



the

CORNUCOPIA

including AGFD abstracts for the
242th American Chemical Society National Meeting

August 28 - September 1, 2011

in

DENVER

NEIL DA COSTA, Program Chair

Dear Readers -

This issue of *the Cornucopia* is the last that the AGFD Division will distribute to the entire membership by surface mail. Starting with the spring 2012 issue a PDF of *the Cornucopia* will be posted for download on the AGFD website 6-8 weeks prior to national meetings. National meeting attendees can still obtain a printed copy of *the Cornucopia* at the AGFD hospitality table.



CONTENTS

page	
2	Message from the Chair
2	Cornucopia editorial staff and contact information
3	Future AGFD programs and other programs
5	Award News
6	Latest installment in the continuing illustrated saga - Mussinan's Memoirs
7	Spring AGFD Reception
8	Puzzle page
9	Membership application - join the team !
10	Roster of officers and committee members
11	Meeting Minutes
13	Schedule of AGFD meetings and merrymaking
13	AGFD technical program w/abstracts

visit our website: <http://agfd.sites.acs.org> - for a pdf of the Cornucopia and much more

deadline for submission of content for next Cornucopia: Jan 15

MESSAGE FROM THE CHAIR

It has been a pleasure serving as Chair of the Agricultural and Food Chemistry Division (AGFD) of ACS. It is also my pleasure to turn the gavel over to our incoming Chair Neil Da Costa. We are in good hands.

The 241st ACS National meeting held in Anaheim CA was a tremendous success with great weather and 25 outstanding sessions supporting the ACS thematic programming *Chemistry of Natural Resources*. This meeting celebrated the achievements of scientists in three International Year of Chemistry (IYC) symposia that highlighted the contribution of women and the achievements of international scientists in agricultural and food chemistry, and helped to increase public appreciation of our globally important field. Prof. Henrick was the recipient of the prestigious Kenneth A. Spencer award.

The theme for the upcoming the 242nd ACS National meeting in Denver, CO will be the *Chemistry of Air, Space and Water*. This meeting is expected to be just as exciting as the Anaheim meeting offering 11 symposia with 18 sessions. AGFD has been selected as a finalist for the ChemLuminary award in recognition of *Innovation and Outstanding Service* to members. Recipient(s) will be announced and the presentation of awards will occur Tuesday, Aug. 30, at the meeting.

We value our member input and would like to encourage you to get involved in directing AGFD programming. Please join us in Denver for the AGFD Future Programs Meeting to be held on Monday, Aug. 29, to share ideas for future symposia. If you are unable to attend the meeting please send your ideas to AGFD chair-elect Neil Da Costa or myself, and we will present your ideas at the meeting.

I have thoroughly enjoyed serving as chair and want to express my sincere gratitude to the AGFD executive committee, symposium organizers, subdivision and committee chairs and councilors for their tireless efforts and numerous contributions that make AGFD the terrific division that it is. I am especially grateful for the support and guidance of past chair Mike Appell and chair-elect Neil Da Costa. These outstanding individuals have made volunteering for ACS and AGFD an enjoyable and rewarding experience

Alyson Mitchell
2011 AGFD Chair
aemitchell@ucdavis.edu



CORNUCOPIA EDITORIAL STAFF & CONTACT INFORMATION

Editor-in-Chief	C. Frey	Pepsi-Cola R&D	carl.frey@pepsico.com	914-742-4832
General Manager	P. White			
Staff	C. Kent, L. Lane, J. Olsen			

FUTURE PROGRAMS

SAN DIEGO - March 25 - 29, 2012

Carotenoid Cleavage Products - Peter Winterhalter, Technische Universität Braunschweig p.winterhalter@tu-bs.de
Sue Ebeler, U. of California - Davis seebeler@ucdavis.edu Russell Rouseff U. of Florida RLR@crec.ifas.ufl.edu

Chocolate: Science and Technology - Joe A. Vinson, University of Scranton vinson@scranton.edu

Graduate Student Symposium - Charles Brine, CJ Brine and Associates brinec11@verizon.net

General Papers and General Posters - Neil Da Costa, International Flavor and Fragrances neil.dacosta@iff.com;
Lauren Jackson, FDA Summit-Argo, Illinois Lauren.Jackson@fda.hhs.gov

Hispanic Foods co-sponsored by AGRO - Michael H. Tunick, Dairy Processing and Products Research Unit,
USDA, ARS, Eastern Regional Research Center michael.tunick@ars.usda.gov Elvira D. De Mejia, Univ. of Illinois -
Urbana-Champaign, Dept. of Food Science and Human Nutrition edemejia@uiuc.

Metabolism and Bioavailability of Bioactives - Alyson Mitchell, University of California, Davis
aemitchell@ucdavis.edu Navindra Seeram, University of Rhode Island nseeram@mail.uri.edu; Fereidoon Shahidi,
Memorial University of Newfoundland, Department of Biochemistry fshahidi@mun.ca

Undergraduate Symposium - Charles Brine, CJ Brine and Associates brinec11@verizon.net

Measuring Flavor Dynamics - Andy J. Taylor, The University of Nottingham andy.taylor@nottingham.ac.uk

Food Allergens - Lauren Jackson, FDA Summit-Argo, Illinois Lauren.Jackson@fda.hhs.gov

Nano-microencapsulation of Bioactives - Ron Huang, Rutgers, Dept of Food Science rhuang@aesop.rutgers.edu

Sample Preparation for Nutraceutical & Functional Food Analysis (Plus Workshop) - Dave L. Luthria USDA,
Beltsville MD D.Luthria@ars.usda.gov

Flavonoid Nutrition and Interactions - Fereidoon Shahidi, Memorial University of Newfoundland, Department of
Biochemistry fshahidi@mun.ca

Nanotechnology for Food and Agriculture - Bosoon Park bosoon.park@ars.usda.gov
Michael Appell Michael.appell@ars.usda.gov

ACS National Meeting Theme for Spring 2012, San Diego - Chemistry of Life.

PHILADELPHIA - August 19 - 23, 2012

AGFD Division Award Symposium - Neil Da Costa, International Flavor and Fragrances neil.dacosta@iff.com

Discovering Active Compounds - John Finley, Louisiana State University Agcenter JFinley@agcenter.lsu.edu;
Navindra Seeram, University of Rhode Island nseeram@mail.uri.edu

Neuroactive Compounds from Natural Products - Agnes M. Rimando; USDA ARS NPURU, 662-915-1037
agnes.rimando@ars.usda.gov

Essential Oils: Natural Materials for Flavor, Fragrance and Bioactives - Neil Da Costa, International Flavor and
Fragrances neil.dacosta@iff.com

General Papers and General Posters - Lauren Jackson, FDA Summit-Argo, Illinois Lauren.Jackson@fda.hhs.gov

continues on the next page

continued from the previous page -

Instrumental Methods for the Analysis of Bioactive Molecules (co-sponsored by AGRO) - G. K. Jayaprakasha; Texas A&M University gjayaprakasha@ag.tamu.edu Bhimu Patil; Texas A&M University b-patil@tamu.edu

Snack Foods - Fereidoon Shahidi Memorial Univ. of Newfoundland, Dept. of Biochemistry fshahidi@mun.ca

Synthesis of Natural Products: New Reagents and Reactions - Michael Appell; USDA-ARS-NCAUR michael.appell@ars.usda.gov Richard Petroski USDA-ARS-NCAUR richard.petroski@ars.usda.gov

Young Scientist Award Symposium - Charles Brine, CJ Brine and Associates brinec11@verizon.net

Fruit and Vegetable Aroma Precursors - Gavin Sacks Cornell University gls9@cornell.edu

Sterling Hendricks Memorial Lectureship - (co-sponsored w/AGRO) Michael H. Tunick, USDA, ARS, EasternRegionalResearchCenter michael.tunick@ars.usda.gov Kim Kaplan, USDA-ARS, Beltsville, MD kim.kaplan@ars.usda.gov Stephen O. Duke, USDA-ARS University, MS sduke@olemiss.edu

Applications and Advances in Centrifugal Particle Chromatography in Natural Products - John Mathy USDA, john.mathy@ARS.USDA.gov

Kenneth A. Spencer Award Symposium - Eckhard Hellmuth, UMKC, Kansas City, MO hellmuthe@umkc.edu

Physical Methods in Food Analysis - Michael H. Tunick, USDA, ARS, EasternRegionalResearchCenter michael.tunick@ars.usda.gov Charles I. Onwulata, USDA, ARS, Eastern Regional Research Center Charles.onwulata@ars.usda.gov

ACS National Meeting Theme for Fall 2012, Philadelphia - Materials for Health & Medicine

NEW ORLEANS - April 7 -11, 2013

Natural Products for Health and Pharmaceuticals and Biotech - John Finley, Louisiana State University Agcenter JFinley@agcenter.lsu.edu

Chemistry of Cajun Cuisine

Chemistry of Reduced Sodium Foods - Lauren Jackson, FDA Summit-Argo, Illinois Lauren.Jackson@fda.hhs.gov

ACS National Meeting Theme for Spring 2013, New Orleans - Chemistry of Energy and Food

INDIANAPOLIS - September 8 - 12, 2013

High Performance Foods

ACS National Meeting Theme for Fall 2013, Indianapolis - Chemistry in Motion

DALLAS - March 16 - 20, 2014

SAN FRANCISCO - August 24 - 28, 2014

Importance of Chirality to Flavor Compounds - Karl-Heinz Engel, Technical University of Munich, Germany, k.h.engel@wzw.tum.de

Other PROGRAMS and SYMPOSIA - unscheduled or beyond 2013

Authentication and Adulteration of Food - Fereidoon Shahidi Memorial University of Newfoundland, Department of Biochemistry fshahidi@mun.ca

continues on the next page

continued from the previous page -

Colorants and Pigments - Fereidoon Shahidi, Memorial University of Newfoundland, Department of Biochemistry
fshahidi@mun.ca Kazuo Miyashita Hokkaido University kmiya@fish.hokudai.ac.jp

Flavor Stability: Chemical Changes in Flavor Molecules, Flavor-Food Matrix Interactions, Flavor Encapsulation - Mathias Sucan mksucan@aol.com

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

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

SAVE THE DATES

May 28 to
June 1, 2012



AGFD invites you to visit the beautiful Greek Isles for the **2012 International Flavor Conference**



A pre-conference ISNFF workshop on nutraceuticals and functional foods is also scheduled for May 26-28.

Look for more details in the next newsletter and online at www.emich.edu/flavor



Join us in Greece in 2012 OPA!!!

AWARD NEWS

Agnes Rimando - 2010/2011 Researcher of the Year

The executive committee of the Ole Miss Section of the ACS selected Dr. Agnes M Rimando, a USDA Research Chemist with the Natural Products Utilization Research Unit as the Researcher of the Year.

Dr. Rimando is internationally known for her research of natural products that provide health and medical benefits, as well as natural product-based pest management agents. She has published extensively and presented research findings at meetings and conferences across the globe. Her current research focuses on pterostilbene, a compound found in blueberries and grapes with potential benefits that include antioxidant activity, the ability to regulate and control cholesterol and sugar levels, and prevent colon cancer. Her research has assisted in the development and production of several dietary supplements that will soon be available in retail locations. A past Chair of the Local section, Dr. Rimando is currently serving on the ACS Council, representing AGFD. She also hosts the annual research poster symposium in the National Center for Natural Products Research at the University of Mississippi. The officers and membership of AGFD congratulate Dr. Rimando and look forward to the continuance of her outstanding career.



MUSSINAN'S MEMOIRS

ANAHEIM JOINT ACS AND CHEERLEADING CONVENTION

What is this? Hey, that's what I wondered myself. Seems like there are equal numbers of chemists and cheerleaders here. As you might imagine, it's extremely difficult to tell them apart!! Hopefully they'll all go home tomorrow so that the line at Starbucks is reduced to only a half mile or so. First things first as usual. To the right you see the latest picture of my granddaughter. As you can see, she's getting bigger and has now taken up stand up paddle boarding.

The second issue is the question of our photo contest. I actually had two entries, but since it's now June 15, I've managed to lose them along the way. Therefore, since this is such a lovely picture, I'm going to submit it again. Look carefully at the photo below..

1. Can you identify the subject on the right?
2. Can you identify the subject on the left
(Creativity in naming counts)?
3. Can you identify the location?
4. How about the year?



Enter now for a once in a lifetime chance (if your lucky) to win a genuine IFF pen and pencil set from 1992 (and may not work) plus an authentic hotel pen! OK enough of that.



To fulfill the duties – symposia good; attendance good. So, Monday afternoon we prepared for our play date. With split second timing, we got lunch, rounded up the group and went for our Enterprise rent-a-car - - - oops! No one was there, and no one was going to be there for 20 min. Undaunted, we raced across to the Marriott, snagged a Hertz and faster than a speeding bullet (maybe that's Superman) we arrived at Warner Bros with 4min to spare. This tour was very good and entertaining. On the way back we decided to get a drink at Roy's. We didn't have much time. They had no tables until 9pm, but Gail Tunick leaped over the railing and snagged one just as someone stood up. We had a great dinner there.

Tonight is our reception. We are going to dinner afterwards, but not to Clancy's again. Gail suggested Bucco de Bo-Peep or something. Should be good. Next stop Denver. Bring your boots and spurs!

continued from the previous page

From the Spring AGFD reception -

(clockwise, starting at right)

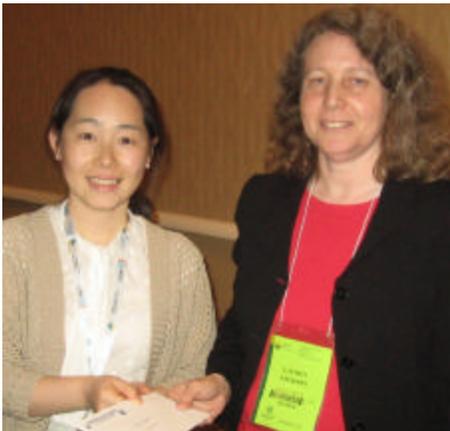
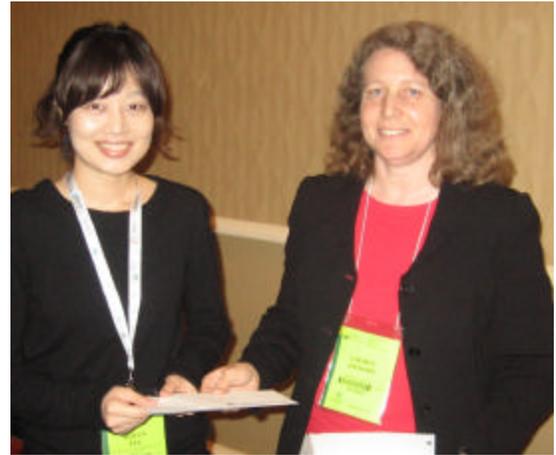
Lauren Jackson presents the second place prize in the Withycombe-Charalambous Graduate Student Research Symposium to Jihyun Lee, University of California-Davis.

Students who participated in the two award symposia.

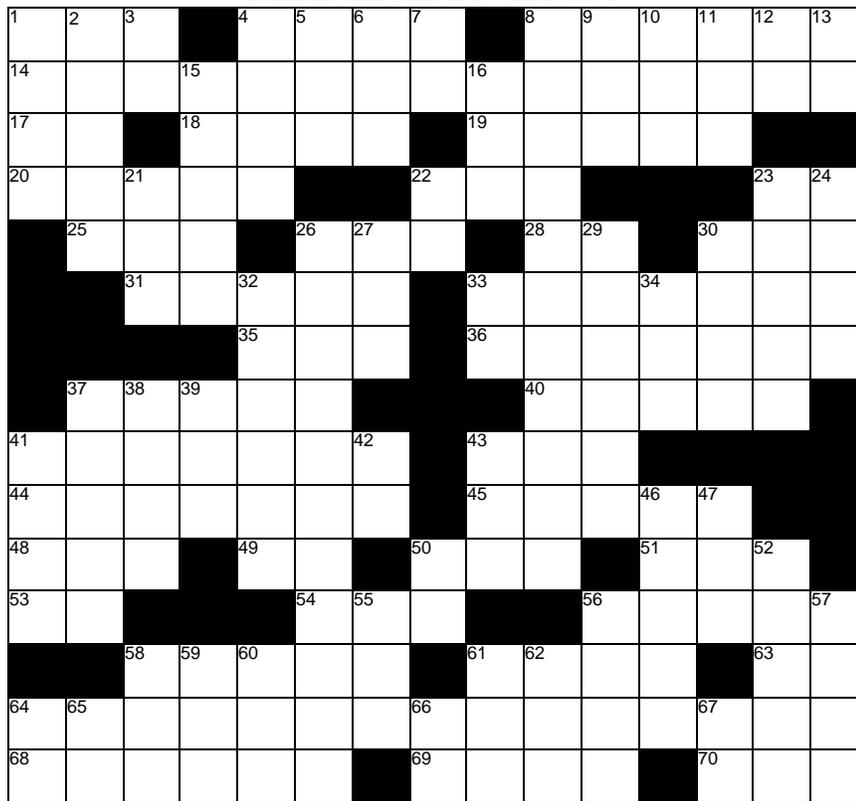
Lauren with Kimberly Hibshman, Lebanon Valley College, winner of the Undergraduate Student Research Award Competition

AGFD Immediate Past Chair Mike Appell passes the gavel to Chair Alyson Mitchell

Lauren presents the first Withycombe-Charalambous Graduate Student Research Symposium prize to Hyeyoung Lee, UC-Davis.



MILE HIGH DIVERSION



A prize to the first to fax
a correct solution to:
Carl Frey at 914-749-3329

Congratulations to the
winner of the coveted
Spring 2011 prize -
Michael Auerbach .
of MARS, Inc

and kudos to other puzzlers -
R. Rauscher, D. Whiteside,
B. Jones, F. Al-Thaer, B. Baldi
N. Pennington, D. Blackwell

ACROSS

- 1 reference to any boat
- 4 he's a jolly good fellow
- 8 ----- lounge
- 14 range west of Denver
- 17 0.9% of the atmosphere
- 18 model's stance
- 19 boring state
- 20 beverage with peppy ads
- 22 briefly frequent
- 23 consumption
- 25 element of Aristotle
- 26 a long way away
- 28 med-- or cil--
- 30 corporate head honcho
- 31 stoneworker
- 33 performer's gifts to fans
- 35 the boy king
- 36 prepares leftovers
- 37 stripteaser
- 40 zero degrees on a
compass
- 41 act of contrition
- 43 cool 60s-70s Pontiac
- 44 once -----, Burma,
now Yangon, Myanmar
- 45 cowboy's loop
- 48 J.K Jerome's *Three
Men --- Boat.*
- 49 Jr's dad
- 50 I.M. guffaw
- 51 snub-nosed dog
- 53 lead-in to a Ph. D
- 54 fatigue fighter
- 56 Roman citrus beverage ?
- 58 neutralization volume
- 61 result of a planted acorn
- 63 cc
- 64 Colorado military school
- 68 20-Across go-with
- 69 World Cup exclamation!!!
- 70 negative prefix

DOWN

- 1 con-man's game
- 2 *Star-Trek* silicon creature
- 3 Chicago commuter option
- 4 proudly boast
- 5 suffers from
- 6 Gator--- or lemon---
- 7 river of Milan, Italy
- 8 Belushi flick:----- *Divide*
- 9 bitter almond toxin
- 10 half of a Heyerdahl title
- 11 grandson of 49 Across
- 12 phot ocell element
- 13 element of genius
- 15 *Tosca* or *Aida*
- 16 ump
- 21 not the brightest
- 22 optional conjunction
- 23 canines
- 24 Bruce Springsteen (w/The)
- 26 CO, UT, AZ, NM nexus
- 27 colony member
- 29 allergy symptoms
- 30 Demo--- or Dixie----
- 32 dictation recorders
- 33 MD or RN workplace
- 34 anthem contraction
- 37 black, navy and green
- 38 Netrebko or Karenina
- 39 *Maple Leaf* --- or *Tiger* ---
- 41 proper mate
- 42 printer measure
- 43 pop art paint: Day ---
- 46 listened in
- 47 Parisian assent
- 50 pre-tape recording medium
- 52 colorful bear
- 55 circular segment
- 56 ---- marsala or ---- scallopini
- 57 laminates
- 58 prefix meaning 3
- 59 food sci. assn.
- 60 also
- 61 Chinese philosophy/path
- 62 *His Master's Voice* company
- 64 --L-CIO (labor union)
- 65 structure determination test
- 66 short for 'for instance'
- 67 Johnny Depp role: '- Wood'

AGFD DIVISION MEMBERSHIP APPLICATION

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

- organizing AGFD symposia at ACS National Meetings and other venues
- providing workshops in AGFD topics
- publishing proceedings of AGFD symposia
- providing cash awards to leading grad students, post docs, and established AGFD scientists
- publishing *the Cornucopia* newsletter
- hosting social gatherings at national meetings

Join the over 2600 members of the AGFD division. At ACS National Meetings you can meet and discuss division activities at the AGFD hospitality table located near the AGFD technical session rooms. Use the membership application form (below) or join on-line at www.acs.org (click on Technical Divisions and then select Join a Division).

APPLICATION FOR AGFD DIVISION MEMBERSHIP (7623P)	
title	
name	
1 st address line	
2 nd address line	
city	
state	
Zip code	
country	
e-mail address	
phone	
check one	MEMBERSHIP FEE
<input type="checkbox"/>	I am an ACS member and wish to join AGFD (\$8.00)
<input type="checkbox"/>	I am not an ACS member and wish to join AGFD (\$10:00)
<input type="checkbox"/>	I am a full time student and wish to join AGFD (\$5.00)
Be cool JOIN AGFD	Return application, with payment, 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 MEMBERS

Chair - Serves 1 year. Presides over Division meetings, & appoints committees
Alyson Mitchell
University of California
One Shields Ave.
Davis CA 95616-8598
530-752-1465 aemitchell@ucdavis.edu

Chair-Elect - Serves 1 year. Substitutes for the chair as needed
Neil Da Costa
International Flavors and Fragrances R&D
1515 Hwy. 36
Union Beach NJ 07735
732-335-2110 neil.dacosta@iff.com

Vice Chair - Serves 1 year. Assists Chair-elect in developing future technical programs.
Lauren S. Jackson
USFDA, National Center for Food Safety & Technology
6502 S. Archer Rd.
Summit-Argo, IL 60501
708-728-4162
Lauren.Jackson@fda.hhs.gov

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.
Cynthia Mussinan
International Flavors & Fragrances R&D
1515 Hwy. 36
Union Beach NJ 07735
732-335-2401 cynthia.mussinan@iff.com

Cornucopia Editor - Edits Division newsletter.
Carl Frey
Pepsi-Cola R&D, 100 E. Stevens Avenue,
Valhalla NY 10595 914-742-4832
carl.frey@pepsico.com

Councilors - Represent Division for 3 years on ACS council.
John Finley (thru '11),
jfinley@agcenter.lsu.edu
Michael Morello (thru '11),
mike_morello@pepsico.com
Agnes Rimando (thru '12),
agnes.rimando@ars.usda.gov
Sara Risch (thru '13),
srisch@sbcglobal.net

Alternate Councilors - Substitute for Councilors that can not attend Council meetings. Serve 3 years.
Charles Brine (thru '12),
brinec11@verizon.net
Keith Cadwallader (thru '11),
cadwlldr@uiuc.edu
Russ Rouseff (thru), rlr@crec.ifas.ufl.edu
Fereidoon Shahidi (thru '13)
fshahidi@mun.ca

At-Large Executive Committee Members - Assist in management of Division. Serve 3 years.
Terry Acree (thru '13), tea2@cornell.edu
Jane Leland (thru '11),
jleland@kraft.com
Robert McGorin (thru '11),
robert.mcgorin@oregonstate.edu
Mathias Sucan (thru '13)
mksucan@aol.com

Awards Committee - Solicits nominations and oversees awards process.
Chair - Steve Nagy
agscience@aol.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
Michael Appell,
michael.appell@ars.usda.gov

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

Membership - Responsible for recruitment and retention of Division members.
Lucy Yu - lyu5@umd.edu

Nominations - Develops slate of officers. Served by Immediate Past Chair.
Michael Appell
Michael.Appell@ars.usda.gov

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

Web Master - Maintains web site.
Victoria Finkenstadt,
victoria.finkenstadt@ars.usda.gov

Flavor subdivision - Develops symposia.
Chair - Kotamballi N.C. Murthy,
kncmurthy@neo.tamu.edu
Chair-Elect - Kevin Goodner,
klg@sensusflavors.com
Vice-Chair - Gavin Sacks,
gls9@cornell.edu
Secretary - Sanjay Gummalla,
sanjay_gummalla@cargill.com

Functional Foods & Natural Products subdivision - Develops symposia.
Chair - Guddadarang Jayaprakasha,
gayaprakasha@ag.tamu.edu
Chair-Elect - Navindra Seeram,
nseeram@mail.uri.edu
Vice-Chair - Gene Lester,
gene.lester@ars.usda.gov
Secretary - Luke Howard,
lukeh@uark.edu

**This space reserved
for your name.**

**Stop by the AGFD hospitality
table and find out how you
can get involved.**

AGFD EXECUTIVE COMMITTEE MEETING MINUTES

Sunday, March 27, 2011 Marriott Hotel, Anaheim, CA

Takes place at each ACS National Meeting

Attendees: Michael Appell, Neil Da Costa, Katya Delak, Robert Hauserman, Chi-Tang Ho, Lauren Jackson, Gene Lester, Steven Meyers, Alyson Mitchell, Michael Morello, Cynthia Mussinan, Agnes Rimando, Sara Risch, James Seiber, Fereidoon Shahidi, Michael Tunick

AGFD Chair Alyson Mitchell called the meeting to order at 5:13 p.m.

