determine antibiotic drugs. Furthermore, protease gene, like tobacco etch virus protease, has been engineered into T7 phage to create a multiplex detection of viable E. coli cells. Compared with T7control phage, our engineered phage resulted in significantly higher levels of reporter enzyme expression, enabling a lower detection limit of E. coli cells. Using this engineered T7 phage, we were able to detect E. coli cells at the concentration of 10 CFU/mL within 7 hours. The uses of engineered phages carrying reporter gene have been demonstrated to become a rapid, sensitive, and reliable strategy to detect viable E. coli cells and determine antibiotic drugs.
AGFD 251 Optimization of a new HPLC method with UV/DAD and ESI-MS\textsuperscript{a} detection for the analysis of non-psychoactive cannabinoids in Cannabis sativa L. Virginia Brighenti, virginia.brighenti@unimore.it, Roberta Tardugno, Stefania Benvenuti, Federica Pellati. Life Sciences, Univ. of Modena and Reggio Emilia, Modena, Italy

Cannabis sativa L. (hemp) has a long history in folk medicine and it is gaining a renewed interest, thanks to the biomedical relevance of the peculiar terpenophenolic constituents, namely the cannabinoids. In general, the main cannabinoids present in fiber type plants are cannabidiolic acid and/or cannabigerolic acid, followed by their neutral counterpart cannabidiol and cannabinigerol, while the content in the psycho-active tetrahydrocannabinoil is below 0.2%. From a medicinal point of view, cannabinoid represent the most interesting cannabinoid, possessing a high anti-oxidant and anti-inflammatory activity as well as neuroprotective, antiangiolytic and anticonvulsant properties. Cannabinoids are usually analyzed by using GC-FID and GC-MS techniques, which lead to the decarboxylation of the native acidic compounds to their neutral forms. The present work was aimed at the development and validation of a new and reliable method for the metabolite profiling of the main bio-active compounds in hemp cultivars of different origin, to select those that could be applied for the preparation of extracts with high pharmaceutical value. The analysis of hemp non-psychoactive phytocannabinoids was performed by developing a RP-HPLC method coupled with UV/DAD and ESI-MS\textsuperscript{a} detection, by taking advantage of a fused-core stationary phase. Ultrasound-assisted extraction with methanol was selected as the extraction technique. The optimized analytical method was completely validated to show compliance with international requirements (ICH guidelines), thus demonstrating to be a valuable tool for the analysis of both acidic and neutral cannabinoids in the raw plant material. The validated method was then applied to the quantification of the main non-psychoactive hemp samples.

AGFD 252 Extraction and isolation of stypodione from Stypododium zonale Marcel R. Denny, mar.den@outlook.com. Chemistry, Univ. of the West Indies Mona Campus, Kingston, Jamaica

A species belonging to the class of Phaeophyceae, Stypododium zonale has been analyzed and for its chemical compositions. This algae inhabits densely populated areas of fish. It survives by releasing Stypodione which is toxic to fishes. Stypodione is a very prominent member of the unique class of pentacyclic marine diterpenoids. The investigation of the Jamaican algal has resulted in the extraction (using methanol chloroform mixture) and isolation of Stypodione (β-benzoquinone). Isolation and characterization was carried out using different chromatography techniques and by analysis of spectroscopic data. Stypodione was identified as the red fragment fraction which eluted in fractions 40-51. This compound has some interesting biological activity, for example inhibiting of various biological processes.

AGFD 253 Scope and limitations of HPLC-HRESI/MS for the analysis of anthocyanins from tropical fruits Coralia Osorio Roa, cosorior@unal.edu.co. Departamento de Quimica, Universidad Nacional de Colombia, Bogota, Colombia

Anthocyanins are a class of polyphenols responsible for the orange, red, purple, and blue colors of many fruits, vegetables, and flowers. In addition to give color, anthocyanins also have an array of health-promoting benefits, as they can protect against a variety of oxidants through a various number of mechanisms. The HPLC-ESI/MS technique has been relevant on the quantitative and qualitative analysis anthocyanins in the last decades. This combination, offers the separation advantages of liquid chromatography combined with the identification advantages of mass spectrometry. However this technique exhibits some limitations related to determine the position of sugar moiety or any other substituent in the anthocyanin ring. A summary of the anthocyanin studies performed in different tropical fruits will show the scope and limitations of HPLC-HRESI (High Performance Liquid Chromatography coupled to High Resolution Electrospray Mass Spectrometry) for the analysis of these compounds. Thus, the qualitative and quantitative anthocyanin composition of four wild tropical (R. megacephalos Focke, Myrciaria aff. cauliflora O. Berg, H. macrocarpa Mull. Arg., and P. cecropifolia Mart.), and two commercial fruits (S. betaceum and R. glaucus) from Colombia was performed on anthocyanin-rich extracts (AREs) obtained by selective adsorption on Amberlite XAD-7. Each extract was analyzed by HPLC–PDA and HPLC–HRESI-MS\textsuperscript{a} in a LCMS-IT-TOF equipment. In some cases these analyses and the coinjection in HPLC using standards allowed identifying the major constituents in each extract. In the case of new compounds, LCMS analyses were useful to define the anthocyanidin type and the molecular weight of sugar moity but mono and bidimensional NMR experiments were needed to elucidate the unequivocal structure.

AGFD 254 Target oriented synthesis and mass spectral characterization of curcumin-phenofuran adduct: Potential insights into the role of this conjugate as anti-diabetic and anti-cancer agent Bishambar Dayal\textsuperscript{2,1}, dayalb77@gmail.com, Dhaval N. Shah\textsuperscript{2,1}, Sagar Patel\textsuperscript{2,1}, Apexa Mehta\textsuperscript{2,1}, Michael A. Lea\textsuperscript{1}. (1) Microbiology, Rutgers New Jersey Medical School, Newark, New Jersey (2) Medicine, Rutgers Univ. New Jersey Medical School, Princeton Jet, New Jersey

Metformin, phenformin and aminoguanidine are all nucleophilic hydrazino compounds which block the formation of fluorescent Advanced Glycation End Products (AGEs). They also prevent glucose-derived collagen cross linked Amadori products in vitro and in vivo. Recently we described a microwave-induced chemical synthesis of curcumin-phenofuran adduct to enhance the efficacy of metformin in preventing the formation of AGEs. We also described combination of metformin with the phytochemicals present in okra seed extract to enhance the efficacy for the inhibiting AGEs and its comparison with different AGE inhibitors. The present studies describe microwave-induced chemical synthesis and mass spectral characterization of curcumin-phenofuran adduct using LC-MS/MS. The mechanism of formation and its analytical data via TLC combined with MS/MS fragmentation revealed a major six membered ring adduct (TLC R\(_f\)=0.53, 90%), a molecular ion peak at M/Z=537 (30% intensity) and a peak at M/Z=310/331 [M-(149+77), 100% intensity] confirming the formation of this adduct. The minor eight membered ring isomer (TLC R\(_f\)=0.69, 10%) exhibited a mass spectral fragment at M/Z=354 [M'- (184), 100% intensity, derived from the fragment 239-55] confirming the formation of eight membered adduct. Although phenformin is 50 times more potent than metformin as an anti-diabetic drug but it is associated with extremely high lactic acidosis side effects. Further studies have also shown anti-cancer effects of phenformin and metformin. These studies elucidated that phenformin has better anti-cancer activity than metformin as demonstrated by significant inhibition of tumor growth. Although the exact mechanisms by which metformin and phenformin reduce cancer risk has not been completely elucidated. But a recent study showed that synergistic anti-cancer effect of phenformin combined with sodium oxamate, a well known lactate dehydrogenase (LDH) inhibitor reduces the side-effect of lactic acidosis. Chemical synthesis and identification of major and minor isomers presented in this study may offer novel therapeutic strategies for inhibiting AGEs as well as anti-cancer treatments.
AGFD 255 Analysis of urinary and fecal metabolites of tea polyphenol EGCG in mice by LC-MS/MS Shuwei Zhang, shzhang.simmi@gmail.com, Shengmin Sang. Lab for Functional Foods and Human Health, Center for Excellence in Post-Harvest Technologies, North Carolina AT State Univ., Kannapolis, North. Many studies in human, animal models, and cell lines suggest potential health benefits from the consumption of tea (Camellia sinensis, Theaceae), including the prevention of cancer, heart disease, obesity, and diabetes. Many of the beneficial effects of tea have been attributed to the strong antioxidative activity of the tea polyphenols: (−)epigallocatechin-3-gallate (EGCG), (−)epigallocatechin (EGC), (−)-epicatechin-3-gallate (ECG), and (−)-epicatechin (EC). Among them, EGCG is the major catechin and may account for 50–80% of the total catechins in tea. The bioavailability and biotransformation of EGCG play a key role in determining the importance of various mechanisms in vivo and designing future intervention studies. However, the metabolic fate of EGCG in animals or humans is not fully understood. The general complexity of the problem of metabolite identification and the need for adequate throughput have led to integration of MS technologies into strategies involving data-dependent MS/MS acquisition and accurate mass acquisition. Using these advanced mass technologies, we recently investigated the metabolic profile of EGCG in mice. Our results showed that the biotransformation of EGCG is much more complicated than what reported in the literature. The phenolic groups of the methylated EGCG (or glucuronidated or sulfated EGCG) can be further methylated, glucuronided and/or sulfated to form multiple conjugated metabolites. In addition, EGCG is a substrate for cytochrome conjugation, glucosidation, and degradation by microbiota. Furthermore, several EGCG related unknown metabolites were also detected as major and minor metabolites in this study.

AGFD 256 Qualitative and quantitative analysis of antioxidant and quinone reductase-inducing phytochemicals present in a Maqui berry (Aristotelia chilensis) botanical dietary supplement C. Benjamin Naman1,2, bnaman@ucsd.edu, Jie Li1,2, Ye Deng2, William J. Keller3, A. Douglas Kinghorn2. (1) Scripps Institution of Oceanography, Univ. of California, San Diego, La Jolla, California (2) Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State Univ., Columbus (3) Nature's Sunshine Products, Inc., Spanish Fork, Utah. Since the passage of the Dietary Supplements Health and Education Act by Congress in 1994, the U.S. market for dietary supplements has increased from about $4 billion to nearly $40 billion per year. One aspect of this growth has been the distribution of previously unavailable exotic fruits and the so-called “super fruits” in extracted form, which together have made a significant consumer impact. These products are often demonstrated or expected to have a high antioxidant capacity, and many have been studied qualitatively and/or quantitatively. In the work to be presented, a commercially available botanical dietary supplement product containing only Maqui berry (Aristotelia chilensis) extract was investigated for potential cancer chemopreventive activity by bioassay-guided fractionation. This yielded 16 natural product isolates, including one compound not previously reported from any natural source and several that were not previously reported or detected in Maqui berry samples. Each molecule was characterized by NMR spectroscopy and HRESIMS. Six phenolic compounds that were present in high abundance and demonstrated hydroxyl radical scavenging or quinone reductase inducing activities in vitro were utilized as authentic standards to develop and validate an LC-DAD-MS method for the quantitative determinations of their occurrence in Maqui berry extracts or other phytochemical samples. This technique is complementary to some other validated protocols for evaluating Maqui berry samples, since they are focused primarily on analyzing anthocyanin and flavonol glycoside contents. This method can thus facilitate extract batch standardizations, quality assurance and control efforts, and natural product drug discovery sample dereplication.

AGFD 257 Identification and quantification of novel cranberry (poly)phenol metabolites in human plasma and urine by UPLC-QTOF MS Ana Rodriguez-Mateos1, San Pedro, CA, anarodriguezmateos@gmail.com, Rodrigo P. Feliciano1, Albert Boeres1, Luca Massacci1, Geoffrey Istas1, Claudia Nunes dos Santos2, Rita Ventura2, Christian Heiss1. (1) Cardiology, Pulmonology and Vascular Medicine, Univ. of Dusseldorf, Dusseldorf, Germany (2) Universidade Nova de Lisboa, Lisbon, Portugal. In recent years, the potential health benefits of cranberry consumption have gained public attention. Cranberries are a rich source of (poly)phenols, in particular proanthocyanidins, anthocyanins, flavonols, and phenolic acids. To date, very few studies have investigated the absorption, metabolism, and excretion of cranberry (poly)phenols in humans. In this work, a fast and sensitive method using UPLC-QTOF-MS was developed for the identification and quantification of (poly)phenol metabolites in human plasma and urine using authentic standards. A total of 60 phenolic metabolites were identified after consumption of cranberry juice by healthy individuals. These included sulfates of pyrogallol, valerolactone, benzoic acids, phenylacetic acids, glucuronides of flavonols, as well as sulfates and glucuronides of cinnamic acids. The most abundant plasma metabolites were small phenolic compounds, in particular hippuric acid, catechol-O-sulfate, 2,3-dihydroxybenzoic acid, phenylacetic acid, isofellic acid, 4-methylcatechol-O-sulfate, a-hydroxyhippuric acid, ferulic acid 4-O-sulfate, benzoic acid, 4-hydroxyphenyl acetic acid, dihydrocaffic acid 3-O-sulfate, and vanillic acid 4-O-sulfate. Some benzoic acids, cinnamic acids, and flavonol metabolites appeared in plasma early, at 1-2h post-consumption. Others such as phenylacetic acids, benzoic acids, catechols, dihydroxycinnamic acid derivatives appear in plasma later (Tmax 4-22h). This work lays important groundwork to start understanding the potential health benefits of cranberries in humans.

AGFD 258 Accuracy of HPLC-MS methods used to assess the absorption, metabolism and excretion of bioactive (poly)phenols: Implications for nutritional and biomedical research Javier Ottaviani, Javier.ottaviani@mss.effem.com, Mars Incorporated, McLean, Virginia. (Poly)phenols are a large group of plant-derived bioactive food constituents that are gaining increasing attention for their putative health benefits in humans. A key aspect to progress in the nutritional and biomedical characterization of these compounds involves understanding their absorption, distribution, metabolism and excretion (ADME). Following dietary intake and absorption, (poly)phenols are extensively metabolized by phase II- and gut microbiome-mediated reactions. Due to the chemical diversity of the resulting metabolites, the quantification of these compounds in plasma, urine, and tissues represents a significant analytical challenge, especially in the absence of reference compounds. In this context, it has become common practice to use unmetabolized parent (poly)phenols as reference standards in order to quantify the corresponding metabolites. However, little is known about the accuracy of this approach. Using HPLC-MS conditions that are representative of methods commonly utilized in this research field, we compared the signal yielded by a particular (poly)phenol, namely (−)-epicatechin, to that of a series of phase II- and gut microbiome-derived (−)-epicatechin metabolites. The results obtained demonstrate sizable differences in the response of the mass spectrometer, which yielded both inaccurate over- and under-estimates of metabolite levels. Further differences were introduced by the use of different chromatographic conditions. Inaccurate quantitative estimates were also obtained when phase II metabolites of other (poly)phenols were quantified by reference to unmetabolised parent (poly)phenols.
AGFD 259 Absorption, distribution, metabolism and excretion of orange juice flavanones in humans Alan Crozier¹, alan.crozier44@gmail.com, Gema Pereira-Caro². (1) Nutrition, Univ. of California, Davis 2) Andalusian Inst. of Agricultural and Fishery Research, Cordoba, Spain. A diet rich in fruit and vegetables is a major factor in the maintenance of good health and in part, these effects are mediated by plant-derived (poly)phenolic compounds. Understanding the fate of these compounds within the body is key to elucidating their mode of action in reducing the incidence of chronic diseases. This talk will focus on the use of HPLC-MS and UPLC-HR-MS to investigate the absorption, distribution, metabolism and excretion (ADME) of flavanones after the ingestion of orange juice by human volunteers, including athletes before and after cessation of training for 7 days, with emphasis on events occurring in the proximal and distal gastrointestinal tract.

AGFD 260 Elucidating metabolic signatures of phytochemical consumption Colin Kay, Colin.Kay@uea.ac.uk. Plants for Human Health Inst., North Carolina State Univ., Kannapolis Characterising anthocyanin metabolites presents many challenges as their structural diversity make extraction and quantification in biological matrices problematic. We utilised an isotopic-labelling approach, feeding 500mg ¹³C-cyanidin-3-glucoside to human volunteers and characterise 59 metabolites of a single anthocyanin. Non-targeted MRM scanning (SCIEX QTRAP) was initially utilised to explore over 200 putative metabolites modelled on established metabolism of similarly structured xenobiotics, following Neutral Loss, and Enhanced MS (EMS) scans. A total of 35 anthocyanin metabolites were verified with the use of commercial and synthetic standards. These included methylated, sulfated and glucuronidated conjugates of benzoic, hippuric, phenylpropionic, caffeic, phenylacetic acids, alcohols and aldehydes. Low sensitivity and specificity and high signal-to-noise prevented detection of many low concentration analytes, therefore targeted methods were employed using MRM to trigger Enhanced Product Ion (EPI) scans using the IDA function, with enhanced resolution (ER) scanning to improve peak sensitivity, allowing structural fingerprinting of an additional 11 sulfate and 13 glucuronide conjugates.

AGFD 261 Development of food-grade filled hydrogels for oral delivery of lipophilic active ingredients: pH-triggered release Zipei Zhang, zipeizhang@umass.edu. Food Sci., Univ. of Massachusetts Amherst It is necessary in the food and pharmaceutical industries to protect and oral deliver the lipophilic active agents, such as oil-soluble flavors, antimicrobials, nutraceuticals, or drugs. Hydrogel particles fabricated from food-grade biopolymers can be used to develop delivery system for these targets. In this study, hydrogel particles were fabricated by electrostatic complexation of a protein (casein) and an anionic polysaccharide (alginate). Relatively small hydrogel particles were formed at pH values just above the isoelectric point of the protein (where both biopolymers are negative) through electrostatic attraction between anionic groups on alginate and cationic groups on casein. Light scattering and confocal fluorescence microscopy indicated that hydrogel particles could keep lipid droplets trapped inside during storage (lower pH conditions), while release the encapsulated lipids under simulated oral conditions triggered by a pH change. These results suggest that our hydrogel particles can be applied for oral delivery of lipophilic active agents.

AGFD 262 Legume proteins as alternative emulsifiers to encapsulate omega-3 oils Cansu E. Gumus, cgumus@umass.edu, David J. McClements. Dept. of Food Sci., Univ. of Massachusetts Amherst There is growing interest among consumers in "clean label" and all plant-based food products. Therefore, the food industry is looking for ways to address consumer concerns about synthetic ingredients. Algae oil is an alternative plant-based source of omega-3 polyunsaturated fatty acids that can be used as a plant-based alternative to fish oil. However, there are issues with incorporating omega-3 fatty acids into foods due to their low water-solubility and oxidative instability, which may be overcome using emulsion-based delivery systems. The aim of this study was to provide a better understanding of the potential use of several legume proteins as natural emulsifiers. The purpose of the current research was to provide a basic understanding of the utilization of plant-based proteins as food emulsifiers, and the range of conditions where they can be successfully used: pH, ionic strength, and temperature. Pea, lentil and fava bean proteins were shown to be effective emulsifiers for the formation and stabilization of algae oil emulsions. Relatively small droplets (< 500 nm) could be formed at low emulsifier levels (2:10 w/w) with high PH levels close to the isoelectric point of the proteins due to a reduction in electrostatic repulsion. The results gained through this study provide practical strategies for the food industry to formulate clean-label omega-3 fortified foods using plant-based ingredients.