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

Cynthia Mussinan gave the **Treasurer's Report**. The investments gained \$11,764 last year. The Boston banquet cost \$11,000 and there apparently have been no proceeds from the Flavor Workshop held there. The treasury has \$461,571.

Steve Meyers and Katya Delak distributed a handout about current programs from the **Office of International Activities**. Mike Morello mentioned the possibility of webinars for those who cannot attend ACS meetings. Gene Lester brought up the emphasis on South American scientists and Hispanic institutions.

Bob Hauserman gave a report on **ACS Books**. AGFD has contributed 26 books since 2006, more than any other division. Chapters go online 4-6 weeks after the book is complete; print copies take 4-5 months. The first full year of the program was 2010, and the number of chapters downloaded has increased by 202% from February 2010 to February 2011. There are now 27,000 chapters online ACS-wide. Scientists and institutions pay once for access to the backlist/archived chapters (those more than one year old) and pay annually to the frontlist/new chapters.

In the **Program Report**, Alyson Mitchell noted that there were 21 sessions and 208 abstracts. There are two **International Year of Chemistry** symposia. Neil Da Costa pointed out that no-shows in the poster sessions cost ACS \$125 each. ACS checks for no-shows and warns those scientists. The Denver meeting has ten symposia, 20 sessions, and two co-sponsored symposia according to Neil. Because of extra costs for obtaining speakers for his symposium, Neil asked for an extra \$750, which was approved. He and Alyson emphasized that abstracts have to be submitted on time. A budget of \$15,000 for Denver was approved. Cynthia Mussinan said that the **International Flavor Conference** will be held in Greece on Memorial Day weekend in 2012, and was approved for placing a deposit of up to \$5000 for the hotel.

Mike Morello gave the **Councilor's Report**. Upcoming **National Meeting themes** include Chemistry of Life (San Diego, Spring 2012), Materials for Health and Medicine (Philadelphia, Fall 2012), Energy and Food (New Orleans, Spring 2013), and Chemistry of Motion (Indianapolis, Fall 2013). Proposed themes for 2014 are Power and Advanced Materials (Dallas, Spring) and Chemistry of a Crowded Planet (San Francisco, Fall). There is an obvious tie-in with AGFD for the New Orleans theme, and Jim Seiber offered to take the lead on it. Meeting attendees will have free access to electronic dissemination of meeting content; other ACS members and non-members will be charged. There is a \$135,000 budget for **Innovative Program Grants**, for which Division Chairs will now have to write letters of support and conflict of interest statements will have to be signed.

Alyson Mitchell reported for Steve Nagy that Peter Schieberle has won the **Award** for the

continued from the previous page

Advancement of Application of Agricultural and Food Chemistry, which was approved by the Executive Committee. Fereidoon Shahidi announced that the determination of the Fellow Awards is in progress. Chi-Tang Ho reported that the Roy Teranishi Graduate Fellowship in Food Chemistry has been won by Jessica Cooperstone, Ohio State University. The Sterling Hendricks Award has been won by Deborah Delmer, and the award symposium will be handled at the Fall Meeting by AGRO. In the absence of Charles Brine, Lauren Jackson ran the Withycombe-Charalambous Graduate Student Award Symposium (first place: Hyeyoung Lee, second place: Jihyun Lee, both from University of California, Davis) and the Undergraduate Student Award symposium (winner: Kimberly Hibshman, Lebanon Valley College). The Young Scientist Award symposium will be held in the fall. Mike Appell reported that AGFD won a ChemLuminary Award last year and was nominated this year for the Graduate Student Award Symposium. Mike Morello suggested that we send the award (a clear plastic flame with the details etched on it) to Charles Brine. Mike Appell and Mike Morello will work on nominating more AGFD members for ACS Fellow Awards.

Alyson Mitchell reported for **Cornucopia** editor Carl Frey and said that the last issue's front-page notice asking for comments about switching to solely electronic copies generated just one response. Paper copies will still be provided at the meetings. Sara Risch suggested mailing the Fall issue as usual and providing only electronic copies after that. This motion was approved. Fereidoon Shahidi suggested e-mailing all AGFD members when a new issue is ready. Carl placed guidelines for symposium organizers in the centerfold of the last issue, and this should be e-mailed to all future organizers.

Hospitality/Public Relations Chair Charlie Brine has arranged the reception for this meeting.

Alyson Mitchell reported for **Membership** Chair Lucy Yu and said that AGFD had 3022 members, including 15 who are celebrating 25 years with the Division.

Mike Appell, the Chair of the **Nominating Committee**, reported that the Councilor terms of John Finley and Mike Morello, the Alternate Councilor term of Keith Cadwallader, and the At-Large Executive Committee terms of Jane Leland and Robert McGorin are all expiring at the end of the year. All have been contacted by Mike and have agreed to serve again. The slate was passed and will be voted upon at the Business Meeting in the fall.

Jim Seiber reported that the **Journal** has a rejection rate of 65%, which is on par with other ACS journals. Some 5000 manuscripts were submitted last year, and the number continues to increase. The number of reviews and perspectives papers has gone up. There are two new Associate Editors and the Journal is looking for another one. They are undergoing a 5-year monitoring by ACS and will have a strategic planning session soon. The Journal's 60th anniversary will be celebrated at a symposium this fall and the papers from it will be published in mid-2012.

In **New Business**, Sara Risch will handle by-law changes that will allow balloting by other than mail. The AGFD dues for next year will remain at \$8. Agnes Rimando is on the International Activities Committee now. Future Programs meetings will be moved to 5 p.m. on the Monday of a National Meeting.

The meeting adjourned at 7:03 p.m.

Submitted by Michael Tunick, AGFD Secretary

Schedule of AGFD Business, Social and Technical Activities

	AGFD Subdivisions - joint meeting	12:15 - 1:15 pm Sunday	August 28
	Executive Committee meeting	5:00 - 8:00 pm Sunday	August 28
	Future Programs meeting	12:15 - 1:15 pm Monday	August 29
	AGFD Business meeting	12:15-1:15 pm Tuesday	August 29
	Poster Session and Social Hour	2:00 - 4:00 pm Tuesday	August 30
AGFD	Award Banquet@ Buckhorn Exchange	6:00 - 8:00 pm Tuesday	August 30

AGFD technical sessions take place at the Colorado Convention Center

SUNDAY MORNING August 28

Section A Colorado Convention Center 505

Young Scientist Award Symposium

C. J. Brine, Organizer C. Brine, Organizer, Presiding L. Jackson, Presiding

8:30 Introductory Remarks.

8:35 1. Physiological interactions of odorants. A. Buettner

9:00 2. Kinetic basis for the control of acrylamide contaminant in foods by flavonoids. Y. Zhang, Y. Ren, Y. Zhang

9:25 3. Sclerotia: An emerging functional food derived from mushroom. K. Wong

9:50 Intermission.

10:05 4. Plant phenolics – from field to fork. J. Lee

10:30 5. Enhancement of anticarcinogenic activities of polymethoxyflavones by biotransformation in mice and rats. H. Xiao

10:55 Concluding Remarks.

Section B Colorado Convention Center 506

Recent Advances in Analysis of Food and Flavors

S. Toth, C. Mussinan, Organizers, Presiding

8:30 Introductory Remarks.

8:35 6. Metabolomics and the quest for understanding quality in flavor chemistry and wine research. M. J. Herderich

9:05 7. Controlling the aroma generation during hazelnut roasting by Sensobolomics and Comparative Metabolome Marker Analysis (COMMA). P. H. Schieberle, J. Kiefl

9:35 8. Discovery of a candidate dietary biomarker indicating coffee consumption by HILIC-UPLC/ToF-MS metabolite profiling. R. Lang, A. Wahl, T. Stark, T. Hofmann

10:05 Intermission.

10:20 9. Analytical and sensory characterizations of chiral 4-mercapto-2-alkanones. K. Engel, M. Wakabayashi, H. Wakabayashi, S. Noerenberg, B. Reichardt, K. Kubota

10:50 10. Confirmation of trace level aroma-impact compounds in cantaloupe (*Cucumis melo* L. var. *cantalupensis* Naudin) by GC-MS/MS analysis. J. Lin, Y. Wang

11:20 11. Convenient synthesis of stable deuterium labeled alkyl pyrazines for use in the stable isotope dilution assays. M. Fang, K. R. Cadwallader

11:50 Concluding Remarks.

PET Recycling: Bridging the Gaps through Innovation
Sponsored by PMSE, Cosponsored by AGFD and SOCED
SUNDAY AFTERNOON August 28
Section A Colorado Convention Center 505

Food for Extreme Environments

N. Da Costa, Organizer, Presiding

1:00 Introductory Remarks.

1:05 12. Soviet/Russian space food from Vostok to Mir. N. C. Da Costa

1:30 13. Nutritional challenges for work and recreation at high altitude. E. W. Askew, S. Wing-Gaia, G. Rodway

2:15 14. Reducing the physiological stress of modern warfare: The role of nutritional science in the U.S. Military. S. M. Pasiakos

2:45 Intermission.

3:00 15. Energy balance and nutritional intervention studies on a Mt. Everest expedition. J. W. Finley

3:30 16. Challenges of developing a food system for a Mars mission. M. R. Cooper

4:15 Concluding Remarks.

Section B Colorado Convention Center 506
Recent Advances in Analysis of Food and Flavors

S. Toth, C. Mussinan, Organizers, Presiding

1:30 Introductory Remarks.

1:35 17. LC/MS/MS method for the analysis of furocoumarins in citrus oil using electrospray ionization. R. Hiserodt, L. Chen

2:05 18. Analytical methods for evaluating the effect of thermal processing on fumonisins in corn-based food. L. S. Jackson, J. Jablonski, K. Voss, D. Ryu

2:35 19. EU essential oils hazard classification: Quantitative multi-component GCMS analysis. J. Broekhans, H. Leijts

3:05 Intermission.

3:20 20. Analysis of trichloroanisole, tetrachloroanisole, pentachloroanisole and tribromoanisole in wines using solid phase microextraction and gas chromatography triple quadrupole mass spectrometry. T. S. Collins, A. Hjelmeland, A. E. Mitchell, S. E. Ebeler

3:50 21. Analysis of flavor-active fatty acid degradation products as well as toxicological relevant compounds during deep-frying with different edible fats and oils. M. Granvogl, A. Ewert, P. Schieberle

4:20 Concluding Remarks.

Chemistry of Air, Space, and Water Plenary
Sponsored by CASW, Cosponsored by AGFD, ENVR, and PHYS

PET Recycling: Bridging the Gaps through Innovation
Sponsored by PMSE, Cosponsored by AGFD and CEI

MONDAY MORNING August 29

Section A Colorado Convention Center 505

AGFD Division Award Symposium - Symposium in Honor of Professor Dr. Peter Schieberle

A. Mitchell, N. Da Costa, Organizers, Presiding

8:30 Introductory Remarks.

8:35 22. Controlling acrylamide formation in heated foods while maintaining color and flavor. D. S. Mottram, J. S. Elmore

9:05 23. Enantioselective analysis: A valuable tool in flavor research. K. Engel
9:35 24. Contribution of methylglyoxal to Maillard flavor reaction. C. Ho
10:05 Intermission.
10:20 25. Flavoromic research applied to Mandarin juice flavor. J. Charve, A. Plotto, G. Reineccius
10:50 26. Progress in analysis of flavour release during eating. A. Buettner
11:20 27. Colorful chemistry of cocoa and chocolate: Flavor creation by processing and eating. P. H. Schieberle
11:50 Concluding Remarks.

Section B Colorado Convention Center 506
Recent Advances in Analysis of Food and Flavors

S. Toth, C. Mussinan, Organizers, Presiding

8:30 Introductory Remarks.

8:35 28. Development of liquid chromatographic techniques for taste compound analysis. D. Jiang, D. Peterson

9:05 29. Anacardic acid profiling in food plants by direct coupling of preparative high-speed countercurrent chromatography and electrospray/APCI mass-spectrometry (prepHSCCC-ESI/APCI-MS/MS). I. Skrjabin, J. Murillo-Velásquez, P. Winterhalter, G. Jerz

9:35 30. Comparison of amino acid analysis in GABA tea via HILIC and ERLIC separation coupled with fluorescence/charged aerosol detection. W. LaFon

10:05 Intermission.

10:20 31. Novel insights into flavor chemistry of asa foetida and overview about trace-level determination of sulfur-containing aroma compounds. A. Degenhardt, M. Liebig, B. Kohlenberg, B. Hartmann, M. Roloff, S. Brennecke, L. Guibouret, B. Weber, G. Krammer

10:50 32. Efficient procedure for isolating methylated catechins from green tea and effective simultaneous analysis of ten catechins, three purine alkaloids, and gallic acid in tea by high-performance liquid chromatography with diode array detection. B. Hu

11:20 33. Headspace solid-phase microextraction (HS-SPME) gas chromatography mass spectrometry (GC/MS) approaches for monitoring early rancidity development in roasted almonds. A. Mitchell, L. Xiao

11:50 Concluding Remarks.

Nitrogen and the Human Endeavor: Chemistry, Effects, and Solutions
Sponsored by CASW, Cosponsored by AGFD and ENVR

MONDAY AFTERNOON August 29

Section A Colorado Convention Center 505

Tropical and Subtropical Fruits: Flavors, Color, and Health Benefits - Flavor and Color

C. Osorio Roa, G. Jayaprakasha, Organizers B. Patil, K. Mahattanatawee, Organizers,
Presiding

M. Steinhaus, Presiding

1:30 Introductory Remarks.

1:35 34. Climate and salinity effects on health promoting and color properties in the pomegranate (*Punica granatum* L.) fruit arils. H. Borochoy-Neori, N. Lazarovitch, S. Judeinstein, B. S. Patil, D. Holland

2:00 35. Plant breeding and genetic approaches to improve flavor and nutrients in vegetables . S. S. Boddupalli

2:25 36. Characteristic volatile compounds from Nagami kumquats (*Fortunella margarita*) and their cell proliferation effect. G. Jayaprakasha, K. Murthy, B. S. Patil

- 2:50 37. Pineapple juice flavor: Key aroma compounds and changes during industrial processing. M. Steinhaus, K. Thomas, P. Schieberle
3:15 Intermission.
3:30 38. Study of the genetic factors that control fruit color variation in pomegranate (*Punica granatum* L.). Z. Ben-Simhon, H. Borochoy-Neori, I. Bar-Ya'akov, R. Harel-Beja, A. Sherman, R. Ophir, D. Holland
3:55 39. High hydrostatic pressure processing as a strategy to increase carotenoid contents of tropical fruits. C. Hernandez-Brenes, R. I. Diaz-De La Garza, D. A. Jacobo-Velazco, P. A. Ramos-Parra, R. Villareal-Lara
4:20 40. Preparative separation and pigment profiling of betalains from fruits of *Opuntia ficus-indica* by ion-pair high-speed countercurrent chromatography (HSCCC). B. Klose, S. Wybraniec, P. Winterhalter, G. Jerz
4:45 Concluding Remarks.

Section B Colorado Convention Center 506
Recent Advances in Analysis of Food and Flavors

S. Toth, C. Mussinan, Organizers, Presiding

1:30 Introductory Remarks.

1:35 41. Monitoring the formation of flavanol–Maillard adducts in model systems relating to cocoa roasting. M. Oruna-Concha, J. P. Spencer, G. R. Gibson, D. S. Mottram

2:05 42. Volatile compound analysis by GC-TOF-MS: Applications and challenges. M. J. Morello

2:35 43. Comparison of fast gas chromatography- surface acoustic wave sensor (FGC-SAW) and capillary GC-MS for determining strawberry and orange juice volatiles. X. Du, R. L. Rouseff
3:05 Intermission.

3:20 44. Beside structure elucidation: Applications of NMR in food analysis. O. Frank, T. F. Hofmann

3:50 45. The power law and dynamic rheology in food analysis. M. H. Tunick

4:20 Concluding Remarks.

Nitrogen and the Human Endeavor: Chemistry, Effects, and Solutions
Sponsored by CASW, Cosponsored by AGFD and ENVR

Undergraduate Poster Session Agricultural and Food Chemistry
Sponsored by CHED, Cosponsored by AGFD and SOCED

MONDAY EVENING August 29 8:00 - 10:00 PM

Sci-Mix

L. Jackson, N. Da Costa, Organizers

73, 80, 81, 84, 86, 89, 94, 95, 99, 100, 104, 107, 108, 110, 111, 115, 116, 117, 118, 121. See subsequent listings.

TUESDAY MORNING August 29

Section A Colorado Convention Center 505

Tropical and Subtropical Fruits: Flavors, Color, and Health Benefits - Health Benefits

C. Osorio Roa, K. Mahattanatawee, B. Patil, Organizers G. Jayaprakasha, Organizer, Presiding

F. Wyzgoski, S. Boddupalli, Presiding

8:30 Introductory Remarks.

8:35 46. Chemoprofiling of Palestine sweet lime (*Citrus limmetioides*) volatiles and their inhibitory role of colon cancer cells proliferation. G. Jayaprakasha, K. Murthy, B. S. Patil

- 9:00 47. Metabolomic models of fruit extracts and chemoprevention. F. J. Wyzgoski, R. N. Reese, L. Paudel, P. L. Rinaldi, M. M. Giusti, J. Johnson, J. C. Scheerens, J. Bomser, A. M. Chanon, J. K. Hardy, C. Wesdemiotis, A. R. Miller, A. Z. Tulio Jr.
- 9:25 48. Antioxidant activity of a anthocyanin-rich Colombian tropical fruits. C. Osorio, L. Santacruz, J. Carriazo, O. Almanza
- 9:50 49. Flavonoid content and antioxidant properties of some tropical and subtropical fruits from the Annonaceae and Citrus genera. D. Barreca, E. Bellocco, C. Caristi, U. Leuzzi, G. Gattuso
- 10:15 Intermission.
- 10:30 50. Acai berries and walnuts: Brain health boosters. S. M. Poulouse, D. F. Bielinski, B. Shikitt-Hale
- 10:55 51. Prevention of biofilm formation and bacterial adhesion after consumption of cranberry juice cocktail. T. A. Camesano, Y. Zhang, Y. Tao, L. Abu-Lail, P. A. Pinzon-Arango, R. Roberto
- 11:20 52. Seed and juice characterization of pomegranate fruits grown in Tunisia: Comparison between sour and sweet cultivars revealed interesting properties for prospective industrial applications. N. Hasnaoui, M. Mars, S. Ghaffari, P. Melgarejo, F. Hernandez
- 11:45 Concluding Remarks.

Section B Colorado Convention Center 506
AGFD International Year of Chemistry (IYC) Symposium

A. Mitchell, Organizer M. Appell, N. Da Costa, Organizers, Presiding

8:30 Introductory Remarks.

- 8:35 53. Studies in the use of algae in fish nutrition. P. W. Perschbacher
- 9:00 54. Non-invasive means to determine stage of maturity in white sturgeon females. A. G. Cavinato, S. A. Servid, J. Van Eenennaam, S. Doroshov, X. Lu, B. Rasco, M. Talbott, W. Sealy, M. Webb
- 9:25 55. Effects of UV irradiation on fish gelatin properties. B. Chiou, C. G. Otoni, R. J. Avena-Bustillos, C. Bilbao-Sainz, P. J. Bechtel, S. H. Imam, G. M. Glenn, W. J. Orts
- 9:50 56. Studies on bioactive compounds from okra seed extracts: Selective inhibitors of advanced glycation end products. B. Dayal, R. Amin, V. Yannamreddy, M. A. Lea
- 10:15 Intermission.
- 10:30 57. Antioxidant polyphenolics in ready to drink tea: How are they really measured? Y. Kim, K. L. Goodner, D. J. Wampler, C. F. Sweeney
- 10:55 58. Breaking up biofilms with *Moringa Oleifera*: Insights into mechanisms. B. Dayal, R. Amin, V. Yannamreddy, M. A. Lea
- 11:20 59. Synthesis of butanolide-containing alkenyl insect pheromones. R. J. Petroski, A. Cossé
- 11:45 Concluding Remarks.

A Sustainable Future: Interface of Energy, Food, Water, and Climate Sustainability
Sponsored by COMSCI, Cosponsored by AGFD, BTEC, and CEI

Sterling B. Hendricks Memorial Lectureship Award
Sponsored by AGRO, Cosponsored by AGFD

TUESDAY AFTERNOON August 30

Section A Colorado Convention Center 505

Tropical and Subtropical Fruits: Flavors, Color, and Health Benefits - Health Benefits

G. Jayaprakasha, K. Mahattanatawee, B. Patil, Organizers C. Osorio Roa, Organizer, Presiding

C. Hernandez-Brenes, S. Jain, Presiding

1:30 Introductory Remarks.

1:35 60. Antitumor activity of garcinol from *Garcinia indica* in PC3 cells and dextran sulfate sodium treated mice. C. Ho, L. Chiou, M. Pan

2:00 61. Issues surrounding the anti-inflammatory actions of the citrus polymethoxylated flavones. J. A. Manthey, T. B. Cesar

2:25 62. L-cysteine supplementation can increase insulin sensitivity by boosting blood levels of hydrogen sulfide and nitrite in type 2 diabetes. S. K. Jain

2:50 63. Development of flavor and antioxidant activity during the ripening of the date palm fruit (*Phoenix dactylifera* L.). C. Wentao, M. Oruna Concha, N. Eid, J. K. Parker, J. P. Spencer

3:15 Intermission.

3:30 64. Bioactive compounds present in *Moringa Oleifera*: Isolation and characterization by thin layer chromatography and electrospray ionization mass spectrometry. B. Dayal, V.

Yannamreddy, R. Amin, M. A. Lea, A. B. Attygale

3:55 65. Phenolic profile and antimicrobial activity of select exotic fruits. C. Engels, D. Lopes-Lutz, C. Nimalaratne, J. Dettmann, P. Esquivel, V. M. Jiménez, M. G. Gänzle, A. Schieber

4:20 66. Passion fruit seed containing high amounts of piceatannol could be a new anti-skin-aging material. Y. Matsui, K. Sugiyama, M. Kamei, T. Takahashi, T. Suzuki, Y. Katagata, T. Ito

4:45 Concluding Remarks.

Section B Colorado Convention Center 506

Food Bioactives and the Journal of Agricultural and Food Chemistry

J. Finley, V. Somoza, Organizers F. Tomas-Barberan, Organizer, Presiding

1:30 Introductory Remarks.