AGFD 263 Structures and interfacial properties of self-assembled protein-polyphenol-polysaccharide ternary complexes Weiping Jin¹, jinweiping1988@163.com, Bin Li², Qingrong Huang². (1) College of Food Sci. and Tech., Huazhong Agricultural Univ., Wuhan, Hubei, China (2) Food Sci., Rutgers Univ, New Brunswick, New Jersey (3) Food Sci., Rutgers Univ., New Brunswick, New Jersey Self-assembly of protein and polyphenol has been studied thoroughly, but effects of co-exist matrix on their structures are not well investigated. Here, influences of glucosamann (GM) and carboxymethylated glucosamann (CM-GM) on structural properties and assembling behavior of gelatin-tannic acid complexes have been discussed. Properties of shape, structure, and aggregated ways of soluble or insoluble complexes were investigated using particle size analysis and small X-ray scattering (SAXS) measurements. As the concentration of tannic acid started from 0.02mg/mL, sizes of soluble complexes did not change much until polyphenol concentration reached the threshold value (0.06mg/mL). To compare the size of Rₚ and Rₚ ratios of Rₚ to Rₚ were in the range of 2-3 indicating insoluble aggregates had a density core and a thick hydration layer. Present results illustrated that effects of GM on protein-polyphenol interaction were attributed to competitive binding and changing of aggregated behavior. For CM-GM, adding tannic acid made complexes that were formed by CM-GM/gelatin coacervates more denser, resulting from reducing size. Due to benefits of Pickering emulsions, protein-based nanocomplexes have been widely developed to stabilize Pickering emulsions. Meanwhile, polysaccharide can regulate particle size and surface wettability of protein-polyphenol.
nanocomplexes. Fluorescence microscopy and Cryo-SEM were used to observe the location of nanocomplexes at the oil-water interfaces. Except for qualitative observation, interfacial shear and dilatational rheology were utilized to study the adsorption behavior of those nanocomplexes at the interface. When the concentration of nanocomplexes went up to 0.1wt%, stabilized Pickering emulsions were obtained due to fast and irreversible adsorption of nanocomplexes onto water-oil interfaces.

AGFD 264 Stabilization of pickering emulsions by polysaccharide-polypeptide nanocomplexes Yike Jiang1, yike9090@gmail.com, Qingrong Huang1. (1) Food Sci., Rutgers Univ, New Brunswick, New Jersey (2) Dept. of Food Sci., Rutgers Univ., New Brunswick, New Jersey The Pickering emulsions which are stabilized by solid particles instead of the traditionally used amphiphilic emulsifiers are becoming an emerging research area in Food Sci. due to their outstanding properties such as superior stabilities against coalescence and Ostwald ripening. Most of work so far on Pickering emulsions was conducted using non-food grade inorganic and organic particles. The food grade particles used as the Pickering stabilizers are majorly focused on either protein/polypeptide or polysaccharide, while less attention was paid to their complexes. The advantages of using the polysaccharide-protein/polypeptide complexes as the Pickering stabilizers are (1) the physical properties of the complexes can be easily controlled so that their interfacial properties are tunable without chemical modification; (2) it saves materials; (3) it saves energy. High energy preparation such as high speed- and high pressure-homogenization are not necessary for preparing the polysaccharide-protein/polypeptide complexes stabilized Pickering emulsions. We recently developed the chitosan (CS)-caseinophosphopeptides (CPPs) nanocomplexes. The CS-CPPs nanocomplexes composed of different CS:CPPs weight ratios were used as the Pickering stabilizers and their physical properties such as particle size, morphology, surface hydrophilicity, and surface tension were investigated. The best formulation of the nanocomplexes was determined by comparing the stabilities (pH and ionic strength), oil fractions, and rheological properties of the Pickering emulsions stabilized by them. We found that the capacity of the nanocomplexes as the Pickering stabilizer increased with the content of CPPs in the system. However, we observed that low pH may affect the stability of the emulsions. To solve this problem, we used a natural crosslinker genipin to covalently crosslink the nanocomplexes. The genipin crosslinked CS-CPPs nanocomplexes with different crosslinking time were used to stabilize Pickering emulsions, which exhibited higher pH stability and stronger gel-like property compared to the CS-CPPs nanocomplexes stabilized emulsions. The significance of the present study is that it provides new perspective of application of the polysaccharide-polypeptide complexes in Food Sci.. It also paves new route of using these nanocomplexes as the nutraceutical encapsulation system since nutraceuticals can be encapsulated in the complexes and/or in the oil phase.

AGFD 265 Ultrasonic treatment of regenerated a-chitin with tunable capacity for stabilization of oil in water emulsion Yuntao Wang, wyt2020@126.com. Huazhong Agricultural Univ., Wuhan, China A-chitin cannot be dispersed directly with ultrasonic treatment because of the strong intermolecular forces. However, in the current work, when a-chitin was first regenerated from a NaOH/urea solvent, the regenerated a-chitin can then be easily dispersed with ultrasonic treatment under weak acidic conditions. The morphology, size, zeta potential, structure and optical transmittance of the dispersed a-chitin solution were characterized by TEM, DLS, XRD and UV spectroscopy respectively. The dispersed chitin was then used for stabilization of oil in water emulsion. It was found that the emulsifying capacity of regenerated chitin was tunable by ultrasonic treatment. The dispersed chitin exhibited excellent emulsifying ability and the resulting emulsion was stable after long-term storage. In short, in this paper, a novel way to prepare dispersed chitin with excellent emulsifying ability was presented, and its emulsifying properties were further evaluated.

AGFD 266 Phytochemical composition of essential oils and in vitro screening of the antimicrobial activity on oral pathogenic bacteria Roberta Tardugno1, robynia@hotmail.com, Ramona Iseppi1, Elisa Franceschini1, Federica Pellati1, Giacomo Bruzzesi2, Moreno Bondi1, Stefania Benvenuti1. (1) Dept. of Life Sciences, Univ. of Modena and Reggio Emilia, Modena, Italy (2) Univ. of Modena and Reggio Emilia, Modena MO, Italy Essential oils (EOs) are complex mixtures of terpenes with interesting antimicrobial activity. In this study, the attention was focused on microorganisms involved in oral diseases, such as caries and periodontitis. A pool of fifteen EOs according their chemical composition was selected and subjected to gaschromatographic analysis (GC-MS, GC-FID), including Illicium verum Hooker, Cinnamomum zeylanicum Ness, Syzygium aromaticum L. Eucalyptus globulus Labill, Leptospermum scoparium J.R. Forst, Mentha arvensis L., Mentha piperita L. Myrtus communis L., Salvia officinalis L., Melaleuca alternifolia Cheed, Rosmarinus officinalis L., L. x intermedia var. Grosso and L. x intermedia var. Sumiens, T. vulgaris L. and Thymus capitatus L. These EOs were then tested on Streptococcus mutans and Lactobacillus species for their antimicrobial activity. According to the in vitro biological screening, promising results were obtained from seven EOs of the initial pool. This preliminary screening represents the first step in order to optimize mouthwashes for further in vivo studies on the most promising EOs.

AGFD 267 Antimicrobial character of lactonic sophorolipids against select bacterial strains commonly associated with foodborne illness Richard Ashby1, rick.ashby@ars.usda.gov, Daniel Solaian1, Xuetong Fan3, Xuejie Zhang3, Modesto Olanya4, Dike Ukuku1. (1) ERRC- ARS-USDA, Wyndmoor, Pennsylvania (2) USDA, Wyndmoor, Pennsylvania (3) USDA - Agric. Res. Service, Wyndmoor, Pennsylvania (4) USDA/ARS/ERRC, Wyndmoor, Pennsylvania (5) Chinese Academy of Agricultural Sciences, Beijing, China Sophorolipids (SLs) are bacterial glycolipid biosurfactants that are produced in relatively low yields via fermentation and possess a much better environmental footprint than petroleumbased surfactants. Sophorolipids were prepared in the presence of palmitic acid, stearic acid, and oleic acid in order to increase structural variability. Structural lactones composed greater than 90% of the SLs produced regardless of substrate. These distinct SLs were then assessed for their antimicrobial behavior against both Gram+ (Listeria) and Gram- (Escherichia coli, Salmonella enterica) bacterial strains that are commonly associated with foodborne illness. Results suggested that Gram+ bacterial strains were more susceptible to the antimicrobial action of SLs than were Gram- strains. Without the thick outer membrane, Gram+ strains are easily accessible for SLs to intercalate into the plasma membrane and disrupt normal membrane function; however, in vitro studies showed that SLs in the presence of 20% ethanol were effective in inactivating E. coli O157:H7 within 2 hours of treatment reducing the population from 7.1 log CFU/mL to a non-detectable level. Transmission Electron Microscopy (TEM) revealed that SLs caused membrane damage in E. coli by separating the outer membrane from the plasma membrane. This phenomenon caused structural damage to the membranes and improved antimicrobial action. In all cases SLs showed an ability to inhibit/kill harmful bacteria which might lead to a larger array of weapons to combat foodborne illness.
AGFD 268 Synthesis of antimicrobial phenolic branch-chained fatty acids Helen L. Ngo, helen.ngo@ars.usda.gov, Karen Wagnner, Zongchen Yan, Alberto Nunez, Robert Moreau, Xuetong Fan. ERRC, ARS, USDA, Wyndmoor, Pennsylvania Natural phenolic compounds with hydroxyl groups on aromatic ring are widespread in plant kingdom. These compounds exhibit a wide range of physiological properties, such as antimicrobial and antioxidant activities. In this presentation, the synthesis of aryl branched-chain fatty acids containing phenolic functionality and their biological activities will be discussed. These phenolic branched-chain lipids have two hydrophilic portions (phenol and carboxylic group) and a hydrophobic region (alkyl chain in the fatty acid moiety), which are found to be good antimicrobial agents. They can be prepared in a one step process by treating unsaturated linear-chain fatty acids (derived from renewable vegetable oils) and excess phenolic with catalytic amounts of modified solid catalysts and small amounts of water at 260 °C. Results showed that under the optimized conditions, the phenolic branched-chain fatty acid products were obtained in up to 70% yield. Investigations of these phenolic branched-chain fatty acids have shown that they not only have antimicrobial properties but also are far more effective antimicrobials than the individual phenolic and parent linear-chain fatty acids. It appears that these types of compounds possess antimicrobial properties due to a balance between the hydrophobic and hydrophilic portions of the molecule, as phenolic branched fatty acids having only a hydrophobic portion but no hydrophilic region or relatively long alkyl chains in their chemical structure showed either reduced or no antimicrobial activity. These hybrid phenolic branched-chain fatty acid molecules could represent a new class of antimicrobials that potentially have food safety, medical and healthcare applications.

AGFD 269 Thiamine dilauryl sulfate (TDS) and organic acid combined treatment to secure microbial safety of selected products Hee Kyung Park, Hao Feng, haofeng@illinois.edu. Dept. of Food Sci. and Human Nutrition, Univ. of Illinois at Urbana-Champaign Many of the food-borne pathogen intervention methods involve the use of chemical antimicrobial agents. Although the chemical methods are popular in the food industry because of their convenience and economy, they often show limited effectiveness. There is a need to develop new sanitizing agents with enhanced antimicrobial potency and minimal impact on the environment and consumers. In this study, the efficacy of thiamine dilauryl sulfate (TDS) combined with organic acids for the inactivation of Escherichia coli O157:H7 on selected produce, meat, and poultry products was examined. The effects of a TDS and malic acid combined wash on the quality of romaine lettuce were also examined. E. coli O157:H7 cell suspensions were treated with TDS, an organic acid, or combinations of them. Produce samples were dip-inoculated, and beef and chicken samples were spot-inoculated, with E. coli cells. The samples were treated for specific time periods, and microbiological analyses were conducted. Romaine lettuce samples vacuum-packaged with N2 gas were evaluated for quality. All of the combinations of organic acid with 0.05% TDS reduced the E. coli populations to undetectable levels. A 5-log reduction was achieved on spinach and lettuce when treated with 1% TDS and 4% malic acid for 1 min., and the time to achieve a 5-log reduction on the chicken skin was 5 min. When 10 g of inoculated alfalfa seeds were treated by TDS + malic acid and Ca(OCl); for 20 min., no E. coli colonies were detected. An off-odor was noted with the TDS + malic acid treatment, but its overall sensory scores were similar to those of the water washed samples. The TDS and organic acid combined treatment may provide an effective kill step in post-harvest and post-mortem processing operations for securing microbial safe of produce, meat, and poultry products.

AGFD 270 Characterization of LAB bacteriocins with the potential for food safety and functional food applications John Renye, john.renye@ars.usda.gov, George A. Somkuti. Dairy and Functional Foods, Agricultural Research Service, Wyndmoor, Pennsylvania For centuries lactic acid bacteria (LAB) have been used as biocatalysts for the production of fermented dairy foods, including cheese and yogurt. Several of these dairy cultures have also been shown to naturally produce antimicrobial peptides call bacteriocins, which have the potential to prevent spoilage and foodborne illness. In addition, LAB which produce broad spectrum bacteriocins have been investigated for their potential as probiotics for inclusion in functional foods. ARS research currently focuses on the identification of novel bacteriocin-producing LAB, and characterization of the molecular mechanisms which regulate peptide expression. These studies have identified two Streptococcus thermophilus strains, ST109 and ST110, which naturally produce broad spectrum bacteriocins encoded within a bacteriocin-like peptide (bip) gene cluster on the bacterial chromosome. The natural production of these bacteriocins is unique in that other characterized strains require the use of a synthetic peptide to induce bacteriocin production. The broad spectrum antimicrobial activity of thermophilin 110, which includes activity against Listeria monocytogenes and streptococcal pathogens, suggests it has potential food safety and probiotic applications. Streptococcus thermophilus and other dairy LAB have also been investigated as microbial production systems for generating potential food-grade bacteriocins with anti-listerial activity, such as pediocin and durancin GL. Duancin GL is a bacteriocin that is naturally produced by Enterococcus durans 41D, which was identified as part of the indigenous microflora in a raw-milk cheese. The genetic elements required for the production of durancin GL have been characterized; and the strain is currently being investigated for its potential to serve as an adjunct culture for preventing the growth of L. monocytogenes.

AGFD 271 Plant-produced colicins for control of foodborne Escherichia coli Chad H. Stahl1, chstahl@umd.edu, Anatoli Giritich2, Yuri Gileva2. (1) Animal and Avian Sciences, Univ. of Maryland, College Park (2) Nomad Bioscience GmbH, Halle, Germany Enterohemorrhagic Escherichia coli (EHEC), such as E. coli O157:H7, cause over 200,000 illnesses annually at a cost to the EU and U.S. economies of approximately €2 billion. These illnesses have been linked to consumption of foods derived from, or contaminated with animal products. Recently, organically grown vegetables have been linked to several such outbreaks. Current interventions to reduce EHEC contamination on food include thermal treatments, organic acid washes, or treatment with other chemicals. All current interventions may negatively impact the taste or quality of the treated food products. With increased interest in the use of natural or bio-based antimicrobial interventions, we have focused on a family of bacteriocins produced by E. coli as a means to compete against other E. coli and closely related bacteria. This family of bacteriocins, called colicins, have diverse modes of antimicrobial action as well as diverse bacterial cell targets. Several colicins have been shown to be highly effective against EHEC strains, both in live animals and on animal derived products. However, strain variation in susceptibility to different colicins suggests that a mixture of several different colicins would be needed to be efficacious against a broad range of EHEC. Additionally, by exploiting variations in mode of action and cellular targets synergistic antimicrobial effects can be realized. We have expressed several colicins in a highly efficient green-plant expression host. This system provides high yields (up to 3 kg active protein per ton of fresh green biomass) and very low manufacturing costs. We have evaluated the efficacy of Col M, Col E7, Col N, Col E1, and Col E3 produced by this system against the “Big 7” EHEC strains. A cocktail of these colicins is capable of causing
significant (2-6 logs) reductions of all of these EHEC strains from a variety of foods at treatment levels of <10 mg of colicin/kg of food product. This efficacy, coupled with its safety and low cost of production make plant-produced colicins a viable intervention for controlling EHEC contamination in a wide variety of foods.

AGFD 272 Bacteriocins producing lactic acid bacteria: Isolation, optimization of growth condition for bacteriocins production and application in foods Lihua Fan, lihua.fan@agr.gc.ca. Agriculture and Agri-Food Canada, Kentville, Nova Scotia. Lactic acid bacteria (LAB) produce a variety of compounds with antimicrobial activity. Among them are bacteriocins, which have attracted great interests due to their antimicrobial effects on spoilage and pathogenic microorganisms and potential applications in food to enhance microbial safety. The objectives of our studies were to isolate and characterize bacteriocins producing LAB strains, determine the optimum growth conditions including pH, culture media and temperature for LAB and bacteriocins production by measuring optical density (OD), bacteriocin activity and viability of LAB, and further explore their application in food. LAB strains were isolated from horticultural commodities and dairy products. The antimicrobial properties of LAB isolates were determined using the agar diffusion bioassay. Bacteriocins producing LAB were identified using 16S rRNA gene sequencing and molecular weight of bacteriocins was determined using SDS-PAGE technique. Antimicrobial effectiveness of LAB and bacteriocins were investigated against a range of spoilage and pathogenic bacteria and fungi. Growth curves of bacteriocinogenic LAB grown under various growth conditions were investigated using a Bioscreen C. For the selected growth conditions, the relationship of pH, OD, bacteriocin activity (AU) and viability of LAB (CFU/ml) were determined. These research findings provided useful information on application of LAB and bacteriocins efficiently in foods to improve food safety and quality. Challenge tests were also conducted on lettuce or cantaloupe juice culture medium as well as on fresh-cut vegetables inoculated with L. innocua at 10^4 CFU/ml. Results showed that bacteriocinogenic LAB such as Lactococcus lactis (7.17) and Enterococcus faecium (13.2) significantly reduced Listeria spp. (p=0.005) during storage at 4 or 20°C. These results suggest that bacteriocins producing LAB would be used for food protection when applied as protective cultures in food system.