1:35 67. From detrimental to beneficial constituents in foods: Tracking the publication trends in JAFAC. J. N. Seiber, L. A. Kleinschmidt

2:05 68. Health benefits of almonds beyond improvements in atherogenic lipoprotein profile. O. Chen

2:35 69. Processing and storage effects on berry polyphenols: Challenges and implications on bioactive properties. L. R. Howard, R. L. Prior

3:05 Intermission.

3:20 70. Mitigating inflammation with foods. A. G. Schauss, X. Wu

3:50 71. Putting health risks into perspective. B. N. Ames

4:50 Concluding Remarks.

Section C Colorado Convention Center Hall D

General Posters

L. Jackson, N. Da Costa, Organizers

2:00 - 4:00

72. Determination of synthetic by-products in the color additive D&C Yellow No. 10 (quinoline yellow) using high-performance liquid chromatography. A. Weisz, H. T. Mai, A. Scher

73. Preparative separation of 1,3,6-pyrenetrisulfonic acid from the color additive D&C Green No. 8 using pH-zone-refining counter-current chromatography. A. Weisz, E. P. Mazzola, Y. Ito

74. Evaluation of a liquid chromatography method for the detection and quantification of aflatoxins in milk thistle supplements. V. Tournas, C. Sapp, M. W. Trucksess

75. Investigation of alkylbenzenes as VOCs in sun-dried salts and its risk assessment. J. Kim, S. Hong, G. Choi, O. Kwon, G. Im

76. Quantitative analysis of residual pesticide of retailed sundried salts in Korea. J. Kim, S. Hong, G. Choi, J. Park, G. Im, O. Kwon

77. Simple quantitative analysis of ethylcarbamate in various fermented food. J. Kim, S. Hong, O. Kwon, G. Im

78. Development of analytical method for lead, cadmium, and methylmercury in Korean functional foods using standard addition method. W. Kim, D. Lee, H. Jin, K. Park, H. Pyo, K. Lee
79. Volatile organic compound migration parameters in nylon MXD6 by the dynamic permeation cell method. Y. Wang, C. Wang, R. Juskelis, Y. Song, J. Koontz
80. Flavor, solvent, and photoinitiator migration parameters in polyethylene terephthalate and nylon 6 by the static permeation cell method. C. Wang, Y. Wang, R. Juskelis, Y. Song, J. Koontz
81. Development of an LC-MS/MS method for quantitation and confirmation of ceftiofur metabolite desfuroylceftiofur cystine disulfide in bovine kidney. S. Feng, C. Chattopadhyaya, P. Kijak
82. Improvement in the analysis of pesticide residues in herbal medicines with different lipid contents. J. Hawng, Y. Jeon, H. Kim, J. Kim, Y. Lee, J. Park, D. Kim, J. Kim
83. Optimization of mycotoxin binding in grains. C. I. Johnston, R. Singleterry, A. Brown, K. Armburst, D. Sparks
84. Determination of components of the color additive FD&C Green No. 3 (Food Green 3) using high performance liquid chromatography. H. W. Yang, A. Scher
85. Glycyrrhizic acid and 18 β -glycyrrhetic acid modulate the lipopolysaccharide-induced inflammatory response by the suppression of NF- κ B through phosphatidylinositol 3-kinase. C. Wang, T. Kao, G. Yen
86. Screening of anthocyanins in red and white cranberry extracts and juice concentrates by HR-MS (Exactive Orbitrap) and LC-MS. A. Z. Tulio, Jr., K. D. White, L. S. Jackson
87. UPLC-UV determination of isoflavones in soy seed. L. Sheng, H. D. Scobell, K. J. Duff
88. Metabolic health benefits of dietary fiber: Comparison of hydroxypropyl methylcellulose and natural dietary fibers in a hamster model. S. Hung, S. A. Young, W. H. Anderson, W. Yokoyama, Y. Hong, H. Kim, G. Bartley, D. R. Albers, M. L. Langhorst, D. M. Williams, D. Dielman, M. Covington
89. Relationship of radical scavenging activities and anthocyanin contents in the 12 colored rice varieties. K. Jang, S. Han, W. Seo, J. Ra, J. Kim, Y. Song, M. Park, H. Kang
90. Neuraminidase inhibitory activities of polyphenolic compounds in the young leaves of 20 barley varieties. K. Jang, W. Seo, S. Han, J. Ra, S. Oh, S. Kim, K. Choi, H. Kang
91. Physicochemical and antioxidative properties of selected barnyard millet (*Echinochloa utilis*) species in Korea. W. Seo, K. Jang, S. Han, K. Choi, S. Kim, S. Oh, J. Ra, H. Kang
92. Alpha-glucosidase inhibitory polyphenols from the grain of native barnyard millet (*Echinochloa utilis*). W. Seo, S. Han, K. Jang, K. Choi, J. Ra, S. Kim, S. Oh, J. Kim, H. Kang
93. Molecular properties and antioxidant activities of polysaccharide-protein complexes from medicinal mushrooms by ultrasound-assisted extraction. Y. Cheung, K. Siu, J. Wu
94. Antioxidative activity of organic vs. conventional milk. M. Paul, D. L. Van Hekken
95. Analysis of black raspberry polyphenols by high field NMR and HPLC-ESI-MS/MS. L. Paudel, J. C. Scheerens, F. J. Wyzgoski, P. L. Rinaldi, R. N. Reese, M. M. Giusti, J. Johnson, N. W. Najjar, J. Bomser, J. K. Hardy, A. M. Chanon, D. Smiljanic, C. Wesdemiotis
96. Determination of the antioxidant capacity of plant parts of *Psoralea esculenta* (prairie turnip) and identification and quantitation of antioxidants. E. Benjamin, E. Rohe, P. L. Weber
97. Preparation of carnosine-containing extracts from chicken and pork and their physiological activities. S. Kim, C. Park, J. Auh
98. Effect of adding milk and sugar on various tea preparations. N. O. Mwebi, J. Brown
99. Potential chemopreventive xanthenes and a new polyisoprenylated benzophenone derivative from *Garcinia humilis*. D. N. Haase, S. Parker, H. Jacobs, S. Badal, S. Francis, R. Delgoda, G. Huang, T. J. Tzeng
100. Microwave-assisted extraction and isolation of red pigment from pitaya peel. R. Huang, B. Huang, H. Huang, S. Chen, X. Lu, N. Li

101. Study on extraction of polysaccharides from longan seeds by cellulase. R. Huang, B. Huang, X. Lu, S. Chen, H. Huang, K. Xu
102. Enzymatic modification of a model homogalacturonan with a pectin methylesterase from papaya: Effects of enzyme-substrate ratios on nanostructure and enzyme mode of action. Y. Kim, R. G. Cameron, G. A. Luzio, P. Vasu, B. J. Savary, M. A. Williams
103. Use of milled-rice co-products in value-added food products. F. Shih, K. Daigle, S. Cheuk
104. Isolation and structural characterization of eel type I collagen. M. Saito, C. Sato, H. Go, H. Hayakawa, N. Uchida, T. Higuchi, H. Suzuki
105. Effects of alcohol compounds on the growth and lipid accumulation of oleaginous yeast *Trichosporon fermentans*. C. Huang, H. Wu, M. Zong
106. Application of high pressure homogenizer for the preparation of *Chlorella vulgaris* nano-suspension. R. Yu, H. Park, D. Lee
107. Preparation of smoked *Bissaria* (*Atherina boyeri*) and utilization of its powder in different popular food products. H. A. Abou Gharbia, E. Abou Tour, A. Abdelnaby
108. Extraction of zein from DDGS for commercial applications. E. Thayer, S. Laskares, A. Beard
109. Characterization of jet-milled rice flour and the effect on resistant starch (type 3 & 4) formation. J. Park, D. Lee, J. Auh
110. Delivering omega-3 lipids into food beverages through a nano-clear o/w emulsion. D. Tang
111. Nano-encapsulation of coenzyme Q₁₀ with octenyl succinic anhydride modified starch. S. Cheuk, K. Daigle, F. Shih, E. Champagne, J. Patindol
112. HPMC reinforced with different cellulose nanoparticles. C. Bilbao-Sainz, J. Bras, T. Williams, T. Sénechal, W. Orts
113. Quality attributes and chemical composition of wheat germ subjected to different heat treatments. H. A. Abogharbia, R. S. Attia
114. Transferring GC carrier gas from helium (He) to hydrogen (H₂) for the determination of fatty acids. H. Zhao, H. D. Scobell, K. J. Duff
115. Cholesterol is a glycoalkaloid precursor in potato plants. E. V. Petersson, N. Nahar, P. Dutta, A. Broberg, R. Åslund-Tröger, L. Jonsson, F. Sitbon
116. Determination of degree of substitution in carboxymethyl cellulose by Fourier transform infrared (FTIR) spectroscopy. J. Ye, Y. Zhang, J. Xiong
117. Allenes in asymmetric catalysis: Rhodium(I)-catalyzed enantioselective addition of arylboronic acids to α -ketoesters. F. Cai, X. Pu, X. Qi, M. I. Antczak, J. M. Ready
118. Organocatalytic methods to transform glycerin into glycerol carbonate. P. Hector, B. A. Hervert
119. Production of activated carbon from hemp by-products by carbon dioxide and steam activation. S. Kim, G. Choi, J. Kim
120. Antioxidant properties of polysaccharide-protein complex isolated from mycelium of a medicinal fungus *Cordyceps Cs-HK1*. K. Siu, Y. Cheung, J. Wu
121. Characterisation of carnauba and other *Copernicia* sp waxes from Brazil. E. S. Brito, A. F. Batista, N. M. Ricardo, E. C. Cabral, M. N. Eberlin, E. J. Pilau, F. C. Gozzo

WEDNESDAY MORNING August 31

Section A Colorado Convention Center 505

Future Agricultural Consumer Safety Demands for the Global Market

Cosponsored by AGRO A. Loaiza, Organizer, Presiding

8:30 Introductory Remarks.

8:35 122. Evaluation of the safety of crop products produced through biotechnology. W. Parrott

9:00 123. Addressing the safety of crop protection products in a global market. W. Jones, R.

McAllister, B. Glenn

9:25 124. Toxicological safety assessment of biotech crops. C. A. Mathesius
9:50 Intermission.
10:05 125. Allergenicity evaluations of proteins introduced into crop products using biotechnology. L. S. Privalle
10:30 126. Analytical methods for testing biotechnology products. J. Chen, P. Doyle
10:55 Concluding Remarks.

Section B Colorado Convention Center 506

Food Bioactives and the Journal of Agricultural and Food Chemistry

F. Tomas-Barberan, J. Finley, Organizers V. Somoza, Organizer, Presiding

8:30 Introductory Remarks.

8:35 127. Formulation of the Total Western Diet (TWD) as basal diet for rodent cancer studies.

K. J. Hintze, R. E. Ward, A. D. Benninghoff

9:05 128. Pleiotropic beneficial effects of 3,3'-diindolylmethane. L. F. Bjeldanes

9:35 129. Antioxidant and anti-inflammatory activity correlate for specific Maillard reaction products. X. Chen, D. Kitts

10:05 Intermission.

10:20 130. Food goes omics: State of the art in curation of chemical data and prospects for epidemiological research. A. Scalbert, I. Romieu, N. Slimani, J. Rothwell, C. Manach, C.

Andres-Lacueva, M. Urpi-Sarda

10:50 131. Structure-/activity relationships of coffee compounds and their implications for optimizing the health benefits of coffee beverages. V. Somoza

11:20 132. Hypoglycemic effect of stilbene glycoside from *Polygonum multiflorum* in KK CgAy/j type 2 diabetic mouse model and its mechanisms. W. Tang, Y. Liu, S. Li, H. Daun, M. Huang, C. Ho

11:50 Concluding Remarks.

Human Exposure and Responses to Toxins from the Air and Water

Endocrine Active Chemicals in the Environment

Sponsored by TOXI, Cosponsored by AGFD, CHAL, and ENVR

WEDNESDAY AFTERNOON August 31

Section A Colorado Convention Center 505

Future Agricultural Consumer Safety Demands for the Global Market

Cosponsored by AGRO A. Loaiza, Organizer, Presiding

1:30 Introductory Remarks.

1:35 133. Pesticide residues in food: The role of dietary risk assessment. M. G. Panek

2:00 134. Secondary standards – barrier or benefit? J. M. Stewart

2:25 135. Remediation of fungicide residues on fresh produce using gaseous ozone. S. S. Walse

2:50 Intermission.

3:05 136. Creating and marketing more sustainable food consumer goods. C. Barcan

3:30 Panel Discussion.

4:15 Concluding Remarks.

Section B Colorado Convention Center 506

Food Bioactives and the Journal of Agricultural and Food Chemistry

J. Finley, Organizer V. Somoza, F. Tomas-Barberan, Organizers, Presiding

1:30 Introductory Remarks.

1:35 137. Phytochemical absorption and metabolism in food based cancer prevention studies.

S. Schwartz

- 2:05 138. Evolution of good polyphenolics from color and flavor problems to health benefits. J. W. Finley, J. Losso, Z. Xu
2:35 139. Agricultural chemistry's toolset for the 21th century. J. B. German
3:05 Intermission.
3:20 140. Translating the basic science of sulforaphane action into a healthy broccoli meal. E. H. Jeffery
3:50 141. High antioxidant potatoes: Acute in vivo antioxidant source and hypotensive agent in humans after supplementation to hypotensive subjects. J. A. Vinson, C. A. Demkosky, D. A. Navarre
4:20 142. Role of dietary factors and phytochemicals in colon cancer risk. R. S. MacDonald
4:50 Concluding Remarks.

THURSDAY MORNING September 1

Section A Colorado Convention Center 505

General Papers

N. Da Costa, L. Jackson, Organizers, Presiding

8:30 Introductory Remarks.

8:35 143. Lemon oil solubilization in mixed surfactant solutions: Rationalizing microemulsion and nanoemulsion formation. J. Rao, D. J. McClements

8:55 144. Computationally modeled self-assembly of higher order structure of collagen peptides. F. Xu, V. Nanda

9:15 145. Metabolic study on reducing effect of functional milk formula on lead exposure in mice. J. Jiao

9:35 146. Complete structural elucidation of isomeric forms of malonylglucoside isoflavones. V. Yerramsetty, B. Ismail

9:55 147. Probing rearrangements occurring in casein micelles during concentration: Addition of soluble caseins. P. Krishnankutty Nair, M. Corredig

10:15 Intermission.

10:30 148. Assessment of groundwater contamination in agriculture areas through lysimetric studies. T. -. Jindal

10:50 149. Composition of the essential oil from *Artemisia vulgaris* L. grown in Pennsylvania, USA and its apoptosis-dependent antitumor activity in promyelocytic leukemia cell line HL-60. J. D. Williams, A. Saleh, D. N. Acharya

11:10 150. Detection of Shiga toxin-producing *E. coli* in environmental samples by immune-PCR. X. He, B. Quinones, S. McMahon, M. Cooley, R. E. Mandrell

11:30 Concluding Remarks.

Section B Colorado Convention Center 506

General Papers

L. Jackson, Organizer N. Da Costa, Organizer, Presiding M. Appell, Presiding

8:30 Introductory Remarks.

8:35 151. Comparative analysis of over the counter milk thistle commercial herbal extracts. M. A. Saleh

8:55 152. Nutritional and nutraceutical properties of strawberry guava and common guava. K. McCook-Russell

9:15 153. Mood and mood disorders: Current therapies, alternative medicine and computational studies. F. H. Lopez-Vallejo, J. L. Medina-Franco, T. L. Peppard, K. Martinez-Mayorga

9:35 154. Screening of small molecules and pectin present on the rind of bacuri (*Platonia insignis*) an Amazonian fruit. W. P. Batista, R. V. Mamede, K. M. Canuto, E. S. Brito

9:55 Intermission.

10:10 155. Acidic polysaccharide analysis by high performance liquid chromatography. X. Yan

10:30 156. Diterpenes profile in coffee: Influence of roasting process. R. C. Dias, A. F. Faria, A. Z. Mercadante, N. Bragagnolo, M. T. Benassi

10:50 157. Synthesis and evaluation of molecularly imprinted polymer microspheres used as detection for Erythromycin Ethylsuccinate in food. J. Lei

11:10 Concluding Remarks.

AGFD Abstracts, 242nd ACS Nat'l Meeting, Denver

AGFD 1 Physiological interactions of odorants Andrea Buettner andrea.buettner@lmchemie.uni-erlangen.de Erlangen Bavaria, Germany. Dept. of Chemistry and Pharmacy - Emil Fischer Center, Univ. of Erlangen-Nuremberg, Germany Sensory Analytics, Fraunhofer Inst. for Process Engineering and Packaging, Erlangen, Germany Odorants are present amongst numerous environmental substances. When they come into contact with the human body, modulation and transformation processes take place depending on whether the substances pass the nasal or oral cavities, or further proceed into the deeper airways or into the gastrointestinal tract. Our studies focus on these diverse modes of interaction, with focus on gastrointestinal modification, adsorption and resorption processes, the passage within the human body, and further transformations. Such chemo-physiological considerations are our basis to understand how odorants proceed either to the chemoreceptive sites responsible for immediate odour sensation, or how they can modulate the response of the human physiology by post-oral or post-inhalation effects. Complexity of these processes will be exemplified, e.g. with odorant-mucosal interactions, or gastrointestinal and post-resorptive biotransformation of odorants in vivo. Implications for odorant action in the human body that are not just related to pure chemosensation are discussed.

AGFD 2 Kinetic basis for the control of acrylamide contaminant in foods by flavonoids Yu Zhang, y_zhang@zju.edu.cn, Hangzhou Zhejiang China; Yiping Ren; Ying Zhang. Dept. of Food Sci. and Nutrition, Zhejiang Univ., Hangzhou Zhejiang, China Zhejiang Provincial Center for Disease Control and Prevention, Hangzhou Zhejiang, China The finding of elevated acrylamide levels in heat processing foods evoked an international health alarm. Our aim was to validate reduction effect and mechanisms of representative flavonoids (homoorientin, EGCG, luteolin-7-O-glucoside, luteolin, genistein and quercetin) on the kinetics of acrylamide in a potato-based model system. The kinetic models were established in the potato microwave model system based on the equal addition levels (10^{-9} mol/L) of flavonoids. Then, kinetic profiles of asparagine, glucose, fructose, acrylamide and melanoidins were determined by previously validated UHPLC-MS/MS method and inhibitory positions of flavonoids were finally confirmed. Our results indicated that flavonoids can significantly inhibit the formation of intermediates such as Schiff base between the reaction of asparagine and fructose, the transform action from glucose to fructose via isomerization, and the formation of acrylamide. However, they cannot inhibit the reaction between asparagine and glucose and no effect on the elimination of acrylamide. Flavonoids can also reduce the formation of melanoidins. However, such effect seems not significant. This kinetics-based research on the reduction mechanism of acrylamide will be in favor of understanding the key reduction position of acrylamide during heat processing and supply theoretical evidence for the development and optimization of relative food processing technologies.

AGFD 3 Sclerotia: An emerging functional food derived from mushroom Ka Hing Wong, bckhwong@polyu.edu.hk, Dept. of Applied Biology and Chem. Tech., The Hong Kong Polytechnic Univ., Hung Hom Kowloon, Hong Kong, Dept. of Applied Biology and Chem. Tech., The Hong Kong Polytechnic Univ., Sclerotium can be described as a nutrient-storage organ of mushroom which can remain dormant during unfavorable conditions until environment is suitable for its fruiting bodies to germinate. Apart from enzymatic preparation as well as biochemical, microstructural, physico-chemical and functional characterizations, our previous ten years' research work on the health promoting effects (such as enhancing passive Ca absorption, immunomodulatory and anti-tumor activities) of both native and chemically modified polysaccharides isolated from three Chinese edible and medicinal mushroom sclerotia, namely *Pleurotus tuber-regium*, *Polyporus rhinoceros*, and *Wolfiporia cocos* will be shared in the seminar. Besides, some on-going projects and future research directions related to the mushroom sclerotium will also be discussed. It is anticipated that finding of our studies would not only provide insights for exploring the use of mushroom sclerotial polysaccharides in cancer immunotherapy, but could also facilitate their development into novel function food ingredients for the rapid growing nutraceuticals industry nowadays.

AGFD 4 Plant phenolics – from field to fork Jungmin Lee, jungmin.lee@ars.usda.gov, U of I Ln, Parma ID, Horticultural Crops Research Unit Worksite, USDA-ARS, Parma ID, Plant secondary metabolites such as phenolics are important to human health, and for the organoleptic properties they impart to fresh and processed foods. Consumers judge appearance, taste, and texture when making purchasing decisions. Thorough identification of phenolic compounds is key to discerning how cultivar selection, breeding strategies, environment, post-harvest conditions, and processing methods ultimately influence food quality. Highlights on elucidation and quantification of phenolics in grapes, berries, and culinary and medicinal herbs will be presented, results of which can improve production and processing. Discussion will include how (1) canopy, cover crop, and nutrient management alter metabolites in wine grapes; (2) winemaking conditions influence wine structure; (3) characterizing cultivar variability in polyphenolics aiding enhanced germplasm selection in berries; and (4) fruit processing methods alter efficiency of phenolic extraction in berry products. The importance of method selection and sample preparation to accuracy and reproducibility in phenolic analyses will also be presented.

AGFD 5 Enhancement of anticarcinogenic activities of polymethoxyflavones by biotransformation in mice and rats Hang Xiao, hangxiao@gmail.com, Amherst MA Previously, we have demonstrated anti-carcinogenic effects of polymethoxyflavones (such as nobiletin and 5-hydroxy nobiletin) isolated from citrus fruits. Biotransformation is one of the key factors that can dictate the in vivo efficacy of food bioactive compounds. Herein, we studied the biotransformation of nobiletin and 5-hydroxy nobiletin in mice and rats. We first developed a highly sensitive HPLC method (with an over 150-fold increase in sensitivity in comparison with previously published method) for the detection of polymethoxyflavones and their metabolites in biological samples. Using this method, we have identified more than 30 urinary metabolites of nobiletin and 5-hydroxy nobiletin. Eight major metabolites have been successfully synthesized for anti-carcinogenic activity test in 10 different human cancer cell lines. Our results demonstrated that certain metabolites were much more potent in inhibiting cancer cell growth than their parent compounds. The structure-activity relationship has been established, which provides important foundation for future in vivo investigation.

AGFD 6 Metabolomics and the quest for understanding quality in flavor chemistry and wine research Markus J Herderich, markus.herderich@awri.com.au, Urrbrae SA Australia . The Australian Wine Research Inst., Adelaide SA, Australia After the first publications more than forty years ago established the principles of metabolomics, metabolomics is now recognised as distinct scientific discipline in its own right and has become an essential technique for an ever increasing number of R&D projects. Yet fundamental breakthroughs based on novel metabolomics approaches, as well as successful applications of metabolomics in R&D still face a number of challenges. Wine composition, flavour and quality are resulting from combinations of grape and yeast metabolites. Consequently, metabolomics approaches are increasingly seen as a critical component of product innovation in the wine industry. Examples will showcase results from targeted and un-targeted metabolomics studies into wine flavor and quality, and yeast strain development projects, with a focus on secondary metabolites. In this context, challenges, success factors and future development needs for metabolomic profiling and quality marker (biomarker) discovery in flavor chemistry and wine research will be discussed.

AGFD 7 Controlling the aroma generation during hazelnut roasting by Sensobolomics and Comparative Metabolome Marker Analysis (COMMA) Peter H. Schieberle, peter.schieberle@Lrz.tum.de, Freising Bavaria, Germany ; Johannes Kiefl Dept. of Chemistry, Food Chemistry, Freising, Germany Roasting is the key process converting raw hazelnuts into a semi-manufactured product with a characteristic aroma. In a previous study, the heat-induced aroma generation in Italian hazelnuts of the variety Tonda Romana was studied by means of the molecular sensory science approach revealing that the pairs 2- and 3-methylbutanal (malty), 2-acetyl- and 2-propionyl-1-pyrroline (roasty, popcorn-like), 2,3-pentandione and 2,3-butandione (buttery), 2-furanmethanethiol and 2-thiophenemethanethiol (coffee-like) as well as 5-methyl-(E)-2-hepten-4-one and 3-methyl-4-heptanone (fruity, hazelnut-like) are among the most important aroma-active compounds. However, further sensory experiments indicated that different aromas are obtained by changing the roasting regime as well as the hazelnut variety. Hence, the aim of the present study was to analyze the heat-induced aroma generation by means of targeted and untargeted approaches, and to correlate the data with the overall sensory impact of the respective samples. The targeted analysis of hazelnuts' Sensobolome comprises the identification and quantitation of key odorants across a larger sample set. The development of a new comprehensive quantitative approach on basis of GCxGC-TOF-MS in combination with stable isotope dilution assays will be presented in detail. Recombination experiments finally verified the effectiveness of the Sensobolomics approach to understand the generation of hazelnut aroma on a molecular basis. Then, by means of GCxGC-TOF-MS, the heat-induced changes of the total volatile hazelnut metabolome were investigated employing the so-called COMMA approach. This way, marker compounds are located by application of an untargeted comparative analysis, and the data are correlated with the overall aroma as well as with the outcome of the Sensobolomics approach. The results showed that a combination of both methods is a useful tool in understanding and controlling the aroma generation during hazelnut roasting.