AGFD 273 Evaluation of toxicity and endocrine disruption potential of the natural antimicrobials or biobased antimicrobials Changqing Wu1, changwui@udel.edu, Chan Ho Jang2, Mingming Guo3. (1) Animal and Food Sci., Univ. of Delaware, Newark (2) Animal and Food Sci.s, Univ. of Delaware, Newark (3) Animal and Food Sci., Univ. of Delaware, Newark. Not all natural antimicrobials or biobased antimicrobials are safe to be used in food industry. To ensure social, industrial and regulatory acceptance of the newly developed antimicrobials, it is essential to determine their toxicity and endocrine disruption (ED) potential. The complex biology of toxicity and endocrine disruption means that neither a single assay nor a single approach can be used to identify chemicals with inherent toxicity and ED characteristics. Comprehensive approaches are recommended to minimize the negative environmental, economical, and social impacts of the new antimicrobials. A multi-tiered approach is proposed to investigate toxicity and ED of the compounds, following the general guidelines of U. S. Food and Drug Administration (FDA), and National Inst. of Environmental Health Sciences/National Toxicology Program. This approach will be developed using a combination of testing methods including both in vitro and in vivo tests to guide the development of inherently safer antimicrobials. A Salmonella mutagenicity test will be used to study short-term genetic toxicology. Human cell lines including MCF-7 human breast cancer cells will be also used to determine the potential toxicities of the new compounds. Specific pathogen free chicken embryos will be used to evaluate the toxic effects of the compounds during developmental stages of vertebrate animal. In summary, a combination of approaches will be used to guide the development of inherently safer antimicrobials. Approaches and findings from our lab will be presented in this presentation.

AGFD 274 Applications of the polysaccharide-polypeptides nanocomplexes in multi-platforms for nutraceuticals encapsulation Yike Jiang1, yike9090@gmail.com, Qingsong Huang2. (1) Food Sci., Rutgers Univ, New Brunswick, New Jersey (2) Food Sci., Rutgers Univ., New Brunswick, New Jersey. Polysaccharide and proteins/polypeptides are important biomolecules in foods. When they are oppositely charged, these molecules can attract each other. The complexion between polysaccharides and proteins/polypeptides does not require chemical reaction, which avoids the use of toxic reagents and undesirable side products. In addition, the physical properties of these complexes such as size and morphology can be controlled by tuning their concentrations, weight ratio, pH, ionic strength. Due to these outstanding properties, the polysaccharide-protein/polypeptide complexes have been widely applied in Food Sci., nutraceuticals, and pharmaceutical areas. We recently developed the polysaccharide-polypeptide nanocomplexes self-assembled from chitosan (CS) and caseinophosphopeptides (CPPs). We herein report two applications of the CS-CPPs nanocomplexes for encapsulating nutraceutical. An application of the CS-CPPs nanocomplexes is to directly encapsulate nutraceuticals. We purified the polyphenol theaflavin-3,3′-digallate (TF-3) from black tea extract and encapsulated TF-3 in the CS-CPPs nanocomplexes. The interactions and microstructure changes involved in the encapsulation process were investigated by multiple techniques such as turbidimetry titration, fluorescence quenching, circular dichroism, small angle- and ultra-small angle X-ray scattering. Another application of the CS-CPPs nanocomplexes is to stabilize Pickering emulsions. Unlike the conventional emulsions which are emulsified by amphiphilic emulsifiers, Pickering emulsions are stabilized by solid particles, usually non-food grade inorganic and organic particles. The food grade particles used as the Pickering stabilizers are majorly focused on either polysaccharides or proteins/polypeptides, while using their complexes are relatively novel. We applied the CS-CPPs nanocomplexes composed of different CS-CPPs weight ratios to stabilize Pickering emulsions and the physical properties of these nanocomplexes such as particle size, morphology, surface hydrophilicity, and surface tension were characterized. These Pickering emulsions were compared in terms of their stability and rheological properties. By incorporating TF-3 in the nanocomplexes and/or oil, TF-3 was encapsulated in these Pickering emulsions at the oil-water interface and/or in the oil phase. These studies pave ways of utilizing the polysaccharide-protein/polypeptide complexes in multi-platforms for encapsulating nutraceuticals.

AGFD 275 Interaction and structure formation between α-lactalbumin and chitosan grafted with poly(ethylene glycol) chains Juan Du1, du2@purdue.edu, Owen G. Jones2. (1) Food Sci., Purdue Univ., West Lafayette, Indiana (2) Nelsen Hall, Purdue Univ., West Lafayette, Indiana. Assemblies are formed in solution between chitosan (CH), a polysaccharide composed of D-glucosamine residues, and the whey protein α-lactalbumin (α-lac) above pH 5 due to strong electrostatic interactions, yet the process is poorly controlled and large phase-separated domains result. To limit the phase-separation process and encourage the formation of micelle-like structures with α-lac, a non-ionic poly(ethylene glycol) (PEG) chain was grafted to amine-groups of CH to form chitosan-graft-poly(ethylene glycol) (CH-PEG). NMR
AGFD 276 De-polymerization of lignin via co-pyrolysis with 1,4-butanediol in a microwave reactor Paul Tarves, Paul.Tarves@ars.usda.gov, Charles A. Mullen, Akwasi Boateng. Sustainable Biofuels and CoProducts, USDA – Agricultural Research Service - Eastern Regional Reserach Center, Lansdale, Pennsylvania Lignin is a low value by-product of the pulp, paper, and cellulosic bioethanol industries and it is generated in very large quantities (~50 million tons per year worldwide). Lignin is an amorphous, three dimensional, biopolymer composed of phenolic units cross-linked via C-C and ether-bonds. Fast pyrolysis of lignin allows for the isolation and utilization of the individual mono-aromatic components, but in extremely low yields and often with operational difficulties. Here we report, batch microwave pyrolysis of lignin at 1200 watts over the course of fifteen minutes in the presence of a microwave absorber (activated charcoal). The liquid products obtained are composed of smaller polymeric components and moderate yields of mono-aromatic compounds. However, the addition of a radical scavenger (1,4-butanediol) to help prevent re-polymerization reactions led to greater reduction in the average molecular weight (~85-90% decrease) and a yield in the monomeric phenols (~3x increase). The results obtained may lead to the development of novel lignin co-processing methods.

AGFD 277 Photoelectrocatalytic oxidation of nitrite using highly ordered anatase form of TiO$_2$ nanotube array photoelectrodes Chan Lu, 21413022@zju.edu.cn, Xishan Guo, Songming Zhu. Institution of Agricultural Bio-Environmental Engineering, Hangzhou, China The main objective of this study was to investigate the photoelectrocatalytic degradation behaviour of nitrite in simulated aquaculture wastewater using highly ordered TiO$_2$ nanotube arrays as the photoanode. The influences of TiO$_2$ nanotube arrays annee temperature, applied bias potential, initial pH, initial nitrite concentration, NaCl concentration were studied. The experimental results indicated that TiO$_2$ nanotube arrays annee temperature, bias potential, NaCl concentration and initial nitrite concentration played important roles in the degradation of nitrite. In addition, pH seemed to have little influence on nitrite removal at the range of 6.5 - 8.5 in solutions contained Cl$. Finally, the reaction mechanism was discussed. Both hydroxyl radicals and active chlorine are responsible for the degradation of nitrite ion.

AGFD 278 Halloysite nanotube/polyethylene nanocomposites as multifunctional active food packaging materials Cuneyt E. Tas, Buke$t Alkan$, Mustafa Baysal$, Filiz Altay$, Fezvi C. Cebeci, Serkan Unal, Yusuf Z. Menceloglu, Hayriye Unal. humal@ sabanciuniv.edu, Ekin Sehit. (1) Faculty of Engineering and Natural Sciences, Sabanci Univ., Istanbul, Turkey (2) Food Engineering, Istanbul Technical University, Istanbul, Turkey (3) NanoTech. Research and Application Center, Sabanci Univ., Istanbul, Turkey Active food packaging materials that are designed to interact with food can greatly contribute to food safety and prevent economic losses caused by spoilage of food products. Halloysite nanotubes/polyethylene (HNT/PE) nanocomposites will be presented as active food packaging materials that can release antibacterial agents to prevent bacterial spoilage and absorb ethylene gas secreted by fruits and vegetables to prevent spoilage caused by overripening. Halloysite nanotubes that are natural clay nanoparticles with hollow tubular structures were utilized as the active component enabling the antibacterial and ethylene scavenging behaviors. Antibacterial essential oil loaded HNTs were incorporated into polyethylene matrix resulting in films that present sustained release of antibacterial agents and reduce the viability of A. hydrophila up to 90%. HNTs were furthermore shown to absorb ethylene gas with a capacity of up to 0.85wt% as determined by gravimetric analysis, which results in corresponding HNT/PE nanocomposite films with significantly higher ethylene scavenging capacity than neat PE films. Antibacterial and ethylene scavenging properties of HNT/PE nanocomposite films were also demonstrated on food samples. Growth of pathogenic bacteria on surfaces of chicken samples packaged with HNT/PE films were reduced compared to samples packaged with neat PE films. HNT/PE nanocomposite films were also shown to slow down the ripening of bananas and retain the hardness of tomatoes and strawberries for longer time than PE films.

AGFD 279 Nanodelivery system: zein nanoparticles for entrapped hydrophobic/hydrophilic bioactives Thamida Chuacharoen, tchuac1@lsu.edu. Food Sci. and Tech., Suan Sunandha Rajabhat Univ., Bangkok, Dusit, Thailand NanoTech. has led to several innovative solutions for delivery of bioactives, which are loaded into engineered nanocarriers designed to optimize the potential of nanodelivered compounds. Because of the ability to either physically entrap or chemically link bioactives, zein has recently gained a reputation as a preferred nanocarrier for hydrophobic/hydrophilic compounds. In this research, hydrophobic lutein was physically entrapped in zein nanoparticles (ZNLT). Another loading mechanism system was folic acid (FA). Not only the health benefits of folic acid, but its ability to target folate-binding receptors in cancer cells makes folic acid outstanding, which was selected as a hydrophilic model. The amino acid side chains of zein can be covalently attached to the activated carboxylic group of folic acid and the link was confirmed by FTIR and $^1$H NMR. The physically loaded zein nanoparticles with entrapped folic acid (ZNFA) were also made as a control. A liquid-liquid dispersion method was successfully used to synthesize the particles with a combined lecithin and pluronic F127 to stabilize the system. The morphology was observed by transmission electron microscopy (TEM). The results revealed that the particle size of ZNLT was 216.5±29 nm with a small polydispersity (less than 0.3) and negative charge (~47.6±1.6 mV). Due to the hydrophobic nature, zein nanoparticles can strongly entrap lutein inside the matrix by electrostatic interactions and hydrogen bonds with 83±5.8% of the entrapment efficiency. The diameter of ZN-FA was 67.2±6.6 nm, which was smaller than 96.8±5.9 nm of ZNFA. The polydispersities of the two systems were less than 0.3 and zeta potential was -27.5±4.4 mV and -20.2±3.6 mV for ZN-FA and ZNFA, respectively. As expected due to the hydrophobicity of zein, the entrapment efficiency of ZNFA was lower than that of ZN-FA (10.53±2.7% compared to 35.51±1.4%), indicating that covalent linking improved the hydrophobic loading ability of zein nanoparticles. Thus, zein nanoparticles could be developed as promising drug nanocarriers for various applications.
AGFD 280 Evaluation of polycyclic aromatic hydrocarbons (PAHs) in edible palm oil produced in the Niger Delta, Nigeria Rafiu O. Raji1,2, Victoria O. Akpambang, veakpambang@futa.edu.ng. (1) Dept. of Chemistry, The Federal Univ. of Tech., Akure, Nigeria, Akure, Ondo, Nigeria (2) Pharmacognosy and Herbal Medicine, Faculty of Pharmacy, Niger Delta Univ., Wilberforce Island, Bayelsa, Nigeria Palm oil is an edible vegetable oil produced from the monococious oil bearing tree, *Elaeis guineensis*, which thrives in tropical and subtropical climate. In Nigeria, the oil palm industry is majorly dominated by small holders who use rudimentary equipment for palm oil processing. Palm oil is an important ingredient in food preparation in Nigeria and can predispose the population to exposure risk, if it contains high levels of polycyclic aromatic hydrocarbons (PAHs). This research aimed to evaluate the levels of PAHs in palm oil samples produced in two states of the Niger Delta, Nigeria, a region prone to pollution due to crude oil exploration and gas flaring activities. The samples were saponified before extraction with n-hexane, purified on solid phase extraction (SPE) columns and analysed using HPLC-FLD. The concentrations in the samples were found to contain <0.001 - 56.8, 0.6 - 57.2, 2.7 - 69.0 and 2.7 - 80.3 (µgKg⁻¹) for BaP, PAH4, PAH8 and ΣPAHs respectively. Approximately, 32% of the total palm oil samples were found to be below the European Union maximum residue limit of 2 µgKg⁻¹ for BaP. The health risk assessment, for a 60 kg person with a daily consumption of 28 g of palm oil, was also evaluated using the margin of exposure (MOE) approach. MOE values obtained were lower than 10,000 for approximately 58% of the samples evaluated. This indicates a potential concern for the health of the consumers of the palm oil. The data obtained from the study has helped to contribute to a scarce data on PAHs in palm oil, an edible vegetable oil from this region.

AGFD 281 Analysis and reduction of possible carcinogenic 4(5)-methylimidazole (MI) in a caramel colorant model system Kwang G. Lee, k Wonglee@dongguk.edu. Dongguk Univ., Jung Gu Seoul, Korea In this study, the 4(5)-methylimidazole levels in various 144 brown colored foods and beverages were determined. The brown colored foods and beverages were 62 processed sugars, 40 coffee, 9 caramel syrups, 18 red ginseng juice, 15 Japanese apricot fruit juice. The amounts of 4(5)-MI in brewed coffee (1821.3 ng/g) was the highest level among the samples. The 4(5)-MI concentration in processed sauce (47.6 ng/g) was the lowest level among the samples. The levels of 4(5)-MI in various samples found as follows: 47.6-1748.5 ng/g in processed sauces, 64.1-1821.3 ng/g in commercial coffee, 115.5-491.9 ng/g in caramel syrups, 91.0-854.1 ng/g in red ginseng juice and 137.6-567.4 ng/g in Japanese apricot fruit juice. Based on the 4(5)-MI levels, the estimated daily intake (EDI) and chronic daily intake (CDI) were calculated. EDI and CDI of red ginseng juice was the highest among all samples, and they were 1618.6 and 1256.8 ng/kg bw/day, respectively. The effect of various food additives on the formation of carcinogenic 4(5)-methylimidazole (4-MI) in a caramel model system was also investigated. The relationship between the levels of 4-MI and various pyrazines was studied. When glucose and ammonium hydroxide were heated, the amount of 4-MI was 556 ± 1.3 µg/mL, which increased to 583 ± 2.6 µg/mL by the addition of 0.1 M of sodium sulfate. When various food additives, such as 0.1 M of iron sulfate, magnesium sulfate, zinc sulfate, tryptophan, and cysteine, the amount of 4-MI was reduced to 110 ± 0.7, 483 ± 2.0, 460 ± 2.0, 409 ± 4.4, and 397 ± 1.7 µg/mL, respectively. The greatest reduction, 80%, occurred with the addition of iron sulfate. Among the 12 pyrazines, 2-ethyl-6-methylpyrazine with 4-MI showed the highest correlation (r = -0.8239).

AGFD 282 Decoding the taste of foods: What makes that cheese taste so good? Mathias Salger, mathias.salger@tum.de, Thomas Hofmann. TU München, Neufahrn, Germany Mammalian taste perception consists of the gustatory taste sensation, i.e. the sweet, bitter, sour, salty and umami basic taste modalities, as well as lingual somatosensory sensitivity resulting from temperature and tactile stimulation as well as chemical activation of chemosensory receptors on the perigemmal fibers. In combination, this sensory detection system provides valuable information on the sensory active ingredients of the food we eat. Although very important for the overall sensory quality of foods, compared to aroma-active volatiles, relatively little attention has been paid to tongue responses induced by non-volatiles. Aimed at creating a valuable foundation for a science-based optimization of food manufacturing processes, a so-called Sensomics approach has been developed in recent years to determine the molecular keys of very authentic taste perception of foods. This concept will be presented using young and matured Gouda and Parmesan cheese as examples. Among the key taste molecules, a series of kokumi-active gamma-glutamyl peptides, the formation pathways of which were clarified by ¹³C-labeling experiments, could be demonstrated to enhance the “matured” character of a cheese. Besides the amino acids, a series of bitter peptides, released from β-casein and α₂-casein, contributed to the long-lasting bitter taste of the Gouda cheese. For the first time, bitter tasting amino acids and peptides were assessed in their interaction with the 25 human TAS2R bitter receptors expressed in cell lines. Interestingly, bitterness of amino acids and peptides was found not to be mediated based optimization of food manufacturing processes, a so-called Sensomics approach has been developed in recent years to determine the molecular keys of very authentic taste perception of foods. This concept will be presented using young and matured Gouda and Parmesan cheese as examples. Among the key taste molecules, a series of kokumi-active gamma-glutamyl peptides, the formation pathways of which were clarified by ¹³C-labeling experiments, could be demonstrated to enhance the “matured” character of a cheese. Besides the amino acids, a series of bitter peptides, released from β-casein and α₂-casein, contributed to the long-lasting bitter taste of the Gouda cheese. For the first time, bitter tasting amino acids and peptides were assessed in their interaction with the 25 human TAS2R bitter receptors expressed in cell lines. Interestingly, bitterness of amino acids and peptides was found not to be mediated by specifically tuned TAS2Rs but brought about by an unexpected complex pattern of highly sensitive TAS2Rs, e.g. L-Phe and L-Trp activated TAS2R1 and TAS2R4, respectively, Trp-Trp-Trp activated also TAS2R14 and TAS2R46, whereas Tyr-Pro-Phe-Pro-Gly-Pro-Ile-His-Asn-Ser and Leu-Val-Tyr-Pro-Phe-Pro-Gly-Pro-Ile-Asn-His both activated TAS2R1 and TAS2R39.

AGFD 283 Changes in the key aroma compounds of dried shiitake mushroom induced by rehydration Philipp Cornelius Schmidberger, Philipp.Schmidberger@itz.tu-muenchen.de, Peter H. Schieberle. Technical Univ of Munich, Freising, Germany Due to their attractive aroma dried Shiitake mushrooms are very popular ingredients in Chinese cuisine. However, previous studies on the aroma compounds of dry Shiitake mushroom only focused on sulfur compounds and C8-carbon compounds while knowledge on the overall set of key aroma compounds is rather scarce. By application of the aroma extract dilution analysis (AEDA) on distillates prepared by extraction/SAFE-distillation from either dried or rehydrated Shiitake (*Lentinula edodes*, respectively), the key aroma compounds could be characterized. In the volatile fraction isolated from rehydrated Shiitake 47 odor-active compounds were located in the flavor dilution (FD) factor range of 8-8192. Among them, 4-hydroxy-2,5-dimethyl-3(2H)-furanone, 3-hydroxy-4,5-dimethyl-2(3H)-furanone, phenylacetic acid, and 2- and 3-methylbutanoic acid showed the highest FD factors. Furthermore, 1,2,3,5,6-pentathiepane and 1,2,4,5-tetrathiane appeared with high FD factors and elicited an aroma reminiscent of Shiitake. For a calculation of odor activity values (OAVs), stable isotope dilution assays were performed for which four isotopically labeled sulfur compounds had to be synthesized for the first time. A comparison of the OAVs of selected aroma-active compounds in dried and rehydrated Shiitake mushrooms revealed considerable changes during incubation with water.