AGFD 8 Discovery of a candidate dietary biomarker indicating coffee consumption by HILIC-UPLC/ToF-MS metabolite profiling Roman Lang, roman.lang@tum.de, Freising Bavaria, Germany; Anika Wahl; Timo Stark; Thomas Hofmann, Technical Univ. of Munich, Freising, Germany Roasted coffee is appreciated for its alluring aroma, typical taste

profile, as well as its stimulatory effect on the central nervous system. With increasing intensity over the last years, coffee moved into the focus of nutritional research since numerous epidemiological studies suggest that coffee consumption may help prevent several chronic diseases, including Alzheimer's disease, Parkinson's disease and type 2 diabetes, among others. In order to evaluate and validate the in vivo function of putatively health beneficial molecules in foods, controlled human intervention studies are required. As the subject's compliance concerning intake or abstinence of a given food is considered mandatory to be monitored by biomarkers, the objective was to identify analytical markers for coffee consumption. Urine samples collected from coffee drinkers were compared with those of non-coffee drinkers using HILIC-UPLC/ToF-MS-based metabolite profiling. Two urinary molecules, found to be contributing most to the dissimilarities between both groups, were identified as N-methylpyridinium (NMP) and trigonelline and their suitability as coffee-specific biomarkers was assessed by means of a pilot coffee intervention study. After the volunteers (5 female, 4 male) consumed a single dose of coffee, morning urine was collected for 10 days while staying abstinent from any coffee. HILIC-MS/MS-SIDA analysis revealed elevated urinary concentrations of trigonelline and NMP for up to 48 (p=0.001) and 72 h (p=0.002), respectively, after coffee consumption when compared to non-coffee drinkers. The analysis of urinary NMP allows to check for coffee consumption within a period of 3 days and, therefore, is proposed as a dietary biomarker which might be used as an analytical probe to control compliance in human intervention studies on coffee.

AGFD 9 Analytical and sensory characterizations of chiral 4-mercapto-2-alkanones Karl-Heinz Engel, K.H.Engel@wzw.tum.de, Freising-Weihenstephan Bavaria, Germany; Hidehiko Wakabayashi; Svenja Noerenberg; Bastian Reichardt; Kikue Kubota; Motoko Wakabayashi, Technische Universitaet Muenchen, Freising-Weihenstephan, Germany, Inst. of Environmental Science for Human Life, Ochanomizu Univ., Tokyo, Japan, Dept. of Food and Nutritional Sciences, Ochanomizu Univ., Tokyo, Japan Sulfur-containing substances play important roles as food volatiles owing to their low odor thresholds. Beta-mercaptocarbonyls are known as high impact aroma compounds exhibiting tropical fruit flavors. The objective of this study was to provide a basis for the analytical and sensory characterization of chiral β -mercaptoalkanones. A homologous series of 4-mercapto-2-alkanones and the corresponding 4-acetylthioesters were synthesized by Michael-type additions of hydrogen sulfide and thioacetic acid, respectively, to 3-alken-2-ones. The enantiomers of the resulting chiral substances could be separated by capillary gas chromatography (GC) using modified cyclodextrin as chiral stationary phase. NMR analysis of diastereoisomeric derivatives and enantioselective lipase-catalyzed kinetic resolution via hydrolysis of the thioesters were shown to be a suitable combination to determine the absolute configurations of chiral thiols. GC-olfactometry using a chiral stationary phase was employed to investigate sensory properties (odor qualities and thresholds) of the enantiomers

AGFD 10 Confirmation of trace level aroma-impact compounds in cantaloupe (*Cucumis melo L. var. cantalupensis* Naudin) by GC-MS/MS analysis Jianming Lin, jianming.lin@firmenich.com, Plainsboro NJ; Ying Wang, North America R & D, Firmenich, Inc., Princeton NJ A thermally gentle sample preparation method combining solid phase extraction (SPE) and gel permeation chromatography (GPC) was used to obtain an authentic aroma extract of fresh cantaloupe purchased from a local farm. More than thirty aroma-impact compounds of the cantaloupe were determined by GC-O analysis. No EI mass spectra were obtained for a number of trace level aroma-impact compounds for their unequivocal identification. The application of GC-MS/MS analysis to unambiguously confirm the identification of trace level compounds were demonstrated on several C9 compounds, e.g. 6Z-nonenal, 2E,6Z-nonadienal, 3Z-nonenyl acetate and 3Z,6Z-nonadienyl acetate.

AGFD 11 Convenient Synthesis of Stable Deuterium Labeled Alkyl Pyrazines for use in the Stable Isotope Dilution Assays Mingchih Fang, fang26@illinois.edu, Urbana IL; Keith R Cadwallader, Univ. of Illinois at Champaign-Urbana, Urbana Illinois GC-MS coupled with the use of stable isotopes as internal standards, so called isotope dilution assays (SIDA), is an extremely accurate way to quantify potent aroma compounds in foods. Despite its any advantages, SIDA is not widely used due to the high cost associated with the purchase and/or synthesis of the isotope standards. The present paper describes a convenient approach for the synthesis of stable deuterium labeled alkylpyrazines. The synthesis involves the chlorination of an alkylpyrazine into a corresponding chloroalkylpyrazines, followed by nucleophilic coupling of a deuterium labeled alkyl magnesium halide (Grignard reagent). 2-Methylpyrazine(d3), 2-ethylpyrazine(d5), 2,6-diethylpyrazine(d10), 2,3(6)-dimethylpyrazine(d3), 2,3(6)-diethylpyrazine(d5), trimethylpyrazine(d3), 2-ethyl-3,6-dimethylpyrazine(d5), 2-ethyl-3,5-dimethylpyrazine(d5), and 2,3-diethyl-5-methylpyrazine(d3) were prepared in good yields (14-82%) and high purities (86-98%). These stable isotopes were used as internal standards in stable isotope dilution assays (SIDA) to accurately and precisely determine selected alkylpyrazines in a commercial peanut butter. Among the pyrazines analyzed, 2,5-Dimethylpyrazine was found in highest abundance. However, this compound was found to have a low odor-activity value due to relatively high odor detection threshold. On the other hand, two pyrazines with low odor thresholds, 2,3-diethyl-5-methylpyrazine and 2-ethyl-3,5-dimethylpyrazine, despite their low abundance, had the highest odor-active values among the 14 pyrazines quantified. Two pyrazines, 2,6-diethylpyrazine and 2,5-dimethyl-3-vinylpyrazine, were synthesized and quantified for the first time in peanut butter.

AGFD 12 Soviet / Russian Space Food from Vostok to Mir Neil C Da Costa, neil.dacosta@iff.com, Union Beach NJ, R&D, IFF, Middletown NJ The Russians were the first to launch a man into space. On 12th April 1961 Yuri Gagarin completed one orbit of the Earth before returning safely. On the second Russian manned flight some small snacks became the first food sampled in space. Since then space food has developed greatly. In more recent years the focus has been on nutrition and counteracting decalcification of the human skeleton which occurs naturally in microgravity. Food growing experiments in space became a regular feature of Russian Salyut space station long duration missions. This was characterized by fruits, vegetables and crop growth in miniature greenhouses and in sustaining small birds and even fish as potential food sources. Also the supply of fresh fruits and vegetables by the Progress supply craft. All amounting to a long term strategy to go to Mars and back. The food flavors have been uniquely Russian to boost morale on long duration trips of up to a year and a half. Thus it has appealed to Russian cosmonauts, but not always their American counterparts who are used to a more Western variety of cuisine. This paper attempts to show the history and development of food in space from the Russian perspective.

AGFD 13 Nutritional challenges for work and recreation at high altitude Eldon W. Askew, wayne.askew@health.utah.edu, Salt Lake City Utah; Stacie Wing-Gaia; George Rodway, Univ. of Utah, Salt Lake City Utah Travel to high altitudes (HA) is accompanied by anorexia, reduced food intake and weight loss. The weight loss at HA consists of both lean body (LBM) as well as fat mass. However, the loss of LBM at altitude is typically 60-70% of the total weight loss and can result in a concomitant loss of muscle strength. Loss of muscle mass at HA is characterized by an "anabolic resistance" where muscle is unable to maintain its protein mass by stimulation of muscle protein synthesis and inhibition of protein breakdown. Reduced nutrient flow to the working muscle contributes to the blunted anabolic stimuli; however oxidative stress damage to sarcolemmal integrity and reduced anabolic sensitivity of skeletal muscle to amino acids are also likely involved. mTOR is a cell signaling factor that senses cellular nutrient and energy levels and redox status. The branch chain amino acid, leucine, may help reduce LBM loss at altitude through its unique stimulation of protein synthesis via mTOR. Preliminary results of a leucine supplementation study involving a 2011 expedition of climbers on Mt Everest will be discussed.

AGFD 14 Reducing the physiological stress of modern warfare: The role of nutritional science in the U.S. Military Stefan M Pasiakos, stefan.pasiakos@us.army.mil, U.S. Army Research Inst. of Environmental Medicine, Natick MA The Military Nutrition Division (MND) of the US Army Research Inst. of Environmental Medicine is an internationally recognized center of excellence conducting research aimed at improving the health and performance of military personnel. Primary nutrition research areas include bioenergetics, healthy weight management, and the development of combat rations that satisfy warrior-specific nutritional requirements. The effects of energy deficiency through reduced energy intake, prolonged physical activity, or combined effects of both, is a focus of current MND investigations, because negative energy balance can lead to loss of musculoskeletal mass and increased susceptibility to injury. Nutritional strategies that promote consumption of high-quality proteins, as integral components of combat rations or higher-protein diets, may attenuate the negative effects of energy deficit on skeletal muscle mass, bone mineralization, and reduce injury risk. Previous MND studies showed that consuming dietary protein at levels nearly twice the current recommended dietary allowance for protein preserves nitrogen balance in response to short-term exercise-induced energy deficit. More recent studies demonstrated reduced whole body proteolysis and increased muscle anabolism during recovery from sustained steady-state exercise after consuming an optimized essential amino acid solution. Findings emphasize the importance of protein for the maintenance of skeletal muscle mass in response to physiological stressors commonly endured by Soldiers. Current endeavors will extend upon these findings by examining effects of prolonged energy deficiency on musculoskeletal health in an attempt to define the optimal level and source of dietary protein intake required for extreme environmental conditions.

AGFD 15 Energy Balance and Nutritional Intervention Studies on a Mt Everest Expedition John W Finley, jfinley@agcenter.lsu.edu, Baton Rouge LA. Louisiana State Univ., Baton Rouge LA Weight maintenance is a major problem in high altitude mountaineering. At extreme altitude the climbers are doing hours of intense work and the same time the resting work rate is high. During an expedition on Mt Everest the energy expenditures were measured on climbers at high altitude. The stress on heart and lungs is enormous because of the increase in hematocrit. The viscous blood requires more energy to pump and the result is a high (often negative) caloric balance even on resting days. Frequently fat is poorly absorbed at high altitude. This was confirmed through fecal analysis. Intervention with added medium chain triglycerides in a variety of foods suggested that there was some improvement in fat absorption, less weight loss and somewhat better performance at altitude. It was also observed that one aspirin a day significantly lowered hematocrit and reduced risk of altitude sickness. Adequate protein consumption remains a major question.

AGFD 16 Challenges of Developing a Food System for a Mars Mission Maya R. Cooper, maya.cooper@nasa.gov, Houston TX (Space Food Systems Laboratory, NASA/JSC, Houston TX The development of space food has been evolving since a Soviet cosmonaut became the first human to eat in space in August 1961. The approach to NASA food provisioning has changed over the last 50 years and will continue to change to accommodate the different mission profiles and vehicle designs. While still maintaining residency on the International Space Station (ISS), NASA is working towards future long duration manned exploration space flights beyond low earth orbit. The primary goal of the NASA Advanced Food Technology Project

is to develop requirements and technologies that will enable NASA to provide the crew with a safe, nutritious and acceptable food system while efficiently balancing appropriate vehicle resources such as mass, volume, and crew time during these exploration missions. Since the duration of Mars missions may be as long as 2.5 years, there will be limited opportunity for resupply of food. This results in the requirement of a shelf stable food system with a shelf life of 3 – 5 years.

AGFD 17 LC/MS/MS method for the analysis of furocoumarins in citrus oil using electrospray ionization

Richard Hiserodt, richard.hiserodt@iff.com, Union Beach NJ, Li Chen International Flavors & Fragrances Inc., Union Beach NJ Furocoumarins are secondary plant metabolites commonly found in the families Umbelliferae and Rutaceae. The basic members of this class of compounds are psoralen and angelicin. Psoralen is linear and considered toxic while angelicin is angular and thought to present little threat to human health. Researchers have shown particular interest in alkoxy analogues of psoralen; particularly at the 5- and 8-positions. 5-Methoxypsoralen and 8-methoxypsoralen have been found to be effective in the treatment of the skin diseases psoriasis and vitiligo using the phototherapy technique PUVA. A mode of action is thought to be monoadduct formation with DNA but formation of diadducts, leading to cross-linked DNA and potential carcinogenic side effects, is also a possibility. In response to this, the International Fragrance Association (IFRA) and the European Commission have agreed to ban the use of furocoumarins in cosmetic products except when they are part of natural essences. When present as the result of natural essences, the total furocoumarin concentration cannot exceed 5 ppm based on the analysis of seven marker furocoumarins. To insure compliance, an LC/MS/MS method using electrospray ionization was developed for the analysis of the seven marker furocoumarins plus seven other furocoumarins. Various aspects of method development will be discussed as well as conclusions from the analysis of citrus oil.

AGFD 18 Analytical methods for evaluating the effect of thermal processing on fumonisins in corn-based

food Lauren S. Jackson, Lauren.Jackson@fda.hhs.gov, Bedford Park IL Joseph Jablonski; Kenneth Voss; Dojin Ryu. Inst. for Food Safety and Health, U.S. FDA, Bedford Park IL Toxicology and Mycotoxin Research Unit, U.S.D.A. Agricultural Research Service, Athens GA Dept. of Nutrition & Food Sci.s, Texas Woman's Univ., Denton, TX The fumonisins are ubiquitous mycotoxins produced mainly by *Fusarium verticilloides* and *F. proliferatum*, primarily in corn. Of the numerous fumonisin analogues, fumonisin B1 (FB1) is the most prevalent. Consumption of corn contaminated with FB1 is a cause of various diseases in animals, and has been correlated with increased risk of human esophageal cancer in regions of the world where corn is consumed as a staple food. While FB1 is relatively heat stable and survives conventional cooking processes such as baking and frying, several studies have suggested that high heat processes such as extrusion reduce toxin levels in finished food products, especially when reducing sugars are present. Fumonisin undergo reactions in foods during processing some of which may alter their bioavailability and toxicity. During thermal processes such as extrusion, FB1 is believed to react with glucose and other reducing sugars to form N-substituted FB1 compounds. In addition, heating has also been shown to result in binding of FB1 to proteins and starches in the food matrix. These heat-induced changes result in the formation of fumonisin derivatives which are not easily detected by conventional analytical methods. Methods (LC-MS/MS and LC-fluorescence) have been developed for detecting and quantifying these "hidden" or "masked" fumonisins in food. These methods have been essential for understanding the toxicological fate of fumonisins in processed food.

AGFD 19 EU essential oils hazard classification: Quantitative multi-component GCMS analysis

Joost Broekhans, joost.broekhans@iff.com, Tilburg Noord-Brabant, The Netherlands; Hans Leijts, International Flavors and Fragrances, Tilburg The Netherlands A quantitative analysis method has been developed for EU hazard classification requirements for essential oils. Method uses dual column GCMS to analyze for 77 analytes. Quantitation is based on full scan extracted ion technique and internal standards. A wide calibration range is needed to cover the range of concentrations observed in nature. Analysis data is automatically processed using a software routine. This paper demonstrates aspects of the method, including dual column approach, calibration, validation, identification criteria and automated data processing. Also, a comparison between full scan extracted ion and SIM quantitation is discussed.

AGFD 20 Analysis of trichloroanisole, tetrachloroanisole, pentachloroanisole and tribromoanisole in wines

using solid phase microextraction and gas chromatography triple quadrupole mass spectrometry Thomas S. Collins tscollins@ucdavis.edu, Davis CA; Anna Hjelmeland Alyson E. Mitchell Susan E. Ebeler Viticulture and Enology, Univ. of California, Davis Agricultural and Environmental Chemistry Graduate Group, Univ. of California, Davis Food Safety and Measurement Facility, Univ. of California, Davis Food Sci. and Technology, Univ. of California, Davis Haloanisoles can impart musty off-aromas in affected wines, with sensory thresholds in the low ng L⁻¹ range; therefore analysis of these low levels in wine can be problematic. Haloanisoles can be analyzed using SPME GC-MS, with limits of quantification at or near the sensory threshold. However, there is a need for rapid methods with improved limits of quantification to support screening programs for corks, barrels and other materials added to wines. We evaluated HS-SPME GC-MS/MS for improved speed and sensitivity for analysis of haloanisoles in wines. TCA, TeCA, PCA and TBA were quantified at low levels with estimated limits of quantification of 0.5 ng L⁻¹(S/N =6). The analysis was rapid with all compounds eluting in less than 7 min. The extraction time of five minutes is significantly shorter than the 20-30 minutes typical of existing methods; if additional sensitivity is required, longer extraction times could be used.

AGFD 21 Analysis of flavor-active fatty acid degradation products as well as toxicological relevant

compounds during deep-frying with different edible fats and oils Michael Granvogl, michael.granvogl@lrz.tum.de, Freising Bavaria Germany; Alice Ewert; Peter Schieberle, Technical Univ. of Munich, Freising, Germany A lot of studies have been undertaken to identify key aroma compounds of foods on the one hand, and to elucidate formation pathways of the so-called "food-borne toxicants" (e.g., acrylamide, furan) on the other hand. But, up to now, the combination of both, the analysis of desirable flavorings and undesirable toxicological relevant compounds is mostly missing. Therefore, the aim of the present study was to join the analysis of aroma-active degradation products and of the formation of selected toxicological relevant compounds during deep-frying of potato slices in different fats and oils varying in their fatty acid composition. After frying, the flavorings were first identified via GC/O and GC/MS and, secondly, quantified via stable isotope dilution assays (SIDA). Additionally, acrolein, acrylamide, and furan were quantified in the chips and in the frying medium using LC-MS/MS and GC/MS techniques. For the acrolein quantitation, two new methods using [¹³C₃]-acrolein as internal standard were developed. The lecture will emphasize the influence of the fatty acid composition on the formation of aroma compounds as well as of food-borne toxicants. For example, a frying fat, which mainly consists of mono-unsaturated or saturated fatty acids, revealed lower acrolein amounts compared to oils containing linolenic acid (e.g. rapeseed or linseed oil). In general, this study could impressively show that the correct choice of the frying fat enables the processing of deep-fried food, which contains less undesirable compounds accompanied by a consumer's well-accepted overall aroma.

AGFD 22 Controlling acrylamide formation in heated foods while maintaining color and flavor

Donald S Mottram, d.s.mottram@reading.ac.uk, Whiteknights, Reading Berkshire, United Kingdom ; J Stephen Elmore Univ. of Reading, United Kingdom It is now almost 10 years since acrylamide, a suspect carcinogen, was first reported in fried and baked potato and cereal products. It was quickly established that the Maillard reaction between asparagine and sugars was the route by which acrylamide was formed and a number of research groups, including that of Peter Schieberle in Munich, showed the important mechanistic steps involved. There was unprecedented activity in academia and the food industry to determine means of mitigating the problem of acrylamide in potato and cereal products. A major issue is that frying and baking produce desirable flavor and color in these products, also through the Maillard reaction, so many of the strategies for acrylamide reduction can have adverse effects on desirable eating quality. This presentation will discuss some of the mitigation strategies that are currently used and relate them to the mechanistic pathways of the Maillard reaction. It will also describe ongoing work to provide crops with lower levels of the essential precursors, in particular asparagine

AGFD 23 Enantioselective analysis - a valuable tool in flavor research

Karl-Heinz Engel, K.H.Engel@wzw.tum.de, Freising-Weihenstephan Bayern Germany. Over the past decades enantioselective analysis has been established as useful technique in flavor research. Owing to the development of chiral stationary phases and their integration into multidimensional systems, the capillary gas chromatographic analysis of chiral volatiles at trace levels has found broad applications. The use of the technique to (i) determine naturally occurring enantiomeric distributions, (ii) to investigate enzyme-catalyzed biotransformations and (iii) to establish structure – sensory activity relationships is presented

AGFD 24 Contribution of methylglyoxal to Maillard flavor reaction

Chi-Tang Ho, ho@aesop.rutgers.edu, Rutgers Univ., New Brunswick NJ Methylglyoxal (MG), also called pyruvaldehyde, is one of the reactive carbonyl species. Major source of MG in food and beverages is the intermediates of Maillard reaction.. Strecker degradation of MG with amino acids leads to various important odor-active flavor compounds, such as Strecker aldehydes and alkylpyrazines. MG tends to react with non-sulfur-containing dipeptides and tripeptides to form various pyrazinone derivatives. With cysteine or cysteine-containing peptides, MG will react with sulfhydryl group rapidly and generate carboxyethylcysteine derivatives. MG also reacts with some polyphenolic compounds to form addition products. The structures of the reaction products between MG and flavonoids such as epigallocatechin gallate and genistein will be discussed. The reactivity of certain polyphenols in foods with MG during food processing may have a great implication on Maillard aroma generation.

AGFD 25 Flavoromic Research applied to Mandarin Juice Flavor

Gary Reineccius, greinecc@umn.edu, St Paul MN; Josephine Charve; Anne Plotto Univ. of Minnesota, St Paul MN Citrus & Subtropical Products Lab, USDA-ARS, Winter Haven FL Flavoromic research is a non-targeted instrumental strategy to investigate chemical stimuli contributing to food flavor, and one application is flavor prediction. The objective of this work was to examine the feasibility of a comprehensive approach combined with chemometrics to predict flavor, irrespective of whether the chemical identity of the instrumental signals was known or not. Sixty mandarin juices from different cultivars and hybrids were evaluated by instrumental (GC- and UHPLC-TOF-MS) and descriptive sensory analyses. The relationships between mass spectral signals and sensory scores were investigated with partial least square regression, and then used to predict juice flavor profile. Several predictive models were developed, compared, and tested by external validation. This can provide information on the chemical compounds associated with a specific flavor characteristic which can assist in developing fruits with enhanced flavor profile through breeding strategies.

AGFD 26 Progress in analysis of flavour release during eating Andrea Buettner, andrea.buettner@lmchemie.uni-erlangen.de, Erlangen Bavaria, Germany . Only for a couple of decades flavour chemists are not only investigating the molecular composition of food aromas, but also their release mechanisms when a meal is presented to the consumer and smelled, or when the food is ingested, chewed and swallowed. Scientists developed numerous approaches to monitor the complex processes taking place during food disruption, mixing and dilution, and to follow the resulting release of odorants in the mouth and their transfer to the nasal cavity. Volatiles being exhaled either from the mouth or nose were analysed either by on-line mass spectrometric techniques, or were trapped and further analysed e.g. for trace but odour potent constituents. Monitored odorant profiles and their dynamics were further evaluated with regard to their correlation with sensory perception. This period of intense research brought about not only a number of novel methodological approaches that were specifically adapted to the requirements of in-vivo analytics. It also dramatically broadened our understanding of the specific “human” aspects in this area of research: individuality and complexity. In view of this, even today our understanding of the final sensing and processing mechanisms of the chemo-sensory stimuli during eating is still limited. This overview presentation will highlight the achievements, and the progress that has been made in flavour release research, but will also address open questions that remained unanswered until today.