AGFD 284 Evaluation of chiral heterocyclic key aroma compounds in cooked Allium-variety – A case study regarding organoleptic and quantitative characteristics Mario Flaim, mario.flaim@gmx.de, Michael Granovöl. (1) Deutsche Forschungsanstalt für Lebensmittelchemie, Freising, Germany (2) Tech Univ. of Munich, Freising Bavaria, Germany Various *Allium* varieties, e.g., onions, leek,
and shallots, are important, ubiquitous vegetables and spices that have been cultivated and used in food all over the world for millennia due to their unique smell. Among the large number of volatiles present in raw and processed *Allium* varieties, sulfur compounds are well-known to be the key odorants characterizing their overall aroma. Most recently, several chiral, heterocyclic alkyl-substituted sulfur compounds, cis-/trans-3,5-diethyl-1,2,4-trithiolane, cis-/trans-3,6-diethyl-1,2,4,5-tetrahydione, and cis-/trans-4,6-diethyl-1,2,3,5-tetrahydione, have been identified as characteristic and potent aroma compounds in cooked onions (*Allium cepa* L.), and were further reported to occur in other *Allium* varieties. Although present in trace amounts, sulfur-containing odorants often play a key role in the overall aroma of foodstuffs, mainly due to low odor thresholds. Despite being often neglected, also stereochemistry is a well-known aspect influencing the sensory properties of aroma compounds, namely odor quality and odor threshold. But, up to now, no comprehensive sensory evaluation and quantitative data considering the stereo-chemistry of cis-/trans-3,5-diethyl-1,2,4-trithiolane, cis-/trans-3,6-diethyl-1,2,4,5-tetrahydione, and cis-/trans-4,6-diethyl-1,2,3,5-tetrahydione in different cooked *Allium* varieties are available. The synthesis of the target compounds mentioned above was carried out, followed by method development for enantiomer separation applying multidimensional GC-MS techniques. After their unequivocal identification in cooked white and red onions, leek, shallots, chives, and spring onions by gas chromatography-olfactometry as well as gas chromatography-mass spectrometry, a stable isotope dilution assay (SIDA) was developed to determine their concentrations in the cooked *Allium* varieties. Quantitative data were completed by sensory evaluation with special emphasis on odor qualities of the isomers and odor thresholds in air.

AGFD 285 Differentiating organic and conventional tomatoes using ultra-performance liquid chromatographic fingerprints Huiping Guo1, guohipin123@sjtu.edu.cn, Weiyong Lu1, Huoying Chen1, Liangli L. Yu2. (1) Inst. of Food and Nutraceutical Science, School of Agriculture and Biological, Shanghai Jiao Tong Univ., Shanghai, China (2) Univ of Maryland, College Park, Maryland Organic foods are generally marketed at much higher prices than their conventional counterparts due to production method and consumer preference. Consequently, analytical technologies to differentiate organic foods from conventionally-grown counterparts is highly needed to ensure food quality and consumer confidence for organic labeling. Tomato is the second most important vegetable worldwide with a good taste and excellent nutritional properties. It is also considered as a functional food because it contains many antioxidants, such as ascorbic acid, vitamin E, carotenoids, flavonoids, lycopene, and phenolic acids. In this work, ultra-performance liquid chromatography (UPLC) techniques combined with multivariate data analysis were applied in differentiating organically grown tomatoes from counterparts that grown conventionally. Principal component analysis (PCA) of UPLC fingerprints could differentiate organic and conventional tomatoes. UPLC-MS analysis were also performed to provide comprehensive information about the chemical compositions of tomatoes. This study will provide fundamental research for tomatoes. Our results indicated that the non-targeted fingerprinting with the chemometric profiling techniques may be utilized in quality assurance of organic tomato products.

AGFD 286 Differentiating cultivation locations and flowering stages of chrysanthemum by UPLC fingerprints combined with chemometric data analysis techniques Li Yanfang1, Zoe Li@sjtu.edu.cn, Weiyong Lu1, Liangli L. Yu2. (1) Inst. of Food and Nutraceutical Science, School of Agriculture and Biology, Shanghai Jiao Tong Univ., Shanghai, China (2) Univ of Maryland, College Park, Maryland Chrysanthemum tea is a flower-based beverage made from chrysanthemum flowers of different cultivation locations or harvested from different flowering stages, which is very popular in East Asia. Various health properties were identified ove to the beneficial components found in chrysanthemum. Different chrysanthemum cultivars may vary in nutritional composition and market value. As a result, it is of great significance to differentiate the high-value chrysanthemum cultivars from the inexpensive ones. Non-targeted fingerprint combined with chemometrics data analysis were used to differentiate chrysanthemum from different cultivation locations in this study. An ultra-performance liquid chromatography (UPLC) fingerprint was obtained for each chrysanthemum sample after sample extraction. Different cultivars of chrysanthemum showed great differences after chemometrics data analysis of principal component analysis (PCA) and partial least-squares-discriminant analysis (PLS-DA). The chemical composition of each chrysanthemum was provided in detail by the UPLC fingerprints and the possible biomarkers were identified. Different flowering stages of bloom chrysanthemum and fetal chrysanthemum could be differentiated by chemometrics data analysis. Our results indicated that the non-targeted fingerprinting with the chemometric profiling techniques may be utilized in quality assurance of chrysanthemum tea products.

AGFD 287 Lateral flow assay exploiting aptamers for the extremely rapid detection of the anaphylactic allergen β-conglutinin Ciara O’Sullivan, ciara.osullivan@urv.cat, Miriam Jauset, Marketa Svobodova. Universitat Rovira i Virgili, Tarragona, Spain β-conglutinin is the predominant conglutinin subunit of lupin and in 2008 β-conglutinin was designated as the Lup an 1 allergen by the International Union of Immunological Societies (IUIS) and lupin was added to the list of substances requiring mandatory advisory labelling on foodstuffs. Aptamers have been developed against β-conglutinin and here we report on a method combining these aptamers with lateral flow for the rapid, facile and quantitative detection of β-conglutinin. Nitrocellulose strips were functionalised with β-conglutinin on the test line and DNA complementary to the aptamer selected against the β-conglutinin on the control line. Gold nanoparticles were prepared and linked to the β-conglutinin aptamer. Magnetic beads were functionalised with an optimised concentration of β-conglutinin, was mixed with β-conglutinin in the sample to be assayed in the presence of the gold nanoparticle functionalised aptamer for by hand agitation for 2 minutes and then wicked onto the lateral flow. A limit of detection of 5.5E-11M was achieved with a total assay time of just 10 minutes.

AGFD 288 Portable optoelectronic nose for rapid monitoring of meat freshness Zheng Li1, chemzheng24@gmail.com, Kenneth S. Suslick1. (1) Univ of Illinois, Urbana (2) Chemistry, Univ. of Illinois at Urbana-Champaign A linearized colorimetric sensor array (CSA) was integrated with a handheld device for the on-site assessment and monitoring of five meat products: beef, chicken, fish, pork and shrimp. The device takes advantage of a commercialized 1D CMOS camera to collect colorimetric data; lower noise level and improved scan rates were achieved compared to other digital imaging tools (Figure 1a). The design of CSA is based on strong chemical recognition between a set of chemo-responsive dyes and meat volatiles; various chemical dyes utilize organically modified silicates as porous and hydrophobic matrices to enhance their reactivity (Figure 1b). This sensor array overcomes the limitations of traditional electronic noses that physical or nonspecific intermolecular interactions dominate the sensor responses. The sensing device was employed for the real-time monitoring of meat products at room temperature over 24 h, which gives distinctive patterns of sensor signal from meat to meat and elevated sensor array response from 0 to 24 h (Figure 1c). Further monitoring of meat products over 96 h shows different levels of spoilage with regards to each
meat product and storage duration in triplicate trials, which can be classified and discriminated using hierarchical cluster analysis (HCA), with the classification accuracy ∼90% (Figure 2). This sensing method proves to be a promising supplement to other available techniques for meat product inspection.

AGFD 289 Ultrasensitive detection of the anaphylatic allergen b-conglutin exploiting lateral flow, tailed primers and isothermal amplification Ciara O'Sullivan, ciara.osullivan@urv.cat, Miriam Jauset, Marketa Sbodova. Universität Rovira i Virgili, Tarragona, Spain

An aptamer was selected against the b-conglutin subunit of lupin, identified as Lup an 1, the subunit causative of anaphylactic allergenicity. This aptamer was used in a competitive assay, with magnetic beads functionalised with b-conglutin, which competes with any b-conglutin present in the sample to be assay for binding to the selected aptamer. Following competition, aptamer was heat / pH eluted and subseq

AGFD 290 Fast method for sugar analysis of instant coffee samples Sachin Patil, sachin.patil@thermofisher.com, Jeffrey Rohrer. Thermo Fisher Scientific, Sunnyvale, California

World consumption of coffee has steadily increased in the past 50 years, growing from 57.9 million bags in 1964 to 142 million bags in 2012. Greater control at each processing step improves the ability to produce a high quality coffee. The carbohydrates are an important constituent of the coffee beans forming about 50% of the green coffee bean dry weight. These carbohydrates undergo complex changes during the roasting process and can affect the final taste and aroma properties of the coffee. Carbohydrate content is used for detecting coffee adulteration. Carbohydrates impact viscosity, which plays an important role in soluble coffee processing. Our lab previously developed a high-performance anion-exchange chromatography with pulsed amperometric detection method for determination of carbohydrates in coffee using the Thermo Scientific Dionex CarboPac™ column with electrolytically generated eluent. The current study updates the fast method with a Dionex CarboPac™ column. Due to smaller particle size this column provides more efficient peaks and better resolution making the sample analysis easier and more reliable. The reduced particle size also allows for a reduction in analysis time. The method proposed here separates nine common carbohydrate sugars in less than six minutes, which allows for shorter sample turnaround times and reduced eluent consumption, and thereby improving the overall process economics. Using this method, carbohydrates present in soluble as well as total carbohydrate extracts of instant coffee were quantified is less than six minutes as shown in Figure 1. The method results in linear response for carbohydrate sugar concentrations from 3 to 800 mg/L with excellent retention time and peak area precisions. The method is robust to matrix effects as demonstrated by high recoveries of spiked carbohydrate sugars from all samples studied.