AGFD 27 Colorful chemistry of cocoa and chocolate: Flavor creation by processing and eating Peter H. Schieberle, peter.schieberle@lrz.tum.de, Freising Bavaria, Germany The characteristic flavor of cocoa, the main ingredient of dark chocolate, is formed as a result of biochemical reactions during fermentation of the cocoa seeds and, secondly, by complex thermo-conversion reactions inside the dried cocoa beans during roasting. But, there is still a lack in knowledge on the key flavor compounds responsible for the attractive odor and taste profile of roasted cocoa, and, in particular, on their precursors and formation pathways. This knowledge is, however, an important prerequisite to create the desired flavor of cocoa during processing. By applying state-of-the-art methods of molecular sensory science, first, the key aroma and taste compounds of roasted cocoa were characterized and quantified. Then, the time course of the formation of selected flavor molecules during fermentation as well as during roasting was quantitatively monitored to allow differentiation between biochemical and thermal formation pathways. On the basis of systematic model experiments, new routes of the Strecker reaction were elucidated showing that different precursors are active in generating the malty and honey-like aromas of Strecker aldehydes during fermentation compared to reactions during roasting and, finally, during mastication in the human mouth. Furthermore, a simple technological step is presented lowering the astringency of cocoa by generating new, velvety tasting compounds.

AGFD 28 Development of liquid chromatographic techniques for taste compound analysis Deshou Jiang, jiang295@umn.edu, Saint Paul MN Devin Peterson, Univ. of Minnesota The identification of taste compounds in foodstuffs is challenged by the development of liquid chromatographic techniques with adequate resolving power and separation speed. This presentation will discuss the development of two dimensional offline reverse phase chromatography for the analysis of taste compounds in food systems. Optimization of the column separation was achieved by the appropriate selection of two orthogonal columns based on the recently established column selectivity comparison function $F_s(-C)$ as well as modifications to the mobile phase pH. The application of this 2D-LC system for the identification of bitter compounds in whole grain foods will also be demonstrated.

AGFD 29 Anacardic acid profiling in food plants by direct coupling of preparative high-speed counter current chromatography and electrospray/APCI mass-spectrometry (prepHSCCC-ESI/APCI-MS/MS) Gerold Jerz, g.jerz@tu-bs.de, Braunschweig Lower Saxonia, Germany; Irina Skryabin; Josue-Alexander Murillo -Velásquez; Peter Winterhalter, Technische Universität Braunschweig, Germany Escuela de Química, Universidad de El Salvador, San Salvador Anacardic acids are phenolic lipids with antibacterial properties against methicillin resistant *Staphylococcus aureus* (MRSA), *Helicobacter pylori* and also anti-tumor activities are known. From aspects of food safety, the occurrence of these cytotoxic compounds in various food relevant plant families had been documented. As a novel preparative scale screening method for sensitive and unambiguous detection of anacardic acids, high-speed countercurrent chromatography with on-line coupling to ESI- and APCI-MS/MS was applied. The anacardic acid metabolite profiles were investigated in food materials of the plant family Anacardiaceae such as *Anacardium occidentale* (cashew nuts), (*Pistacia vera*) (pistachio nuts), and also in senescent *Ginkgo biloba* leaves (*Ginkgoaceae*). The selection of ESI-/APCI-MS single ion-traces gave the direct access to molecular weights and fragment-ion-data of the eluting anacardic acids. All preparative separations were monitored in the negative ionization mode for ESI and APCI-MS (scan range m/z : 100-1500). The indicative and most prominent MS-MS fragment ion of anacardic acids is generated by the neutral loss of m/z 44 indicating the cleavage of the phenolic carboxyl group. Preparative scale HSCCC-ESI-/APCI-MS/MS (injection amount approx. 500 mg) had been shown to be a valuable tool for metabolite profiling in complex natural product crude extracts and determined the presence and structural identities of anacardic acids. Preparative substance peaks were detected by ESI-/APCI-MS and directly pooled for further 1D- and 2D-NMR spectroscopy, and also gravimetric non-standard based quantification.

AGFD 30 Comparison of Amino Acid Analysis in GABA Tea via HILIC and ERLIC Separation Coupled with Fluorescence/Charged Aerosol Detection William LaFon, william.lafon@unilever.com, Unilever, Englewood Cliffs NJ
GABA (gamma-aminobutyric acid) tea is a popular leaf tea in Japan that has been produced for over 20 years. The amino acid content of these teas is important for flavor characteristics and contribution to health. This content can be assayed using HPLC techniques that maximize sensitivity and resolution of hydrophilic components in the tea matrix, thus two modes of aqueous normal phase chromatography were evaluated for analysis of key amino acids in GABA tea. Column phase chemistry and method eluent composition were carefully selected and tuned to optimize separation parameters of chosen analytes for ultraviolet, fluorescence and charged aerosol detection

AGFD 31 Novel insights into flavor chemistry of asa foetida and overview about trace-level determination of sulfur-containing aroma compounds Andreas Degenhardt, andreas.degenhardt@symrise.com, Holzminden Niedersachsen, Germany; Margit Liebig; Birgit Kohlenberg; Beate Hartmann; Michael Roloff; Stefan Brennecke; Laurence Guibouret; Berthold Weber; Gerhard Krammer, Symrise AG, Holzminden, Germany
Asafoetida is an important condiment based on an oleogum resin with an onion-like aroma obtained from various plants of the genus *Ferula* (family Umbelliferae), which are cultivated in countries like India. Since the aroma and taste of Asafoetida is significantly dominated by sulfur compounds, a combination of specific analytical and sensorial techniques was selected to investigate the flavor profile. In particular the combination of high temperature liquid chromatography (LC taste®) with preparative GC isolation of the volatile compounds showed good results with regard to the correlation of taste effects and newly identified substances. Furthermore, the flavor contribution of the individual compounds in the context of food matrices has been investigated. In this study, high temperature liquid chromatography was applied for the characterization of taste active substances together with aroma compounds at the first time in order to link the observed effects to the complete flavor profile. In this study a specific focus is given to the selection process of analytical methods for the trace-level quantification of sulphur-containing aroma compounds.

AGFD 32 Efficient procedure for isolating methylated catechins from green tea and effective simultaneous analysis of ten catechins, three purine alkaloids, and gallic acid in tea by high-performance liquid chromatography with diode array detection Bing Hu, binghu@rci.rutgers.edu, Rutgers Univ., New Brunswick NJ
In this study, catechin Monomers with high purity (>97%), including EGC, EGCG, EC, ECG, EGCG3"Me, and ECG3"Me, were successfully isolated by just two times separation with Toyopearl HW-40S column chromatography eluted by 80% ethanol. Then, epimers of epicatechins, monomers of C, GC, GCG, and CG with high purity (>98%), were prepared from the obtained EC, EGC, EGCG, and ECG by heat-epimerization and semi-preparative chromatography methods. The chemical structures of the prepared monomers were all confirmed by ESI-TOF-MS and 1H-NMR. In addition, a new liquid chromatographic method was developed for simultaneous determination of fourteen components in tea including gallic acid, four major tea catechins, four of their epimers, two methylated catechins, and three purine alkaloids within 15 min total analysis time. These components were separated on an ODS-100Z C18 reversed-phase column by linear gradient elution with formic acid solution (pH 2.5) and methanol. The detection limits (S/N = 3) were generally on the order of 0.1–1.0 ng (0.3-2 pmol) for most components at the applied wavelength of 280 nm. Method replication generally resulted in intraday and interday peak area variation of <6% for most tested components in green, oolong, black and pu-erh tea. Recovery studies for the quantified compounds in green and oolong tea were generally within the range of 92-106% with CV less than 4.39%. Therefore, this method is sensitive, reproducible, and represents a 2.5-7 fold reduction (15 min, as opposed to 40-105 min) in HPLC analysis time from existing analytical methods for analysis of purine alkaloids, GA, tea catechins including their epimers and O-methylated derivatives.

AGFD 33 Headspace solid-phase microextraction (HS-SPME) gas chromatography mass spectrometry (GC/MS) approaches for monitoring early rancidity development in roasted almonds. Alyson Mitchell, aemitchell@ucdavis.edu, Davis CA
Lu Xiao Roasting is critical to the production of a wide array of almond products; many of which undergo long-term storage. While offering unique flavor, roasting can promote reactions that lead to lipid oxidation and the development of off-odors and aromas associated with rancidity. Rancidity development during storage significantly shortens the shelf-life of roasted almonds. To control almond quality and better predict storage shelf-life, markers are needed for evaluating early rancidity in roasted almonds before sensorial changes can be detected. To address this, a headspace solid-phase microextraction (HS-SPME) method using DVB/CAR/PDMS fibers was developed, coupled to GC/MS for monitoring changes in a range of pyrazines, alcohols and aldehydes in roasted almonds undergoing accelerated and room temperature storage. Pyrazines, alcohols (C4-9) and aldehydes decreased in the first week of roomtemperature storage. Levels of hexenal increased 3-fold between weeks 2-4 of storage, while levels of pyrazines did not change after initial losses.

AGFD 34 Climate and salinity effects on health promoting and color properties in the pomegranate (*Punica granatum* L.) fruit arils Hamutal Borochoy-Neori, hamutalborochoy@rd.ardom.co.il, Hevel Eilat, M. P. Hevel Eilat Israel; Doron Holland; Bhimanagouda S. Patil; Naftali Lazarovitch; Sylvie Judeinstein, Southern Arava Research and Development, Hevel Eilat, Israel
Newe Ya'ar Research Center, Agricultural Research Organization, Ramat Yishay Israel
Dept. of Horticultural Science, Vegetable and Fruit Improvement Center, Texas A&M Univ., College Station TX 77843-2119, Ben-Gurion Univ. of the Negev, Sede-Boqer Campus, Israel
Pomegranate (*Punica granatum* L.) became a commercially important

crop in recent years due to multitude health promoting properties attributed to different parts of the fruit. Worldwide pomegranate production has expanded greatly in traditional as well as new locations of diverse climatic and water conditions. The pomegranate industry demands fruit with intense red color and high antioxidant content. It is therefore especially important to investigate the effects of climate and water quality on pomegranate anthocyanin and total polyphenolics accumulation. Our current research has focused on the edible part of the fruit, specifically, the arils. A diverse selection of pomegranate cultivars was employed. To explore climate effect, fruit that developed and ripened under a wide range of temperature regimes were studied. To explore water quality effect, fruit from plants irrigated with a wide range of salinities, from 0.5 to 9 dS m⁻¹, were studied. Aril anthocyanins were analyzed by RP-HPLC and phenolics content was determined by the Folin-Ciocalteu assay. Both abiotic factors considerably affected the accumulation of polyphenolics and anthocyanins in the pomegranate arils. Cooler temperatures enhanced the accumulation of both health promoting and pigment compounds. Increased salinity enhanced polyphenolics accumulation but reduced that of anthocyanins. Climate also affected significantly the relative proportions of delphinidins and cyanidins and their level of glucosylation. Our results on climate and salinity effects on pomegranate color and antioxidant traits can benefit the current breeding and agricultural efforts to enhance pomegranate fruit quality, especially in face of global warming and water quality deterioration.

AGFD 35 Plant breeding and genetic approaches to improve flavor and nutrients in vegetables sekhar s boddupalli, sekhar.s.boddupalli@monsanto.com, Global Consumer R&D, Monsanto Vegetables Division, Woodland CA During the past 20 years, there has been a dramatic increase in obesity and diabetes across the globe. Escalation in prevalence and progression of this global, diet-linked epidemic is generally attributed to caloric-rich, nutrient-poor diets, increase in aging population and a sedentary lifestyle. Significant scientific support exists that increased consumption of vegetables is associated with lower risk of chronic diet-linked diseases. In spite of the inherent nutritive value and need for enhanced consumption, there is not enough consumption of vegetables due to perceived poor taste, appearance appeal and convenience. Enhancing the levels of precursors to essential nutrients and phytonutrients in vegetables would have favorable impact on consumer sensory appeal at the same time delivering higher nutritional value. Significant opportunity exists to integrate advances in breeding technology, high throughput analytical, and molecular nutrition tools to address unmet consumer need and also meet the global demands of agricultural productivity. Germplasm diversity for various consumer and agronomic traits along with whole genome sequence information, molecular markers, biochemical pathway insights, and high throughput phenotyping enable rapid innovation of new crop varieties for enhancing consumption and ensuring crop productivity. Progress in deploying plant breeding coupled with high throughput genetic and molecular approaches to enhance flavor and nutrition in vegetables will be presented.

AGFD 36 Characteristic volatile compounds from Nagami kumquats (*Fortunella margarita*) and their cell proliferation effect G.K. Jayaprakasha, gjayaprakasha@ag.tamu.edu, College Station TX; K.N.C. Murthy; Bhimanagouda S. Patil VFIC, Horticultural Sciences, Texas A&M Univ., College Station TX Kumquats, a citrus fruit of *Fortunella* species, have been used in traditional herbal medicine especially for cold and cough. The fruit varies in shape from round to slightly oval of 2 cm diameter. The genus *Fortunella* is taxonomically close to *Citrus*. To best our knowledge, systematic study on identification of characteristic flavoring compounds and their health benefits is limited. In the present study, fresh nagami kumquats were subjected for the isolation of volatile components by hydro-distillation using Clevenger type apparatus. The chemical constituents were analyzed by GC-MS using dimethylpolysiloxane capillary column. Fifteen volatile compounds were identified by mass spectral fragmentation and Kovats indices. The major hydrocarbon identified was d-limonene along with oxygenated compounds. The identified oil was subjected for proliferation inhibition activity studies using human androgen dependant prostate cancer (LNCaP) cells. The volatile oil exhibited time dependant inhibition of LNCaP cells proliferation. Treatment of 100 µg/ml of volatile oil for 72 h resulted in 50% proliferation inhibition suggesting the significant activity of kumquats volatile oil. The activation of program death induction was found to be the key mode for proliferation, which was confirmed through western blot analysis of LNCaP cells treated with 100 µg/ml. The constituents of volatile oil has resulted in elevation of Bax/Bcl2 ratio, activation of death inducing protein (p53), caspase-3 and caspase-8 the key markers for apoptosis induction. The constituents have also demonstrated their ability to inhibit inflammation inducing markers, suggesting possibility of association of anti-inflammatory activity along with induction of apoptosis. Taken together, the monoterpenes rich volatile oil of *Fortunella margarita* has a beneficial role in prevention of cancer cells proliferation and the results suggest further studies using in vivo system for better applications. These results are based on the work supported by the USDA-NIFA # 2010-34402-20875 "Designing Foods for Health" through the Vegetable & Fruit Improvement Center.

AGFD 37 Pineapple juice flavor: Key aroma compounds and changes during industrial processing Martin Steinhaus, martin.steinhaus@lrz.tum.de, Freising Germany ; Karin Thomas; Peter Schieberle Deutsche Forschungsanstalt für Lebensmittelchemie Freising, Germany Pineapples are one of the most important tropical fruit crops. They are mainly consumed as fresh fruit, but also processed to canned fruits and juice. Screening for aroma-active compounds in a fresh pineapple juice, characterized by a pleasant fresh, fruity aroma using aroma extract dilution analysis revealed eighteen substances with high FD factors. Their quantitation by stable isotope dilution assays resulted in 13 compounds that exceeded their odor thresholds. The aroma of an aqueous pineapple juice model solution based on these natural odorant concentrations

perfectly resembled the aroma of the original juice, thus indicating that the key aroma compounds were included. Subsequently, changes in major aroma-active compounds during industrial NFC juice processing were studied. Results indicated that losses in major odorants as well as the formation of methional from its precursor methionine during processing accounted for the development of a kind of "cooked"-like off-flavor in the industrially manufactured pineapple juice.

AGFD 38 Study of the genetic factors that control fruit color variation in pomegranate (*Punica granatum*

L.) Doron Holland, vhhollan@agri.gov.il, Ramat Yishay Israel; Zohar Ben-Simhon; Hamutal Borochoy-Neori; Irit Bar-Yaakov; Rotem Harel-Beja; Amir Sherman; Ron Ophir, Newe Ya'ar Research Center, Agricultural Research Organization, Ramat Yishay, Israel Southern Arava Research and Development, Hevel Eilat Israel Dept. of Fruit Tree Sciences, Volcanic Center, Agricultural Research Organization, Bet Dagan, Israel Different pomegranate varieties display high variability of fruit color ranging from green to dark purple. Skin and aril color in pomegranate is determined by anthocyanin molecules. Apart from being important for the commercial value of the fruit, anthocyanins help to protect the fruit from radiation damage and are important for human diet as free radical scavengers and inhibitors of lipid peroxidation. Our study is aimed towards understanding the genetic factors that are responsible for the high variation observed in skin color, type of anthocyanin molecules and rate of pigment accumulation during pomegranate fruit development. The sequence of over 200 genes potentially involved in the anthocyanin biosynthetic pathway was determined and expression data for some of the genes was associated with anthocyanin content in several pomegranate cultivars that prominently differ in their skin color. The molecular genetic data combined with phenotypic analysis of segregating populations is expected to reveal the genetic factors that determine color variation in pomegranates.

AGFD 39 High hydrostatic pressure processing as a strategy to increase carotenoid contents of tropical

fruits Carmen Hernandez-Brenes, chbrenes@itesm.mx, Centro de Biotecnología-FEMSA, Monterrey Nuevo Leon, Mexico ; Rocio I Diaz-De La Garza Daniel A Jacobo-Velazco; Perla A Ramos-Parra; Raul Villareal-Lara DEPT. OF BIOTECHNOLOGY AND FOOD ENGINEERING, TECNOLÓGICO DE MONTERREY, MEXICO BIOTECHNOLOGY RESEARCH CENTER-FEMSA, TECNOLÓGICO DE MONTERREY, MEXICO DEPT. OF AGROBIOTECHNOLOGY AND AGRIBUSINESS, TECNOLÓGICO DE MONTERREY, NUEVO LEON, Mexico Avocado (*Persea americana*), papaya (*Carica papaya*) and mango (*Mangifera indica* L.) contain bioactive molecules that protect human cells against the detrimental effect of reactive oxygen species. High hydrostatic pressure (HHP) processing has been pointed as an effective alternative to stabilize tropical fruit pulps due to retention of flavor and desirable sensory characteristics. Project objectives were to evaluate the HHP processing stability of carotenoids from avocado, papaya and mango pulps and of plant cell oxidative stress biomarkers. HHP processing (600MPa/3min) caused an increase in total carotenoid concentrations (~56%) for avocado pulp. Neoxanthin b showed the highest percentage increase (513%) followed by a-cryptoxanthin (312%), a-carotene (284%), b-cryptoxanthin (220%), b-carotene (107%) and lutein (40%). Papaya pulps presented increases in phytofluene (224%), phytoene (222%), lycopene (207%), β -cryptoxanthin (145%) and β -carotene (131%), while mango carotenoids remained unchanged. Higher concentrations of extractable carotenoids have been attributed to possible changes in the permeability of cells and chloroplast membranes induced by HHP processing. Herein evidence was provided that HHP application caused oxidative stress within the tissue, and intact RNA molecules were found in pressurized samples suggesting that the cells are metabolically active and biosynthesizing plant cell antioxidants.

AGFD 40 Preparative separation and pigment profiling of betalains from fruits of *Opuntia ficus-indica* by

ion-pair high-speed countercurrent chromatography Gerold Jerz, g.jerz@tu-bs.de, Braunschweig Lower Saxonia, Germany ; Bettina Klose; Slawomir Wybraniec; Peter Winterhalter Inst. of Food Chemistry, Technische Universität Braunschweig, Braunschweig Germany Analytical Flavor Research, Symrise AG, Holzminden, Germany Faculty of Analytical Chemistry, Inst. C-1, Dept. of Chemical Engineering and Technology, Cracow Univ. of Technology, Cracow, Poland *Opuntia* varieties play an important role as a drought tolerant plant resource for fruit, fodder and land conservation. *Opuntia* fruits moved to the scientific focus due to nutritional values and their potential health properties such as treatment of diabetes. Pigment profiling of betaxanthins and betacyanins occurring in yellow, orange and violet *Opuntia ficus-indica* fruits from Sicily had been realized by using two chromatographic dimensions including preparative ion-pair HSCCC and subsequent off-line LC-ESI-MS/MS analysis of the recovered fractions. Countercurrent chromatography as an all liquid chromatographic technique is commonly applied in preparative scale isolation procedures where solely immiscible biphasic solvent systems are used. For separation of the highly instable and polar betalain structures, suitable solvent systems not inducing degradation of these pigments are t-butylmethylether, n-butanol, acetonitrile and water. Different perfluorinated carboxylic acids were used as ion-pair modifiers for the preparative recovery by HSCCC of charged betalains from *Opuntia* fruits. Minor concentrated lipophilic betacyanins such as 15R- and 15S-phyllocactin were identified by LC-ESI-MS-MS, so far not known in violet pigmented *Opuntia* fruits

AGFD 41 Monitoring the formation of flavanol-Maillard adducts in model systems relating to cocoa

roasting Donald S Mottram, d.s.mottram@reading.ac.uk, Whiteknights, Reading Berkshire, United Kingdom; Maria-Jose Oruna-Concha; Jeremy P E Spencer; Glenn R Gibson Univ. of Reading, United Kingdom Previous studies have shown that reactive carbonyl compounds such as glyoxal (GO) and methylglyoxal (MGO), which are formed as a result of the Maillard

reaction, can react with polyphenol compounds, such as flavanols. Under the high temperature conditions that occur during the processing of food ingredients, like coffee beans, such reactions will contribute to the loss of nutritionally beneficial polyphenols. This presentation discusses the application of LC-MS-MS in the identification and quantitation of adducts of MGO and GO with epicatechin (EC) the main flavan-3-ol present in cocoa. Reactions were carried out in both aqueous and low moisture model systems at temperatures and times typical of the roasting of cocoa beans (120-140°C for between 5 and 30 min). The results confirmed the formation of previously identified adducts (mono- and di-MGO/GO adducts) and show major effects of heating conditions. In addition larger molecules derived from EC units joined by GO bridges were produced.

AGFD 42 Volatile compound analysis by GC-TOF-MS: applications and challenges Michael J. Morello, mike.morello@pepsico.com, PepsiCo Global R&D, Barrington IL Advances in GC-TOF-MS have enabled fast data collection. The increased data collection rates enable faster chromatography to be coupled with peak deconvolution. Examples of the use of GC-TOF-MS for analysis of a juice sample, a grain sample, and a comparison of rPET samples will be used to illustrate benefits of fast data collection rates. Challenges in using this technology will also be addressed.

AGFD 43 Comparison of fast gas chromatography- surface acoustic wave sensor (FGC-SAW) and capillary GC-MS for determining strawberry and orange juice volatiles Xiaofen Du, xdu@ufl.edu, Lake Alfred FL; Russell L. Rouseff Univ. of Florida, Inst. of Food and Agricultural Sciences, Lake Alfred FL The development of rapid, simple and less costly techniques for volatile analysis has been an active area of research in recent years. Fast gas chromatograph-surface acoustic wave sensor (FGC-SAW) is a new instrumental approach, which employs a solid phase volatile trap coupled with a short (1 m) capillary column and a single quartz surface acoustic wave (SAW) detector. Headspace FGC-SAW analyses typically take 15-30 s whereas an equivalent GC-MS run will typically take 20-60 min. As expected, less chromatographic resolution is observed for such a short analysis time. Considering the short column, the observed resolution is surprising. For strawberries, 19 peaks were observed with the FGC-SAW and 80 peaks for the GC-MS. For orange juice, 15 peaks were observed with the FGC-SAW and 60 peaks for the GC-MS. The major volatiles in strawberry puree were esters; whereas main compounds in orange juice were terpenes. Although the resolution and identification of fruit volatiles using FGC-SAW was inferior to GC-MS, the usefulness of the data to distinguish strawberry cultivars and orange juice quality was roughly equivalent. Both GC-MS data and data from FGC-SAW showed similar trends of total volatiles with strawberry fruit maturity and similar clustering patterns in principle component analysis (PCA). Both techniques could differentiate 10 strawberry cultivars as well as between fresh orange juice and temperature abused orange juice. However, the FGC-SAW could not detect trace volatiles associated with microbial contamination such as guaiacol and 2,3-butanedione.

AGFD 44 Beside structure elucidation: Applications of NMR in food analysis . Oliver Frank, oliver.frank@tum.de; Thomas Frank Hofmann Technical Univ. of Munich, Freising Germany NMR spectroscopy is today one of the most important spectroscopic tools for the chemist. Experiments like COSY, TOCSY, NOESY, ROESY as well as HSQC and HMBC are widespread spectroscopic methods used routinely for the structure elucidation of e.g. bioactive compounds in foods. Beside these techniques, NMR spectroscopy offers much more to food scientists. NMR is by definition a quantitative spectroscopic tool due to the fact that the intensity of a resonance line is directly proportional to the number of resonant nuclei. This enables the possibility of precise quantification of natural products in complex mixtures as well as the purity assessment of isolated substances as reference compounds. Moreover, detection of a specific binding between a macromolecule and a ligand is an important task for the understanding of biochemical regulation processes as well as interactions between different constituents in foods e.g. macromolecules like melanoidins and taste active compounds. An elegant experiment for this purpose is the so called saturation transfer difference (STD). The difference of a standard NMR spectrum and a spectrum recorded with selective saturation of the receptor, yields in a STD-NMR spectrum, which contain only NMR signals of molecules with contact to the receptor/macromolecule during the saturation period. Therefore these spectra are particularly capable to detect binding processes. All signals of non-binding molecules are subtracted in the difference NMR spectra and this allows an unequivocal identification of molecules even in mixtures binding to a biopolymer or a receptor protein. Examples of one or the other technique will be presented in the presentation.

AGFD 45 The power law and dynamic rheology in food analysis Michael H. Tunick, michael.tunick@ars.usda.gov, Eastern Regional Research Center, USDA-ARS, Wyndmoor PA, Protein networks impart functional and structural characteristics to food, and should be examined to gain an understanding of properties of the product. Food matrices are investigated nondestructively by small amplitude oscillatory shear analysis, which provides information on viscoelasticity, including values for elastic modulus (G') and viscous modulus (G''). Relationships between frequency (ω) and viscoelastic data are obtained from frequency sweeps by applying the power law, where $G' = a \omega^x$ and $G'' = b \omega^y$. The power law was applied to the investigation of Queso Fresco cheeses subjected to various pressure treatments and storage conditions. Power law equations for G' and G'' revealed decreases in values of x and increases in values of y during aging at 4°C. The release of excess whey during storage created a stronger and more elastic protein matrix that was less sensitive to changes in frequency. Other cheeses show the opposite trend -- the matrix degrades over time because of proteolysis. Values for b and y were always lower than

those of α and χ , which indicates that viscous dissipation of energy was not as pronounced as elastic energy storage. The power law may be applied to dynamic rheology of food to gain an understanding of the nature of the protein matrix.

AGFD 46 Chemoprofiling of Palestine sweet lime (*Citrus limmetioides*) volatiles and their inhibitory role of

colon cancer cells proliferation Bhimanagouda S. Patil, b-patil@tamu.edu, College Station TX; G.K. Jayaprakasha; K.N.C. Murthy Vegetable and Fruit Improvement Center, Dept. of Horticultural Sciences, Texas A&M Univ., College Station TX Citrus juice is the most appreciated juice beverage world-wide, due to its characteristic aroma. Volatile compounds are especially important to the flavor of orange, lime, lemon and grapefruit juice, including alcohols, aldehydes, esters, ketones and hydrocarbons. Most of the citrus fruits accumulate high concentration of citric acid and soluble sugars. Generally vacuolar pH of acid limes will be 2.0 and in case of Palestine sweet lime (*Citrus limmetioides*) the pH is 5.0. To our knowledge, there is no report on chemical composition of volatile oil from Palestine sweet lime (PSL). In the present study, PSL were juiced and subjected to hydro-distillation for four hours to obtain volatile oil. The chemical composition was analyzed by gas chromatography coupled with mass spectra. Volatile compounds were separated on Rtx-5 Sil MS column. Fifteen compounds were identified by comparing the retention indices, co-injection with standards and matching their mass spectral fragmentations. Hydrocarbons were found to be most abundant compounds present in this volatile oil. This oil demonstrated significant dose dependant inhibition of colon adenocarcinoma (SW480) cell proliferation with inhibition of more than 40% cells at 75 $\mu\text{g/ml}$ at 24 h. Furthermore, induction of apoptosis by the compounds were confirmed through translocation of phosphatidylserine upon incubation of cells with volatile oil at 50 $\mu\text{g/ml}$. Immunoblotting of the SW480 cells treated with volatile oil at less than 50 $\mu\text{g/ml}$ clearly demonstrated induction of apoptosis and suppression of inflammatory marker NF κ B. Furthermore, its down-stream products are the most possible cause for cytotoxicity. This is the first report on chemoprofiling and anti-proliferative role of volatile oil from PSL. These results are based on the work supported by the USDA-NIFA # 2010-34402-20875 "Designing Foods for Health" through the Vegetable & Fruit Improvement Center.

AGFD 47 Metabolomic models of fruit extracts and chemoprevention Faith J Wyzgoski, wyzgoski.1@osu.edu, R. Neil Reese; Liladhar Paudel; Peter L. Rinaldi; M. Monica Giusti; Jodee Johnson; Joseph C. Scheerens; Joshua Bomser; Ann M. Chanon; James K. Hardy; Chrys Wesdemiotis; A. Raymond Miller; Artemio Z Tulio Jr, The Ohio State Univ., Mansfield OH

South Dakota State Univ., Brookings SD Dept. of Chemistry, Univ. of Akron, Akron OH Dept. of Food Sci. and Technology, The Ohio State Univ., Columbus Dept. of Horticulture and Crop Science, The Ohio State Univ., Ohio Agricultural Research and Development Center, Wooster Dept. of Human Nutrition, The Ohio State Univ., Columbus Ohio U.S. FDA, Summit - Argo Illinois US Recent studies have shown that freeze-dried black raspberries (*Rubus occidentalis* L.) are effective in preventing the proliferation of cancer cells, most notably with respect to colon and oral cancers. Seeking to better understand these results, our interdisciplinary research group employed nuclear magnetic resonance (NMR)-based metabolomic methods to build statistical models to discern the relationships between constituents of black raspberries with respect to inhibition of proliferation of growth of HT-29 colon cancer cells. Studies were conducted with highly variable black raspberry samples obtained from fruit in varying stages of ripeness. When NMR data were regressed against cell assay results using partial least squares regression analysis, regression vector values were calculated and correlated with specific compounds found in black raspberries. Rankings of the regression vector values showed that the major chemopreventive contributors were anthocyanins, cyanidin 3-O-rutinoside, cyanidin 3-O-(2(G))-xylosylrutinoside and cyanidin 3-O-glucoside. However, other phenolic compounds which included hydroxybenzoic and ellagic acid derivatives were also found to be important. Advanced NMR experiments coupled with HPLC-ESI-MS/MS were conducted on additional black raspberry extracts to aid in their identification. Our work indicates that these metabolomic techniques could be applied to a variety of fruit extracts to study chemopreventive effects.

AGFD 48 Antioxidant activity of anthocyanin-rich Colombian tropical fruits Coralia Osorio,

cosorior@unal.edu.co, Bogota DC, Colombia ; Liliانا Santacruz; José G. Carriazo; Ovidio Almanza. Departamento de Química, Universidad Nacional de Colombia, Bogota, Colombia Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia A screening of anthocyanin composition (qualitative and quantitative) and antioxidant activity of four wild tropical fruits from Colombia was achieved. *Rubus megalococcus* Focke (Rosaceae), *Myrciaria aff cauliflora* D. Bery (Myrtaceae), *Hyeronima macrocarpa* Mull. Arg. (Euphorbiaceae), and *Hyeronima macrocarpa* (Euphorbiaceae) fruits were separately extracted with methanol-acetic acid (19:1, v/v). In each case, the lyophilized extract obtained after solvent evaporation under vacuum was applied on an Amberlite XAD-7 column for the selective adsorption of anthocyanins. The column was washed with water, and the anthocyanin-rich extracts (AREs) were obtained after elution with methanol-acetic acid (19:1, v/v). Each extract was analyzed by HRESI-MS and MS/MS in a LCMS-IT-TOF equipment in order to characterize the anthocyanin pigments. The comparison of these results with standards allows identifying the major constituents in each extract. Electron Paramagnetic Resonance (EPR) is a highly specific and sensitive technique for direct detection and quantification of free radicals generated by ex vivo or in vivo chemical reactions, and is based on the absorption of microwave energy by unpaired electrons when they are in a magnetic field. Thus, the antioxidant activity of AREs was measured with stabilized radical EPR spectroscopy. The ARE of *Hyeronima macrocarpa* exhibited the highest radical scavenging activity in comparison with the other extracts, using ABTS and DPPH as free radicals. A second-order kinetic model was followed in all

of the cases. These results suggested that the studied fruits are promising not only as source of natural pigments but also as antioxidant materials for food industry. Financial support: IFS (International Foundation of Sciences).

AGFD 49 Flavonoid content and antioxidant properties of some tropical and subtropical fruits from the Annonaceae and Citrus genera Davide Barreca, barrecad@isengard.unime.it, Viale F. Stagno d[apos]Alcontres 31, Messina Italy; Ersilia Bellocco; Corrado Caristi; Ugo Leuzz; Giuseppe Gattuso. Dipartimento di Chimica Organica e Biologica, Università di Messina, Messina Italy We have investigated the composition and properties of some tropical and subtropical fruits belonging to the Annonaceae and Citrus genera. RP-HPLC-DAD-MS-MS analysis showed that cherimoya (*A. cherimola*) is characterized by the abundance of flavan-3-ols (epicatechin and procyanidins), kumquat (*C. japonica*) by a dihydrochalcone (phloretin-di-C-glucoside) and flavones, sweet lemon (*C. limetta*) by flavanones (neohesperidin and eriocitrin) and flavones, and citron (*C. medica*) by flavones (dosmetin-di-C-glucoside, neodiosmin) and flavanones. Cherimoya extracts possess remarkable radical scavenging ability towards DPPH•, ABTS•+, O₂•- and OH•- (IC₅₀ 100–490 gallic acid equivalents), and they have been tested for their anti-peroxidation and cytoprotective effects on tert-butylhydroperoxide-treated cells, and for their ability to avoid protein and DNA degradation by HOCl and Fenton-type reactions. As for kumquat, crude juice, selected flavonoid fractions and the main dihydrochalcone component have been tested separately against DPPH• and ABTS•+, gaining insight on the constituents responsible for antioxidant activity.

AGFD 50 Acai berries and walnuts: Brain health boosters Shibu M Poulouse, shibu.poulouse@ARS.USDA.GOV, Boston MA; Donna F Bielinski ; Barbara Shikitt-Hale Neuroscience, USDA-ARS, Human Nutrition Research Center on Aging at Tufts Univ., Boston MA Neuroinflammation (INF), oxidative stress (OS) and loss of protein homeostasis in the brain have been implicated in the alarming rise of age-related diseases, which will reduce the quality of life while raising medical costs. We investigated whether supplementing brain cells with extracts from walnuts or acai berries would reduce chemically-induced inflammation and OS, along with activating the brain's natural housekeeping functions. Thus, BV2 microglia, HT22 hippocampal neurons and autophagy-deficient ATG5 -/- fibroblast cells were pre-treated with acai berry or walnut extracts, then subjected to stress with lipopolysaccharide (LPS), dopamine (DA) or bafilomycin (BF). Acai pulp extracts rich in unique polyphenols and phytosterols at 50-250 µg/ml significantly (p<0.01) reduced the LPS/DA-induced OS/INF, measured in terms of TNFα expression and phosphorylation of NFκB and p38-MAPK. Similar effects were also observed for walnuts at 30-90 µg/ml. Significant reversal of BF-induced autophagy inhibition was observed for both extracts (p<0.05), with altering effects on markers such as p62, MAP1B-LC3, beclin1 and mTOR. Overall, the results indicate multiple health-promoting effects of walnuts and acai berries on brain cells.

AGFD 51 Prevention of biofilm formation and bacterial adhesion after consumption of cranberry juice cocktail Terri A Camesano, terric@wpi.edu, Yuxian Zhang; Yuanyuan Tao; Paola A Pinzon-Arango; Regina Roberto; Laila Abu-Lail Chemical Engineering, Worcester Polytechnic Inst., Worcester MA A double-blind, placebo-controlled pilot clinical trial on the effect of cranberry juice cocktail (CJC) consumption on biofilm formation and bacterial adhesion was conducted in 10 healthy women between the ages of 18 and 27. A single dose of 16 oz. of CJC or a placebo beverage was given to the volunteers, and urine samples were collected in the following 48 hours. Bacteria (*E. coli* B37, CFT073, BF1023, HB101, and *S. aureus* ATCC43866) were cultured in the urine samples supplemented with media and the amount of biofilm formed was measured using a crystal violet absorbance assay in a 96-well plate. In the urine of volunteers who had consumed CJC, biofilm formation was inhibited within 24 hours after CJC consumption, and biofilm formation started to increase after 48 hours by 49-67%. *S. aureus* showed the least biofilm formation after incubation with post-CJC urine. While *E. coli* CFT073 is a commonly studied uropathogenic *E. coli* strain and it expresses P fimbriae, *E. coli* B37 and BF1023 are antibiotic resistant and do not contain P fimbriae. Atomic force microscopy measurements of bacterial adhesion also revealed that cranberry metabolites could block bacterial adhesion, and changed the conformation of molecules on the bacterial surfaces. This is the first study to show that biofilm formation in antibiotic resistant *E. coli* and a wide range of uropathogens, including *S. aureus*, can be prevented in the urine of healthy women who have consumed CJC. We also demonstrated the duration of the benefit, noting that anti-biofilm activity in the urine peaks between 24 and 48 hours after drinking CJC, depending on the bacterial strain studied.

AGFD 52 Seed and juice characterization of pomegranate fruits grown in Tunisia: Comparison between sour and sweet cultivars revealed interesting properties for prospective industrial applications Nejib Hasnaoui, nejibhasnaoui@yahoo.fr, Medenine Medenine, Tunisia ; Messaoud Mars; Sana Ghaffari; Pablo Melgarejo; Francisca Hernandez U.R. Agrobiodiversity, Higher Agronomic Inst., Chott Mariem Sousse , Tunisia Laboratory of Aridland and Oases Cropping, Inst. of Arid Regions, Medenine Medenine, Tunisia Dept. of Plant Production and Microbiology, Univ. of Miguel Hernández, Alicante Orihuela, Spain Tunisian pomegranate genetic resources consist of sweet and sour cultivars, showing large morphometric variability. In the present work we characterized seeds and juice contents of sugars and organic acids of 5 sour and 7 sweet pomegranate cultivars. Results showed that citric acid was predominant in sour pomegranates, while malic acid was the most prevalent in sweet ones. Paradoxically, sour cultivars have higher sugar content than the sweet ones. A strong correlation was found between sourness and citric acid content, which is assumed to be the major factor that determines

sour taste in pomegranate fruits. Besides, some of the seed parameters showed a significant positive correlation with acidity. Sweet cultivars were appropriate for fresh consumption and juice production due to several attributes in addition to their sweetness. Equally, sour pomegranate showed several characteristics that could be of great interest for food and nutraceutical industries.

AGFD 53 Studies in the Use of Algae in Fish Nutrition Peter W Perschbacher, pperschbacher@uaex.edu, Dept. of Aquaculture/Fisheries, Univ. of Arkansas at Pine Bluff, Pine Bluff AR Algae are and will be increasingly important in aquaculture feeds. Tilapia have evolved on an algae diet in Africa. Astaxanthin is currently derived from algae and has increased survival and added red coloration. Efforts to reduce or eliminate fish protein and oil from diets are focusing on algal meals. Algae are also being considered for biofuel and carbon sequestration purposes, both of which will increase algal byproducts. Our studies found natural sources of algae were utilized by Nile tilapia *Oreochromis niloticus* co-cultured with channel catfish *Ictalurus punctatus* and added 1000 lbs/a of tilapia at little cost. Spirulina replaced 50% of supplemental feed of Nile tilapia in indoor tanks with no decrease in growth and increased HUFAs (highly unsaturated fatty acids) by 50%. Additional studies at UAPB are finding EFAS (essential fatty acids) from algal oil outperformed those of several other vegetable oils

AGFD 54 Non-invasive means to determine stage of maturity in white sturgeon females Anna G Cavinato, acavinat@eou.edu; Sarah A Servid; Joel Van Eenennaam; Serge Doroshov; Xiaonan Lu; Barbara Rasco; Mariah Talbott; Wendy Sealy; Molly Webb Eastern Oregon Univ., La Grande, Oregon Univ. of California Davis, Washington State Univ., Montana State Univ., Bozeman Fish Technology Center, USFWS Sturgeon farming is becoming a major supplier of caviar to the domestic and international market. Currently, the only means by which to accurately assess stage of maturity in sturgeon is calculation of the oocyte polarization index (PI; ratio of the distance between the germinal vesicle and the animal pole to the animal-vegetal oocyte diameter). This technique is accurate but time consuming. The current technique employed by the white sturgeon caviar industry, to sort females prior to harvest, is to biopsy the ovary and visually assess whether the eggs are firm and of adequate size. This technique could result in decreased caviar yield due to harvesting females at the early stages of ovarian maturity (high PI). The long-term goal of this study is to develop a less invasive, fast and accurate predictor of maturity. Ovarian maturity of sturgeon grown in California and Idaho farms was assessed using short wavelength near infrared spectroscopy (SW-NIR) and Fourier transform infrared spectroscopy (FT-IR), and compared to the actual oocyte PI in the fall of 2009 and 2010. Fish were segregated into groups of maturity using oocyte PI and harvested at the predicted optimal time in the spring to determine whether our alternative techniques (SW-NIR and FT-IR) could accurately predict oocyte PI. To date, SW-NIR can successfully predict oocyte PI with 64-84% accuracy, and FT-IR can successfully predict oocyte PI with approximately 90% accuracy, suggesting that these tools may be useful alternative methods for pre-screening females prior to harvest.

AGFD 55 Effects of UV irradiation on fish gelatin properties Bor-Sen Chiou, bor-sen.chiou@ars.usda.gov Caio G Otoni; Roberto J Avena-Bustillos; Cristina Bilbao-Sainz; Peter J Bechtel; Syed H Imam; Greg M Glenn; William J Orts Bioproduct Chemistry and Engineering, U.S. Dept. of Agriculture, Albany CA Processed Foods Research, U.S. Dept. of Agriculture, Albany CA Dept. of Biological and Agricultural Engineering, Univ. of California Davis, SubArctic Research Unit, U.S. Dept. of Agriculture, Kodiak AK Commercial cold-water fish and tilapia gelatin samples were irradiated with UV radiation. At higher UV doses, the gel strengths of the cold-water fish and tilapia gelatin samples increased by more than 50% and 16%, respectively. This indicated that UV radiation had a greater effect on cold-water fish gelatin properties. Also, irradiated samples had higher viscosity, gelation temperature, and melting temperature values. In addition, gel electrophoresis results showed that samples treated with higher UV doses contained higher concentrations of immobile gelatin bands. These results indicated that UV radiation might have caused some cross-linking between gelatin chains.

AGFD 56 Studies on Bioactive Compounds from Okra Seed Extracts: Selective Inhibitors of Advanced Glycation End Products Bishambar Dayal, dayalbi@umdnj.edu, Ritesh Amin; Vineela Reddy Yannamreddy; Michael A Lea, UMDNJ-New Jersey Medical School, Newark NJ Advanced Glycation End Products (AGEs) have been associated with the micro-vascular complications in diabetes and other progressive age-related neurodegenerative diseases. Glycation alters the protein structure and stability in vivo as a result of high glucose concentrations. Recent studies from our laboratory indicated that okra seed extracts inhibit the formation of advanced glycation end products (AGEs) during the incubation of bovine serum albumin with glucose. Briefly, protein glycation in the absence and presence of Okra seed extracts were prepared by incubating BSA (0.1mg/ml) at 37°C with 1M glucose in 0.4mM phosphate buffer, pH 7.4 containing 0.1% sodium azide. Low molecular weight reactants and unbound sugars were removed by extensive dialysis. The degree of protein glycation was assessed after 90 days by tryptophan fluorescence, AGE-induced cross-linking by SDS-PAGE and MALDI-TOF Mass Spectrometry. Fluorescence spectra (excitation at 360 nm and read at 460nm) of BSA solution with okra seed extracts showed significant inhibitory potential (45-50%) at 0.1mg/ml concentration in a dose dependent manner. Intensity of fluorescence spectra combined with densitometry measurements exhibited 50% inhibition of glycation of BSA with Okra seed extract. We observed the fluorescence emission spectra altered upon glycation when incubated with okra seed extracts in vitro and thus inhibited the

advanced glycation end products. Glycosylation of BSA in the presence of okra seed extracts leads to a change in the conformation of the protein probably due to an increased exposure of tryptophan residues. Thus the bioactive compounds present in Okra Seed Extracts may very well serve the same mechanisms of inhibition in vivo as well.

AGFD 57 Antioxidant polyphenolics in ready to drink tea: How are they really measured? Youngmok Kim, ymk@sensusflavors.com, Kevin L Goodner; Daniel J Wampler; Christian F Sweeney Dept. of Research and Development, Sensus, LLC, Hamilton OH Ready to drink (RTD) tea is a growing market segment due to its convenience, refreshing flavor and health benefits. Even though many RTD tea manufacturers claim their antioxidant level on the label, most consumers do not know how it is measured and what it really means. Currently, two different analytical testing methods are being used to determine polyphenol content in RTD teas. Folin-Ciocalteu method for tea polyphenol determination is standardized by the ISO and US tea association. HPLC analysis was also standardized by ISO but it is only limited to green tea polyphenol determination. According to polyphenolic analysis on 23 commercial RTD teas conducted in Sensus tea research and development center, all RTD teas contain significantly higher amount of polyphenolics when measured by Folin's method than by HPLC analysis. In the present study, which method delivers real polyphenolic value in RTD teas and what makes the difference will be discussed.

AGFD 58 Breaking up Biofilms with Moringa Oleifera: Insights into Mechanisms Bishambar Dayal, dayalbi@umdj.edu, Ritesh Amin; Vineela Reddy Yannamreddy; Michael A Lea. UMDNJ-NJMS, Newark NJ We carried out a systematic examination of the antimicrobial activities of different sections of the tropical fruit Moringa Oleifera and found that seed cover (seed coat) had the highest antimicrobial properties than the skin, the innerskin skeleton and the seeds. Although Moringa seeds have been reported to act directly upon microorganisms resulting in growth inhibition but to our surprise seed cover had a dramatic effect and thus prevented the formation of biofilm itself. These experiments were carried out using strain NJ 9709-Staphylococcus epidermidis, a resistant strain to almost all antibiotics. Since the parent glucosinolates do not possess much biological activity, hydrolysis with the myrosinase enzyme converts them into active products. We have studied the mass spectrometric studies of the Seed Cover section of the Moringa and found an intact glucosinolate, 4-(*a*-L-rhamnopyranosyloxy) benzyl glucosinolate) which on hydrolysis with myrosinase results a compound 4-(*a*-L-rhamnopyranosyloxy) benzyl isothiocyanate. We believe the antimicrobial effects of seed cover are attributed to this compound. Our results raise the possibility of new drugs that can dissolve biofilms across a variety of bacterial species. Mechanical implications of dismantling biofilm communities in infectious diseases in light of recent new studies (Science 2010 and Appl. Environ. Microbiol 2011 will be discussed.