AGFD 291 Variations in the enantiomeric composition of thujone-containing essential oils Jack D. Williams1, jwilliams@mercyhurst.edu, Kristin A. Anderson1, Jessica A. Yazarians2, Gregory R. Boyce2, (1) Chemistry and Biochemistry, Mercyhurst Univ., Erie, Pennsylvania (2) Chemistry and Physics, Florida Gulf Coast Univ., Fort Myers

The enantiomeric composition of common thujone-containing essential oils was determined using headspace solid phase microextraction followed by gas chromatography-mass spectrometry (HS-SPME-GC-MS). Significant variability was observed in the enantiomeric excesses of several common phytochemicals including thujone, camphor, and linalool in the essential oils of Thuja occidentalis, A. fragrantissima, Tanacetum vulgare, Artemisia vulgaris, and Artemisia herba-alba. Salvia officinalis L. and Salvia labiundulaefolia were found to possess a high enantiomeric excess favoring the unusual enantiomers (+)-α-thujone and (-)-β-thujone which were unreported in nature prior to this study. Since racemic thujone is not commercially available, a three-step synthesis of racemic thujone was developed to afford the standard sample required for the initial chiral resolution.

AGFD 292 Improved method for determination of biofuel sugars by HPAE-PAD Sachin Patil, sachin.patil@thermofisher.com, Jeff Rohrer. Thermo Fisher Scientific, Sunnyvale, California

Measurement of the breakdown of lignocellulose into fermentable carbohydrates is used to monitor the efficiency of biomass-to-biofuel conversion, and is directly related to target biofuel yield and the process economics. Hence, this is a crucial step in biofuel production process. Although, development of robust analytical methods still remains a challenge. High performance anion-exchange chromatography with pulsed amperometric detection (HPAE-PAD) can be used to determine carbohydrates in these samples. HPAE-PAD has been shown to deliver fast carbohydrate determinations in biomass hydrolysates using the Thermo Scientific™ Dionex™ CarboPac™ column. Determination of carbohydrates in acid-hydrolyzed corn stover samples was shown in Thermo Scientific Application Update 192 (AU192). The method uses electrolytically generated hydroxide eluent resolve nine common biomass sugars (fucose, sucrose, arabinose, galactose, glucose, xylose, mannose, fructose, and cellobiose). The current work updates the system used for the carbohydrate analysis in AU192. The new system combines flexibility and ease-of-use with high sensitivity and selectivity, bringing a new level of convenience and cost effectiveness to simple sugar analysis. Here nine common carbohydrate sugars are separated in less than eight minutes, which allows for shorter sample turnaround times and reduced eluent consumption, and thereby improving the overall process economics. Using this method, biofuel carbohydrates present in 10 different biofuel samples were quantified. Figure 1 shows a representative chromatogram for standard containing the eight common biofuel carbohydrates and fucose as an internal standard at 0.6 g/L. All the peaks are well resolved and the separation is completed within 8 minutes. The method is linear from 0.005 to 2 g/L for the eight target carbohydrates. The retention time and peak area percent relative standard deviations (%RSDs) are less than 1.26% for all biofuel carbohydrates indicating excellent method precision. More over the method proposed here is robust and does not show significant change in retention time and peak area after 200 injections of biofuel samples. In summary, the method proposed here will improve the reliability of biomass-to-biofuel efficiency calculations.
AGFD 293 Metabolomics characterization of bottled wine: impact of environmental parameters

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(1) Chesapeake Biological Lab, Solomons, Maryland (2) TUM, Munich, Germany (3) Université de Bourgogne, Dijon, France (4) BGC, Helmholtz Zentrum München, Munich, Germany (5) Laboratoire de Stress, Défences et Reproduction des Plantes, Université de Reims Champagne-Ardenne, Reims, France

From a chemical composition point of view, wine is the result of complex interplays between environmental, genetic and human factors. Metabolic compositions of grapes and related wines are complex and include primary (e.g., sugars, organic acids, amino acids) and secondary metabolites (e.g., flavonoids, anthocyanins and other pigments). The idea of wine metabolomics is to provide a comprehensive chemical picture of a complex wine system, through the analysis of as many metabolites and different compound classes as possible. Direct injection ion cyclotron resonance Fourier transform mass spectrometry (FTICR-MS), which provides unrivalled resolution, ultra-performance liquid chromatography mass spectrometry (LC-MS), which increases the scope of detectable metabolites and allows the separation between isomers, Nuclear Magnetic Resonance (NMR) spectroscopy which provides detailed structural compositions and Excitation Emission Matrix Fluorescence (EEMF) have been combined. Powerful statistical tools and relevant databases were used in combination to the analytical platforms in order to provide an unprecedented synoptic description of the chemical composition diversity of wine. Such tools were applied to the characterization of chemical composition specifically related to aging, in verticals series including very old wines considered as evolution end points. The study of series of wines reveals that chemical spaces related to oenological practices (SO\textsubscript{2} addition at pressing, permeability of the stopper) could be deciphered although the vintage signatures were confirmed to be the most significant. Finally, non-targeted analyses of wines from different appellations revealed that terroir-related signatures could be read, in particular after a few years of bottle ageing.

AGFD 294 Estimation of total phenolic compounds in leaf tissues of American chestnut (Castanea dentata), Chinese chestnut (Castanea mollissima), and their back-cross breeding generations Jinyan She, shejinyan@hotmail.com. Chemistry, Mississippi State Univ.

American chestnut tree (Castanea dentata) was one of the dominant tree species in Appalachian Mountains, and plays an important role in the ecology system. However, it was nearly eliminated by chestnut blight caused by cryphonectria parasitica. Studies show that phenolic compounds produced by plants are significant to their defense mechanisms against fungal pathogens. In this study, we developed an analytical methodology to estimate the total phenolic content in leaf tissues of American chestnut (Castanea dentata), Chinese chestnut (Castanea mollissima), and their back-cross breeding generations (B3F2 and B3F3) using Folin Ciocalteu reagent assay with UV/Vis spectrophotometry. The preliminary results from leaf tissues extraction in solvent to sample ration 5:1, methanol/water (95%:5% v/v), pH 2, and 765 nm showed that the variations among these four tree species are significant (p < 0.05). In addition, the kinetics solid-liquid extraction of phenolics was elaborated using Peleg, first/second order, and power law models.

AGFD 295 Microwave-induced chemical synthesis of oxidized lanosterol and cholesterol derivatives using KMnO\textsubscript{4}-CuSO\textsubscript{4} catalyst: Potential target molecules for clearing up protein aggregation in diabetes patients suffering from cataract formation Bishamber Dayal\textsuperscript{1}, dayalb77@gmail.com, Jesse Chou\textsuperscript{2}. (1) Medicine, Rutgers Univ. New Jersey Medical School, Princeton Jct (2) Undergraduate Participant, Dept. of Chemistry, Princeton Univ., New Jersey

Recent exciting studies reported in ("Ophthalmology: Cataracts dissolved", July 2015) described that cholesterol like molecules, lanosterol and 25-hydroxycholesterol, have the potential to treat and clear up cataracts in individuals suffering from Type-2 diabetes and other age-old diseases. Cloudy vision in subjects with cataracts is primarily caused by eye lens protein (α-, β-, and γ-crystallins) aggregation, which clump together to cause cataracts. Although cataract formation is also caused by genetic mutations in eye lens proteins, a vast majority results from clumped aggregated proteins damaging eye lens in hyperglycemia Type-2 diabetes conditions. Since 25-hydroxy cholesterol and lanosterol have been tested and implicated to be responsible for clearing up cataracts in animal studies, we have initiated a small molecule synthesis of oxidized and epoxidized cholesterol and lanosterol like molecules via a facile microwave-induced preparation using KMnO\textsubscript{4}-CuSO\textsubscript{4} catalyst. The resulting oxidized compounds were resolved and analyzed via analytical and preparatory TLC, and structures were confirmed by Fast-Atom Bombardment Mass Spectrometry (TLC-FABMS). Results: 3-acetate 24,25-lanosterol epoxide exhibited M/Z= 485. In the presence of KCl it showed [M’ + 2K’ + H’] (M/Z=564), 3,24-diketo, 25-hydroxy lanosterol exhibited M/Z=457. Cholesterol epoxide M/Z=401, 4,5-epoxy 25-hydroxy cholesterol M/Z=417, Epoxidation of cholesterol palmitate with this reagent provided [M’ + H’ + Na’ + Cu’\textsuperscript{2+}] = 727. We believe MW-Induced rapid synthesis of such small oxidized lanosterol and cholesterol derivatives may be helpful in studying the unfolding process of proteins as well as clearing up cataract formation in patients suffering from Type-2 diabetes. Such molecules may have the potential to be better therapeutic targets for the prevention and treatment of cataracts in both diabetes and Alzheimer’s disease patients.
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