AGFD 59 Synthesis of butanolide-containing alkenyl insect pheromones Richard J Petroski, Richard.Petroski@ars.usda.gov; Allard Cossé Dept. of Crop Bioprotection Research, USDA, Agricultural Research Service, Peoria Illinois A pheromone is a natural substance, produced by an insect to attract members of its own species. Pheromones can be used to manage beneficial insects, used for the biological control of insect pests or invasive weeds. Racemic alkene-4-olides were prepared by Grignard reaction of alkenyl bromides with 4-(tetrahydro-pyran-2-yloxy)-butryaldehyde, followed by cleavage of the THP protective group with pyridinium *p*-toluenesulfonate in ethanol, then oxidation of the resulting 1,4-diol with tetra-*n*-propylammonium perruthenate and 4-methylmorpholine *N*-oxide as co-oxidant. Chiral alken-4-olides were prepared using organocuprate chemistry to construct key intermediate chiral 1,2-epoxyalkenes from alkenyl bromides and chiral epichlorohydrins. Two-carbon homologation with 2,4,4-trimethyl-2-oxazoline afforded chiral 4-hydroxy carboxylic acids, protected as their oxazoline derivatives. Hydrolysis of the protective group, in a mixture of 3N HCl and THF, yielded the desired alkene-4-olides. The butanolide-containing compounds could be used in monitoring systems to evaluate the establishment and spread of newly released populations of Emerald Ash Borer (EAB) parasitoids

AGFD 60 Antitumor activity of garcinol from Garcinia indica in PC3 cells and dextran sulfate sodium treated mice Chi-Tang Ho, ho@aesop.rutgers.edu, Li-Yu Chiou; Min-Hsiung Pan Food Sci., Rutgers Univ., New Brunswick New Jersey Dept. of SeaFood Sci., National Kaohsiung Marine Univ., Kaohsiung, Taiwan Republic of China Garcinol, derived from Garcinia indica and other related species of tropical fruits. It has been found that garcinol has several health promoting effect including anticancer. In this study, we showed that garcinol could inhibit cell proliferative in PC3 prostate cancer cell by inducing apoptosis in a concentration and time-dependent manner. We further observed that garcinol induced apoptosis in PC3 cells through modulation of mitochondrial functions regulated by reactive oxygen species. Significant therapeutic effects were demonstrated in vivo by treating nude mice bearing PC3 tumor xenografts with garcinol. In addition, we further evaluated the anti-inflammatory effect of garcinol on dextran sulfate sodium (DSS) induced colitis. Garcinol was administrated daily per oral route for 7 days and significantly attenuated DSS induced aberrant crypt foci and dose-dependently prevented shortening of colon length. Furthermore, garcinol inhibited DSS-induced iNOS and COX-2 expression. These results show that garcinol may have significant applications for cancer chemotherapy.

AGFD 61 Issues surrounding the anti-inflammatory actions of the citrus polymethoxylated flavones John A. Manthey, John.Manthey@ars.usda.gov Thais B. Cesar Citrus and Subtropical Products Laboratory, U.S. Dept. of

Agriculture, Winter Haven FL Dept. of Food and Nutrition, Sao Paulo State Univ., Araraquara, Brazil The polymethoxylated flavones in citrus peels have been widely investigated for their in vitro and in vivo biological properties in mammalian cells. While the in vitro anti-inflammatory actions of the PMFs have been widely studied, there appears to be conflicting results about their in vivo actions. Animal dosing by direct injection typically results in potent inhibition of inflammation, while results obtained with oral dosing are mixed. In contrast, an early study of the immune-response driven inflammation in the Arthus Reaction exhibited excellent response to oral doses of PMFs. Evidence has also shown that the biological actions of the metabolites of the PMFs in animals may also be important to the overall effects of these compounds. Factors influencing the efficacies of oral doses of PMFs in different inflammation models need to be explored further.

AGFD 62 L-cysteine supplementation can increase insulin sensitivity by boosting blood levels of hydrogen sulfide and nitrite in type 2 diabetes. Sushil K. Jain, sjain@lsuhsc.edu, LSU Health Sciences Center, Shreveport LA Garlic is a rich source of sulfides. Recent studies reveal several physiological roles of H₂S, including vasodilator, antioxidant, anti-inflammatory and anti-atherosclerotic effects in in vitro and animal studies. Diabetic patients have lower blood concentration of H₂S. This study examined the hypothesis that supplementation with L-cysteine, an endogenous precursor of H₂S, replenishes blood levels of H₂S and lowers insulin resistance and vascular inflammation markers in type 2 diabetes using Zucker diabetic rats (ZDF) rats as a model. Starting at age of 6 wks, ZDF rats were supplemented orally (daily gavages, 8 wks) with saline-placebo (D, n=8) or L-cysteine (LC, n=12, 1 mg/KgBW) and fed a high calorie diet. 6 weeks age rats without any supplementation were considered baseline (BL) rats. Fasting blood levels of D rats showed lower H₂S, and elevated GHb, MCP-1 and insulin resistance when compared with BL in which there was no onset of diabetes. LC supplementation significantly (p<0.05) increased blood levels of H₂S (37%) and NO₂ (30%) and lowered levels of GHb (9%), MCP-1 (31%), TNF- α (31%) and HOMA insulin resistance (25%) compared with levels seen in saline-supplemented D. The blood levels of GHb and IR showed a significant negative correlation (p<0.05) with concentrations of H₂S and nitrite in LC supplemented ZDF rats. This is the first report showing L-cysteine supplementation can increase circulating levels of H₂S and NO₂ in a diabetic animal model, and needs to be explored as an adjuvant therapy for the reduction of vascular inflammation in the diabetic patient population

AGFD 63 Development of flavor and anti-oxidant activity during the ripening of the date palm fruit (Phoenix dactylifera L.) Jane K. Parker, j.k.parker@reading.ac.uk, Whiteknights, Reading Berkshire, United Kingdom ; Cui Wentao; Maria-Jose Oruna Concha; Noura Eid; Jeremy P.E. Spencer Dept. of Food and Nutritional Sciences, Univ. of Reading, Reading, United Kingdom The fruits of the date palm (Phoenix dactylifera L.) are highly nutritious. They contain high levels of carbohydrate and dietary fiber and are rich in vitamins, salts and minerals. They have a delicate flavor which is not well characterized. In this study, the flavor of different varieties of date palm fruit at different stages of ripening, including kimri, khalal, rutab and tamr were analysed. Volatile flavor compounds were extracted by dynamic headspace extraction and the more polar flavor compounds including phenols, furanones and pyranones were obtained by solid phase extraction prior to analysis by GC-MS. GC-Olfactometry was used to confirm the more odor-active components of each extract. Some of the important volatile compounds are derived from the polyphenol content of the dates. The polyphenols present in the dates at the four ripening stages were also characterized, as well as the total antioxidant activity.

AGFD 64 Bioactive Compounds present in Moringa Oleifera: Isolation and characterization by Thin Layer Chromatography and Electro-Spray Ionization Mass Spectrometry Bishambar Dayal, dayalbi@umdnj.edu, Vineela Reddy Yannamreddy; Ritesh Amin; Michael A Lea; Athula B Attygale. UMDNJ-New Nersey Medical School, Newark Dept. of Chemistry, Chemical Biology and Biomedical Engineering, Stevens Inst. of Technology, Hoboken NJ Recently, we initiated a systematic study to examine the antimicrobial and anticarcinogenic activities of different sections of the tropical fruit Moringa Oleifera. We found strong polyphenolic and antioxidant activity in the skin, the inner skin skeleton, seed coat and the seeds of the Moringa Oleifera. Isolation and structure elucidation via thin-layer chromatography (TLC) /electro spray ionization-mass spectrometry (ESI-MS) of microwaved methanolic extract of inner skin skeleton provided 4-(a-L-rhamnopyranosyloxy) benzyl glucosinolate, an intact glucosinolate in addition to allyl isothiocyanates, and thiocyanates presumably by the hydrolysis of the enzyme myrosinase. Collision-induced dissociation mass spectra of anions present in Moringa Oleifera exhibited product ion at m/z 97, characteristic of sulfate moiety (HSO₄⁻) in their molecular structure. The other characteristic fragment ion, m/z 195 was assigned to 1-thiohexose anion. Two minor peaks at m/z 259, 275 represented glucose 1-sulfate anion formed by the loss of phenyl isothiocyanates and glucose 1- thiosulfate anion respectively. The ion at m/z 570 (100% intensity) corresponds to 4-(a-L-rhamnopyranosyloxy) benzyl glucosinolate. The acetyl derivative of intact glucosinolate provided m/z 612. To our knowledge, the intact acetyl derivative of 4-(a-L-rhamnopyranosyloxy) benzyl glucosinolate has not been reported in the literature. We believe that the isolation and structure elucidation of this intact glucosinolate and its acetyl derivative having antimicrobial and anticarcinogenic activity will be useful in the prevention and treatment of cancer and neurodegenerative diseases.

AGFD 65 Phe nolic profile and antimicrobial activity of select exotic fruits Christina Engels, engels@ualberta.ca, Daise Lopes-Lutz; Chamila Nimalaratne; Judith Dettmann; Patricia Esquivel; Víctor M. Jiménez; Michael G. Gänzle; Andreas

Schieber Agricultural, Food and Nutritional Science, Univ. of Alberta, Edmonton Canada Escuela de Tecnología de Alimentos, Univ. of Costa Rica, San Pedro, Costa Rica CIGRAS, Univ. of Costa Rica, San Pedro Costa Rica Exotic fruits are an abundant source of secondary plant metabolites, especially phenolic compounds. Despite a larger number of studies, our knowledge about their chemical structures and biological activities is still very limited. This is, among other factors, a result of the lack of analytical methods and reference compounds. Using liquid chromatography-mass spectrometry, we determined the profile of phenolic compounds extracted from two members of the Anacardiaceae family, mango (*Mangifera indica* L.) and jocote (*Spondias purpurea* L.), as well as from Amazon grape (*Pourouma cecropiifolia* Martius), which belongs to the Moraceae family. Phenolic acids, flavonoids including anthocyanins, and hydrolyzable tannins were characterized on the basis of their UV-Vis and mass spectra. Gallotannins isolated from mango kernel extracts using high-speed counter-current chromatography displayed strong antibacterial activity against several food-borne pathogens such as *Listeria monocytogenes*, whereas the growth of beneficial lactobacilli was not affected.

AGFD 66 Passion fruit seed containing high amounts of piceatannol could be a new anti-skin-aging

material Yuko Matsui, y-matsui-jd@morinaga.co.jp, 2-1-1 Shimosueyoshi, Tsurumi-ku, Yokohama Kanagawa, Japan ; Kenkichi Sugiyama; Masanori Kamei; Toshio Takahashi; Tamio Suzuki; Yohtaro Katagata; Tatsuhiko Ito Research Inst., MORINAGA & CO., Ltd., Japan Dept. of Dermatology, Yamagata Univ. School of Medicine, Yamagata Univ., Japan Faculty of Agriculture and Life Science, Hirosaki Univ., Japan Health Care Division, MORINAGA & CO., Ltd., Japan Passion fruit, the fruit of *Passiflora edulis*, is grown in the tropical region and there are studies on the effect of polyphenols from the fruit. Here, we focused on the effect of passion fruit in cultured human melanoma and fibroblast cells to investigate the inhibition of melanogenesis and promotion of collagen synthesis. Passion fruit was divided into rind, pulp and seed to compare each activity in the cells. Treatment of melanoma cells with the seed extracts inhibited melanogenesis, and the production of total soluble collagen was also elevated in dermal fibroblast cells. The removal of polyphenols from the seed extracts led to the abolishment of these effects. We found out that piceatannol (3,4,3',5'-tetrahydroxy -trans-stilbene), is the major polyphenol in passion fruit seed, and that piceatannol and its related compounds are responsible for the seed extract's effects observed.

AGFD 67 From detrimental to beneficial constituents in foods: Tracking the publication trends in JAFC

James N. Seiber, jnseiber@ucdavis.edu; Loreen A. Kleinschmidt Dept. of Food Sci. & Tech., Univ. of California, Davis Dept. of Environmental Toxicology, Univ. of California, Davis A large part of the research focus on food constituents in the 20th century was toward health detrimental contaminants—pathogens, toxins, chemical residues, and food additives. This is reflected in the publications in the *Journal of Agricultural and Food Chemistry* and other journals. This era witnessed the formation of FDA and EPA, the rise and fall of DDT and other synthetic chemicals, as well as artificial sweeteners, preservatives and coloring/flavoring agents that attracted consumer and regulatory attention. During the last 25 years or so, the emphasis in food chemistry and biochemistry has trended more toward health beneficial chemicals in foods, as examination of phytonutrients, nutraceuticals and functional foods yielded information on naturally occurring constituents—polyphenolic antioxidants, unsaturated fatty acids, soluble fibers and many other classes of constituents that ward off chronic diseases and promise a healthier life and lifestyle. This presentation will address the changes in emphases in published research to the present, and follow trends that indicate the directions that food chemistry/biochemistry and related sciences might follow in the future.

AGFD 68 Health benefits of almonds beyond improvements in atherogenic lipoprotein profile

Oliver Chen, oliver.chen@tufts.edu, Jean Mayer USDA Human Nutrition Research Center on Aging, Tufts Univ., Boston MA Almonds are a rich source of unsaturated fatty acids. Such a lipid composition profile contributes importantly to their beneficial impact on atherogenic lipoprotein profiles. In addition, phytochemical constituents in almonds including fiber, phytosterols, tocopherols, and polyphenols may also benefit CVD risk via mechanisms other than improvements in lipoprotein profiles, such as antioxidation, anti-inflammation, and glucoregulation. Such benefits have been demonstrated in a number of clinical studies. Almond consumption augmented plasma alpha-tocopherol in healthy adults in a dose-dependent manner. Antioxidant actions of almond constituents were demonstrated in young male Chinese smokers with enhanced antioxidant enzyme activities and decreased DNA damage products. Given that almonds are a low glycemic index food, they decreased glycemic excursion of co-consumed carbohydrate foods in healthy individuals. Inclusion of almonds in a breakfast meal increased satiety both acutely and after a second-meal in adults with impaired glucose tolerance. We also found that almonds replacing 20% calorie intake in patients with type 2 diabetes improved glycemic control and attenuated oxidative stress and inflammation. Patients with polycystic ovary syndrome had a reduced free androgen index after almond consumption. The increased growth of bifidobacteria by almond constituents demonstrated in invitro studies implicates their potential prebiotic effect. Thus, constituents in almonds could decrease risk of cardiovascular disease beyond cholesterol reduction.

AGFD 69 Processing and storage effects on berry polyphenols: Challenges and implications on bioactive

properties Luke R. Howard, lukeh@uark.edu; Ronald L. Prior Dept. of Food Sci., Univ. of Arkansas, Fayetteville AR Berry fruit are rich in polyphenols, namely anthocyanins and tannins, compounds that possess numerous health-promoting properties.

Berries are commonly consumed as canned, pureed, juiced and jellied products due to limited seasonal availability and shelf-life of fresh berries. Berry polyphenols are susceptible to losses during processing and storage due to various physical and biochemical changes. Juicing results in the most marked losses of anthocyanins and tannins due to exclusion of seeds and skins in the pomace, but flavonols are well retained. With the exception of juices, losses in anthocyanins and tannins during ambient temperature storage of processed products exceed those that occur during processing. Increase in polymeric color indicative of the formation of anthocyanin-tannin complexes is a common phenomenon in all stored berry products. Challenges associated with preventing berry polyphenol losses during processing and storage will be discussed as well as potential implications of processing and storage-induced changes on bioactive properties.

AGFD 70 Mitigating Inflammation with Foods Alexander G. Schauss, alex@aibmr.com, Xianli Wu. Natural and Medicinal Products Research, AIBMR Life Sciences, Puyallup Washington Dept. of Physiology and Biophysics, Univ. of Arkansas, Little Rock Constant overproduction of pro-inflammatory cytokines leads to chronic inflammation. Unlike acute inflammation, which is essential for healing, chronic inflammation can delay healing and if left unchecked lead to a host of diseases, such as atherosclerosis. There is growing evidence that some dietary polyphenols can play an important role in maintaining health and even reversing the progression of chronic diseases. Recent studies have shown that the pulp of a tropical palm fruit, acai (*Euterpe oleracea* Mart.), exhibits extraordinary antioxidant and anti-inflammatory properties. When added to the diet compounds in the pulp have been shown to significantly inhibit the development of atherosclerotic lesions. Such findings add to the body of evidence that dietary polyphenols and other classes of compounds found in fruits, berries, vegetables, nuts, and foods of marine origin, can play an important role in attenuating and mitigating chronic pro-inflammatory processes associated with chronic diseases.

AGFD 71 Putting health risks into perspective Bruce N Ames, bames@chori.org, Nutrition and Metabolism Center, Childrens Hospital Oakland Research Inst., Oakland CA Most of the world's population, even in developed countries, has inadequate intake of one or more of the ~30 essential vitamins and minerals (V/M) that a varied and balanced diet should provide. Triage theory (PNAS 2006 103;17589) posits that, as a result of recurrent shortages of V/M during evolution, natural selection developed a metabolic rebalancing response to shortage. The rebalancing favors V/M-dependent proteins needed for short-term survival and reproduction while starving those proteins only required for long-term health. Triage theory predicts that the consequence of moderate shortages of even a single V/M, though insufficient to cause overt clinical symptoms, will impair functions essential for long-term health. This impairment will result in insidious damage (e.g. increased DNA damage) that, over time, leads to the acceleration of age-associated diseases (e.g. increased cancer). Analyses (AJCN 2009 90;889, J Nucleic Acid 2010 doi:10.4061/2010/ 725071, FASEB J 2011 doi:10.1096/fj.11-180885) show that a triage perspective is both correct and useful. Animal cancer tests, which are done at the maximum tolerated dose (MTD), are being misinterpreted to mean that minuscule doses of synthetic chemicals such as pesticides are relevant to human cancer. 99.99% of the pesticides we eat are naturally present in plants to ward off insects and other predators. Over half of all chemicals tested, whether natural or synthetic, are carcinogenic in rodent tests. A plausible explanation is that the MTD causes chronic cell killing and consequent cell replacement, a risk factor for cancer that can be limited to high doses. Reducing our exposure to traces of dietary synthetic pesticides is expensive and will not plausibly reduce cancer rates. Fruits and vegetables are effective dietary sources of V/M, and making them more expensive, e.g. organic food, could increase cancer in the poor.

AGFD 72 Determination of synthetic by-products in the color additive D&C Yellow No. 10 (Quinoline Yellow) using high-performance liquid chromatography Adrian Weisz, Adrian.Weisz@fda.hhs.gov, College Park MD; Hao T. Mai; Alan Scher U.S. FDA/Center for Food Safety and Applied Nutrition, College Park MD D&C Yellow No. 10 (Y10, Colour Index No. 47005) as well as its lakes (Y10 precipitated onto an insoluble substratum) are U.S.-certified color additives used in drugs and cosmetics. Y10 consists primarily of a mixture of the sodium salts of the monosulfonic acid isomers of 2-(2-quinolinyl)-1H-indene-1,3(2H)-dione with up to 15% of the disodium salts of the disulfonated positional isomers. A variant form of this dye, used for coloring foods in Europe (identified as E 104), contains mostly a mixture of the di- and trisulfonated isomers. During manufacture, sulfonated by-products may be produced and carried into the final material. Y10 and its lakes are subject to batch certification by the U.S. FDA to ensure compliance with certain chemical specifications including those for sulfonated quinaldines and sulfonated phthalic acids. Currently, those by-products are determined by a labor-intensive procedure that includes gravity-elution column chromatography followed by spectrophotometric quantification. The present work reports the development of a simpler-to-implement HPLC method for determining the specified by-products.

AGFD 73 Preparative separation of 1,3,6-pyrenetrisulfonic acid from the color additive D&C Green No. 8 using pH-zone-refining counter-current chromatography Adrian Weisz, adrian.weisz@fda.hhs.gov, College Park MD; Eugene P. Mazzola; Yoichiro Ito. FDA/Center for Food Safety and Applied Nutrition, College Park MD Biochemistry and Biophysics Center/NHLBI/National Inst.s of Health, Bethesda MD D&C Green No. 8 (G8, Colour Index No. 59040, mainly the trisodium salt of 8-hydroxy-1,3,6-pyrenetrisulfonic acid) is a color additive used in drugs and cosmetics in the U.S. It is manufactured by sulfonating pyrene to form the tetrasulfonic acid compound, followed by hydrolyzing one of the sulfonic acids to yield the monohydroxytrisulfonate, which is isolated as the trisodium salt. During manufacture, various contaminants

may be produced, including 1,3,6-pyrenetrisulfonate (PTS). G8 is subject to batch certification by the U.S. FDA (FDA) to ensure compliance with certain chemical specifications including “not more than 6 percent” of PTS. To develop analytical methods for batch certification of G8, purified PTS is required as reference material but is not commercially available. The present study describes the separation of preparative quantities of PTS from a sample of G8, using pH-zone-refining counter-current chromatography, and its identification and characterization by NMR, LCMS, and HPLC.

AGFD 74 Evaluation of a liquid chromatography method for the detection and quantification of aflatoxins

in milk thistle supplements Valerie Tournas, valerie.tournas@fda.hhs.gov, College Park MD, Chelsea Sapp; Mary W. Trucksess Center for Food Safety and Applied Nutrition, FDA, College Park MD JIFSAN/Univ. of Maryland, College Park MD Milk thistle (MT) botanical supplements are widely consumed because of their possible liver-health-promoting properties. The presence of moulds and mould toxins (mycotoxins) such as the aflatoxins (AF) in botanicals has been reported in many studies. Currently, there is no published method for determining AF in milk thistle. A method validated for mycotoxins in botanicals was investigated and applied to milk thistle. The method consisted of acetonitrile/water extraction, immunoaffinity column cleanup, liquid chromatography separation, and photochemical reaction post column derivatization and fluorescence detection. The average recoveries for AF added to milk thistle seeds, herb, oil-based liquid extract, and alcohol-based liquid extract were >76%. The mean relative standard deviation was <10%. The limit of detection (LOD) was 0.03 ng/g and the limit of quantification was 0.15 ng/g. The method exhibited good accuracy, precision and reproducibility for the determination of AF in milk thistle products. A total of 83 MT samples from the U.S. market were analyzed. AF was detected in 18% of the samples with levels ranging from 0.04 – 2.0 ng/g. This is the first study reporting on AF contamination of milk thistle botanical supplements.

AGFD 75 Investigation of alkylbenzenes as VOCs in sun-dried salts and its risk assessment

Jin Hyo Kim, setup75@korea.kr, 150 Suin-ro, Gweonseon-gu, Suwon Gyeong-gi, Republic of Korea ; Su-Myeong Hong; Geun-Hyoung Choi; Oh-Kyung Kwon; Geon-Jae Im. Chemical Safety Division, National Academy of Agricultural Sciences, Suwon Gyeong-gi, Republic of Korea Toluene, ethylbenzene and three xylenes are known as toxic alkylbenzenes in crude oils. The alkylbenzenes were investigated in sun-dried salts retailed in Korea. The total contents of toluene, ethylbenzene, o-xylene, m-xylene, and p-xylene were analyzed with GC-MS through the extraction with hexane. The domestically produced sun-dried salts were monitored up to 1.11 mg/kg (toluene), 3.11 mg/kg (ethylbenzene), 0.59 mg/kg (o- and m-xylenes), and no detected as p-xylene. On the other hand, the imported sun-dried salts were showed up to 0.89 mg/kg (toluene), 1.32 mg/kg (ethylbenzene), 0.50 mg/kg (o- and m-xylenes) and 0.46 (p-xylene). Furthermore, hazard quotient of targeted contaminants and hazard index were estimated to be much lower than 1.0 in risk assessment. These results suggested that the associated health risks of alkylbenzenes in sundried salts might be negligible.

AGFD 76 Quantitative analysis of residual pesticide of retailed sundried salts in Korea

Jin Hyo Kim, setup75@korea.kr, Gweonseon-gu, Suwon Gyeong-gi, Republic of Korea; Su-Myeong Hong; Geun-Hyoung Choi; Jong-Min Park; Geon-Jae Im; Oh-Kyung Kwon Chemical Safety Division, National Academy of Agricultural Sciences, Suwon Gyeong-gi, Republic of Korea Coastal waters might be contaminated with pesticides that originally came from agricultural fields. Thus, we screened pesticides residues through the qualitative analysis of 160 pesticides with LC-MS/MS in sundried salts, and only one pesticide, tricyclazole, was ultimately confirmed on the chromatogram. The confirmed pesticide was analyzed quantitatively with GC-NPD, and only three out of 20 samples contained the pesticide, with maximum concentrations of 1.7 µg/kg. The amount was not considered to pose a health risk. However, sundried salts may possibly be contaminated with agricultural pesticides due to the manufacturing process. The results presented here suggest that dried salts should be continuously monitored for pesticide residues.

AGFD 77 A simple quantitative analysis of ethylcarbamate in various fermented food

Jin Hyo Kim, setup75@korea.kr, Gweonseon-gu, Suwon Gyeong-gi, Republic of Korea ; Su-Myeong Hong; Oh-Kyung Kwon; Geon-Jae Im Chemical Safety Division, National Academy of Agricultural Sciences, Suwon Gyeong-gi, Republic of Korea Ethylcarbamate is known as a toxic chemical in fermented food, and we try to study the best procedures for accurate quantization of this in various fermented food. Thus, we investigated the major disturbance and revised the clean-up procedure for quantification with GC-ToFMS in a few fermented types (alcohol, acetic acid and so on). When we followed referenced method, we identified a major disturbance, diethyl succinate, in alcohols, and it was easily removed with 1 % Et₂O in hexane. And we successfully got over low recovery with simple pH adjustment (around 10) in acetic acids. Finally, we optimized a clean-up procedure and GC-ToFMS condition for ethylcarbamate quantification in various fermented foods. (LOD = 0.8 ~ 1.2 mg/kg)

AGFD 78 Development of analytical method for lead, cadmium, and methylmercury in Korean functional

foods using standard addition method Wooseok Kim , woodol2@hanmail.net, Seoul Junggu Pildong 3-ga, Republic of Korea ; Donghun Lee, y4109101@hanmail.net, Seoul Junggu Pildong 3-Ga, Republic of Korea ; Heeun Jin, cindy8190@hanmail.net, Seoul Junggu Pildong 3-Ga, Republic of Korea ; Kyung Su Park; Hee Soo Pyo; Kwang-Guen Lee Dept. of Food Sci. and Biotechnology, Dongguk Univ., Seoul Junggu Pildong Republic of Korea Adavanced Analysis Center, Korea Inst. Science

and Technology, Seoul Sungbuk-Gu Hwarangro, Republic of Korea Intergrated Omics Center, Korea Inst. Science and Technology, Seoul Sungbukgu Hwarangro, Republic of Korea Currently, many people are consuming functional foods for their health. However, functional foods may contain various trace elements such as heavy metals. In particular, Pb, Cd and MeHg have harmful effects to humans and longer half-lives than other organic hazardous materials. So far, few analytical methods for these three trace elements in functional foods have been investigated. For integrated exposure assessment of trace elements in Korean functional foods, the development of robust analytical method is required. This study evaluated the accurate analytical method for Pb and Cd in functional foods using ICP-MS and standard addition. The method for analyzing MeHg by SPME-GC-MS and standard addition method was also evaluated. Functional food samples were categorized by their matrix (solid, semi-solid, liquid). The levels of Pb and Cd were analyzed with wet-digestion method using microwave. Samples were scanned before analyzing Pb and Cd by ICP-MS. Calibration of the standard addition method was done using a three-point calibration curve. Analysis of the methylmercury method was established with a response surface method in an effort to optimize extraction condition of MeHgEt as a function of sample matrix. Methylmercury was analyzed with SPME-GC-MS using a derivatization reagent (NaBEt₄). LOD of Pb and Cd were 0.09 ng/ml and 0.1 ng/ml, respectively. LOQ of Pb and Cd were 0.27 ng/ml and 0.3 ng/ml, respectively. Z-score and recovery rate using CRM were less than 1.0 and 98%, respectively. In the methylmercury analysis, optimized conditions for a solid matrix were as follows: extraction time (30 min), temperature (100°C) and volume of NaBEt₄ (500 mL). With a semi-solid matrix, the optimized extraction time, temperature and volume of NaBEt₄ were 5 min, 100°C and 500 mL, respectively. In a liquid matrix, the optimized extraction time, temperature and volume of NaBEt₄ were 30 min, 25°C and 100 mL, respectively.

AGFD 79 Volatile organic compound migration parameters in nylon MXD6 by the dynamic permeation

cell method John Koontz, John.Koontz@fda.hhs.gov, Yang Wang; Chen Wang; Rima Juskelis; Yoonseok Song. National Center for Food Safety and Technology, U.S. FDA, Bedford Park IL National Center for Food Safety and Technology, Illinois Inst. of Technology, Bedford Park Diffusion coefficient data for organic compounds in high-barrier polymer food packaging is lacking. Nylon MXD6 is a specific grade of nylon 6 used in multilayer packaging due to its high oxygen-barrier properties, unique rheological properties, and processing conditions. The migration parameters of low molecular weight volatile organic compounds, including methanol, acetaldehyde, methylene chloride, diacetyl, chloroform, toluene and ethyl butyrate, were determined using the dynamic permeation cell method. Nylon MXD6 films (20 µm) were placed between two temperature-controlled test cell blocks inside an organic vapor permeability analyzer, and allowed to equilibrate at 40, 66, 100 or 121 °C. The permeation of organic vapor through nylon MXD6 film was monitored at each temperature in real time by a flame ionization detector. Diffusion coefficients were evaluated to determine whether the Piringer and Limm diffusion models were conservative predictors of chemical migration from the polymer in contact with foods to validate their use in the regulatory review process.

AGFD 80 Flavor, solvent, and photoinitiator migration parameters in polyethylene terephthalate and nylon

6 by the static permeation cell method John Koontz, John.Koontz@fda.hhs.gov; Chen Wang; Yang Wang; Rima Juskelis; Yoonseok Song. National Center for Food Safety and Technology, U.S. FDA, Bedford Park IL National Center for Food Safety and Technology, Illinois Inst. of Technology, Bedford Park IL The migration properties of a flavor compound (d-limonene), an organic solvent (dichloromethane), and a photoinitiator for printing inks (benzophenone) through food packaging polymers, polyethylene terephthalate (PET) and nylon 6, were studied. Glass permeation cell systems were used to determine the migration rates of the non-volatile surrogate compounds through films of PET (13 µm) and nylon 6 (15 µm). Miglyol 812 was used as a fatty food simulant added to the receptor chamber, while the donor chamber was filled with 1-10% surrogate compounds spiked in Miglyol 812. The permeation cell was maintained at 40, 66, 100 or 121 °C for up to 30 days of polymer film exposure time. Non-volatile surrogates migrating into the receptor chamber through the polymer were quantified by headspace GC/MS. Diffusion coefficients were obtained and evaluated to determine whether the Piringer and Limm diffusion models were conservative predictors of chemical migration from the polymers into foods to validate their use in the FDA's food contact notification program.

AGFD 81 Development of an LC-MS/MS method for quantitation and confirmation of ceftiofur metabolite

desfuroylceftiofur cystine disulfide in bovine kidney Shixia Feng, shixia.feng@fda.hhs.gov; Chaitali Chattopadhyaya; Phil Kijak Center for Veterinary Medicine, U.S. FDA, Laurel MD Ceftiofur is a cephalosporin β-lactam antibiotic that is widely used for treating certain respiratory diseases in cattle. The regulatory method is an HPLC-UV method which is very laborious, non-specific and is becoming obsolete. Ceftiofur residue violations have been frequently reported and therefore an improved method is needed. Our goal is to develop a rapid and sensitive LC-MS/MS method for the determination and confirmation of ceftiofur metabolite desfuroylceftiofur cystine disulfide (DCCD) in bovine kidney tissue, the target tissue. The new method utilizes a simple extraction by phosphate buffer, SPE cleanup, a deuterated internal standard, and LC-MS/MS in positive ESI mode for detection and quantitation. The average accuracy for control kidney samples (from six different sources) fortified at 50 – 1000 ng/g was 98 – 100% with CV < 10%. The lower limit of confirmation was 50 ng/g. The validation of the method in other tissue matrices such as muscle is underway.

AGFD 82 Improvement in the analysis of pesticide residues in herbal medicines with different lipid contents

Jeong-In Hawng, jekim@knu.ac.kr, Sangyuk-dong, Buk-gu, Daegu Daegu Metropolitan city, Republic of Korea ; Young-Hwan Jeon; Hyo-Young Kim; Ji-Hwan Kim; Yoon-Jeong Lee; Ju-Young Park; Do-Hoon Kim; Jang-Eok Kim Dept. of Applied Biosciences, College of Agriculture & Life Science, Kyungpook National Univ., Daegu Daegu Metropolitan city, Republic of Korea Division of Herbal Medicine Research, Korea FDA, Osong Chungchengpook-do, Republic of Korea Because lipids in herbal medicines have similar chemical characteristics to pesticides, they can be interfering substances for pesticide residue analysis. The residue analysis of pesticides with different polarities has been studied from herbal medicines with different lipid contents using official analysis methods by the Korea FDA. Using these methods, it was discovered that lower recoveries of pesticides with lower polarities were obtained in herbal medicines with higher lipid contents, and that emulsions formed during liquid-liquid extraction. In order to improve the problems, we used acetonitrile as a extraction solvent for eliminating lipids, and a macroporous diatomaceous earth (MDE) column rather than a liquid-liquid partitioning step. The applicability of the method was evaluated on recoveries of bifenthrin, chlorpyrifos and acetamiprid from Platycodon root, Safflower and Persicae semen. The recoveries ranged from 80 to 100% for whole samples, indicating that it is possible to analyze for pesticide residues in herbal medicines without the effects of lipid and emulsion.

AGFD 83 Optimization of mycotoxin binding in grains

Christopher I Johnston, cij4@msstate.edu, Starkville MS; Rebecca Singleterry; Ashli Brown; Kevin Armbrust; Darrell Sparks Dept. of Biochemistry, Molecular Biology, Entomology, and Plant Pathology, Mississippi State Univ., Mississippi State MS Office of the State Chemist, Mississippi State Univ., MS Aflatoxins are toxic metabolites produced by the fungus species *Aspergilli*. Crops contaminated with these mycotoxins pose a carcinogenic threat to livestock and humans when consumed. The presence of aflatoxins in grains has been shown to decrease by using silicates as binding agents. The US FDA (FDA) limits the percentage of binding agent that can be used in foodstuff and feed thus necessitating the discovery of optimal percentages of grain versus binder. Once the grain/binder mixture has been digested, the pH environment of the gut can alter the silicate's binding activity and, in many instances, neutralize its binding ability and releases aflatoxins from the silicates entering the blood stream. A binding study of Alltech® binder 290293 and Sigma® Distillers Grain and Solubles was performed which found an optimal Aflatoxin binding percentage of 72.51 % utilizing a 2 % binder versus grain mixture that is permissible in feed by the FDA. Furthermore, a pH study was conducted and determined that at lower pH, the silicate binder investigated loses some of its ability to bind aflatoxin.

AGFD 84 Determination of components of the color additive FD&C Green No. 3 (Food Green 3) using high

performance liquid chromatography Huei Hsuan Wendy Yang, hueihsuan.yang@fda.hhs.gov, College Park MD; Alan Scher Center for Food Safety and Applied Nutrition, U.S. FDA, College Park MD FD&C Green No. 3 (G3, Food Green 3, Colour Index No. 42053) is a triphenylmethane dye used for coloring food, drugs, and cosmetics in the U.S. During its manufacture, various positional isomers, intermediates, subsidiary colors, and residual leuco base may be produced or carried over into the final product. G3 is batch-certified by the U.S. FDA to ensure compliance with limiting specifications set forth in the U.S. Code of Federal Regulations (CFR). Formerly, the intermediates were determined by a labor-intensive procedure that included separation by gravity-elution column chromatography and quantification by UV spectrophotometry. Similarly, the subsidiary colors were determined by a multi-step procedure that involved separation by thin-layer chromatography and quantification by visible spectrophotometry. The leuco base was determined by a liquid chromatographic method developed for its determination in a related color additive. The present study reports the development of a rapid high-performance liquid chromatography (HPLC) method for determining in one analysis the CFR-specified leuco base, intermediates, and subsidiary colors found in G3.

AGFD 85 Glycyrrhizic acid and 18β-glycyrrhetic acid modulate the lipopolysaccharide-induced

inflammatory response by the suppression of NF- κ B through phosphatidylinositol 3-kinase Gow-Chin Yen, gcyen@nchu.edu.tw, , Taichung Taiwan, Taiwan Republic of China ; Chung-Yi Wang; Tzu-Chien Kao Dept. of Food Sci. and Biotechnology, National Chung Hsing Univ., Taichung, Taiwan Republic of China The roots and rhizomes of licorice (*Glycyrrhiza*) species have been used extensively as a natural sweetener and an herbal medicine. The aim of this work was to study the anti-inflammatory effects of glycyrrhizic acid (GA) and 18 β -glycyrrhetic acid (18 β GA) from licorice in a LPS-stimulated macrophage model. The results showed that GA and 18 β GA significantly inhibited the production of LPS-induced NO, prostaglandin E2 (PGE2) and intracellular ROS without cytotoxic effects in cells. Western blotting and RT-PCR analyses revealed that GA and 18 β GA significantly blocked protein and mRNA expression of iNOS and COX-2 in LPS-induced macrophages. Both GA and 18 β GA inhibited the activation of NF- κ B, PI3K p110 α and p110 β and the production of LPS-induced TNF- α , IL-6, and IL-1 β , in a concentration-dependent manner. These results indicate that GA and 18 β GA may contribute anti-inflammatory effects by attenuating the generation of excessive NO, PGE2, and ROS and suppressing the expression of pro-inflammatory genes by inhibiting NF- κ B and PI3K activation.

AGFD 86 Screening of anthocyanins in red and white cranberry extracts and juice concentrates by HR-MS

(Exactive Orbitrap) and LC-MS Artemio Z. Tulio, Jr., artemio.tulio@fda.hhs.gov, Kevin D. White; Lauren S. Jackson Center for Food Safety and Applied Nutrition, U.S. FDA, Bedford Park IL Center for Food Safety and Applied Nutrition, Office of

Regulatory Science, Division of Analytical Chemistry, Spectroscopy and Mass Spectroscopy Branch, U.S. FDA, College Park MD A high-resolution Exactive Orbitrap mass spectrometer (HR-MS) was employed for the screening of anthocyanins in red (RCE) and white cranberry extracts (WCE), and red (RCC) and white cranberry concentrates (WCC). Results of Orbitrap screening were compared to LC-MS analysis. Exact mass measurements revealed the presence of eight and six anthocyanin glycosides in RCE and WCE, respectively, whereas, six and five anthocyanins were detected in RCC and WCC, respectively. In contrast, only five anthocyanins each were detected in RCE and RCC by LC-MS. However, no anthocyanin compounds were found in both WCE and WCC due to lower level of LC-MS sensitivity and also due to less inherent anthocyanins in white cranberry. In this study, Exactive orbitrap provided a rapid method for qualitative screening of anthocyanin compounds in cranberries using accurate mass measurements. In addition, HR-MS is ideally suited for general screening of unknown compounds and in the absence of reference standards for berry juice and concentrate products.

AGFD 87 UPLC-UV determination of isoflavones in soy seed Li Sheng, lsheng@epibas.com, Henry D Scobell; Keith J. Duff Dept. of R&D, EPL Bio Analytical Services, Niantic IL Isoflavones are extracted from ground soybean seed with a mixture of methanol and water. After being hydrolyzed with NaOH and neutralized with acetic acid, the acetyl and malonyl isoflavones are transformed to glycosides. A UPLC/UV assay was developed to quantify the glycoside and aglycone forms including daizin, daidzein, glycitein, genistin and genistein using calibration curves of the six external standards. The linearity of this method is 0.1 µg/mL – 100 µg/mL, or 4.8 mg/Kg Dry Basis (DB) – 480 mg/Kg DB. Excellent accuracy and precision were obtained during method validation. At least forty samples can be analyzed per day using this method. The UPLC run in this method takes 12.5 minutes which is much shorter than the HPLC test (44.5 min) of the AOAC method.

AGFD 88 Metabolic health benefits of dietary fiber: Comparison of hydroxypropyl methylcellulose and natural dietary fibers in a hamster model Shao-Ching Hung, schung2@dow.com, Midland Michigan; Scott A Young; William HK Anderson; Wallace Yokoyama; Glenn Bartley; Yun-Jeong Hong; Hyunsook Kim; David R Albers; Marsha L Langhorst; David M Williams; Demetrius Dielman; Margaret Covington The Dow Chemical Company, Midland Michigan Western Regional Research Center USDA, Albany California The hypolipidemic and hypoglycemic effects of dietary fibers have attracted significant attention for the prevention and treatment of metabolic syndrome. Previously we have shown that hydroxypropyl methylcellulose (HPMC) supplementation resulted in reductions in plasma cholesterol and postprandial glucose levels. The present study was designed to compare the metabolic effects of 8% HPMC and natural dietary fibers, pectin, psyllium, and xylan, consumption in golden Syrian hamsters fed high-fat diets. After eight weeks of feeding, 8% HPMC supplementation showed better efficacy in both LDL-cholesterol and glucose reductions compared to the natural fibers, while decreases in plasma total cholesterol levels were observed for all dietary fibers. Additionally, hepatic lipid and fecal fat levels were investigated to provide insights in lipid metabolism and absorption influenced by the dietary fiber. Finally, the expression levels of hepatic genes of proteins involved in cholesterol and fatty acid metabolism were examined for elucidating the underlying physiological mechanism.

AGFD 89 Relationship of radical scavenging activities and anthocyanin contents in the 12 colored rice varieties Ki Chang Jang, kcjang2001@korea.kr, 20th, Jeompiljaero, Miryang Gyeongnam, Republic of Korea ; Sang-Ik Han; Woo Duck Seo; Ji-Eun Ra; Jun Young Kim; You Chun Song; Mi Jin Park; Hang Won Kang Dept. of Functional Crop, Rural Development Administration, Miryang Gyeongnam, Republic of Korea The aim of this research was to evaluate the total polyphenolic, protein, lipid and anthocyanin contents of grains from 12 colored rice varieties. Contents were also evaluated for their relationships with DPPH and ABTS radicals scavenging activities. Three anthocyanins, cyanidin-3-O-glucoside (Cy-3-G), petunidin-3-O-glucoside (Pt-3-G), and peonidin-3-O-glucoside (Pn-3-G), were also characterized by ultra performance liquid chromatography. The highest anthocyanin content was in 'Heugjinju' [(Cy-3-G):113.63±0.13, (Pt-3-G): 0.04±0.01, (Pn-3-G): 8.98±0.34 mg/100g], whereas no anthocyanins were detected in 'Hongjinju' and 'Jeogjinju'. Furthermore, the highest antioxidant activity was observed in 'Heugjinju' (IC50, DPPH: 246.94±11.95, ABTS: 19.96±1.03 mg/mL), whereas 'Jeogjinju' exhibited the lowest activity. To determine the correlation between total polyphenolic content, anthocyanin content and antioxidant activity, linear regression analysis was carried out. The results show that total polyphenolic content was correlated strongly with antioxidant activity; the correlation coefficients squared were 0.8512 (DPPH) and 0.7839 (ABTS). Overall results suggest that total phenolic contents can be a key factor in antioxidant activity of colored rice and 'Heugjinju', 'Heugseol', and 'Sintoheugmi' may be very important sources concerning nutritional value.

AGFD 90 Neuraminidase inhibitory activities of polyphenolic compounds in the young leaves of 20 barley varieties Ki Chang Jang, kcjang2001@korea.kr, 20th, Jeompiljaero, Miryang Gyeongnam, Republic of Korea ; Woo Duck Seo; Sang-Ik Han; Ji-Eun Ra; Seong-Hwan Oh; Sang-Yeol Kim; Kyung-Jin Choi; Hang-Won Kang Dept. of Functional Crop, Rural Development Administration, Miryang Gyeongnam, Republic of Korea Young barley leaf extract is a good natural source of vitamins and minerals. It is made from barley leaves harvested 2 weeks after seeding. The barley leaves were freeze-dried for 3 d and then ground. The ground leaves contain fat 5.3%, protein 33.1%, and a variety of vitamins, minerals and polyphenolic compounds. In this context, a methanol extract of young leaves in 20 barley varieties were evaluated for their

inhibitory effect on recombinant virus H1N1 neuraminidase. The influenza neuraminidase (E.C. 3.2.1.18) is an antiviral target of high pharmaceutical interest because of its essential role in cleaving sialic acid residues from surface glycoproteins and facilitating release of virions from infected cell. Seven phenolic compounds, ferulic acid, isovitexin, luteolin, homoorientin, saponarin, lutanarin, and chlorogenic acid were isolated from this methanolic extract, and determined those structures by 1D and 2D nuclear magnetic resonance (NMR), including COSY and HMBC experiments. Among the isolated compounds, luteolin, isovitexin, homoorientin, saponarin, lutanarin, and chlorogenic acid inhibited the rvH1N1 neuraminidase with an IC₅₀ of 11.5, 15.8, 9.8, 17.8, 15.5, and 61.0 μ M, respectively. Whereas ferulic acid, at concentrations up to 200 μ M, did not inhibit rvH1N1 neuraminidase.

AGFD 91 Physicochemical and antioxidative properties of selected barnyard millet (*Echinochloa utilis*)

species in Korea Woo Duck Seo, swd2002@korea.kr, Nei-Dong, Miryang Gyeongnam, Republic of Korea ; Ki Chang Jang; Sang-Ik Han; Kyung Jin Choi; Sang Yeol Kim; Seong Hwan Oh; Ji Eun Ra; Hang Won Kang Dept. of Functional Crop, National Inst. of Crop Science, Miryang, Republic of Korea The purpose of this study was to analyze and report the nutritional and physicochemical properties of 13 barnyard millet varieties (*Echinochloa* spp.) in Korea. Among the varieties, IT153600 exhibited the highest total protein (14.75 \pm 1.7%), lipid (6.92 \pm 1.1%), and amino acids contents (137.10 \pm 3.1 mg/g), and had a high germination rate (98.9 \pm 1.8%). For fatty acid composition, the highest linoleic acid (67.6 \pm 2.5%) content was found in K141285. K141286 varieties exhibited the highest amylose content. The highest mineral content was found in IT153604. Based on excellent agricultural properties, K141285 was selected and investigated for its antioxidant effects using 1,1-diphenyl-2-picrylhydrazyl (DPPH) and 2,2-azino-bis-(3-ethylbenzthiazoline-6-sulfonic acid) (ABTS). The 80% methanol extract of K141285 showed significantly high total phenolic (38.45 \pm 0.45) and flavonoid (28.71 \pm 0.27) contents. These results suggest that all of the selected barnyard millet (*Echinochloa* spp.) varieties can be considered to be new functional crops due to their anti-oxidative effects and high nutrient contents.

AGFD 92 Alpha-glucosidase inhibitory polyphenols from the grain of native barnyard millet (*Echinochloa utilis*)

Woo Duck Seo, swd2002@korea.kr, Nei-dong, Miryang Gyeongnam, Republic of Korea ; Sang-Ik Han; Ki Chang Jang; Kyung-Jin Choi; Ji-Eun Ra; Sang-Yeol Kim; Seong-Hwan Oh; Jun Young Kim; Hang-Won Kang Dept. of functional crop, National Inst. of Crop Science, Miryang Gyeongnam, Republic of Korea The grain of barnyard millet (*Echinochloa utilis*) were extracted into five different polar solvents: ethylacetate, butanol, ethanol, 50% ethanol and water. The ethylacetate extracts showed the lowest IC₅₀ value against α -glucosidase (70.2 mg/ml). To investigate the compounds responsible for this effect, activity guided fractionation of barnyard millet grain by chromatography yielded ten polyphenolic compounds which were identified as N-p-coumaroyl serotonin (1), feruloyl serotonin (2), tricin (3), tricin methylester (4), luteolin (5), luteolin-7-glucoside (6), beta-sitosterol (7), protocatechuic acid (8), vanillic acid (9) and 4-hydroxy benzoic acid (10). Interestingly, compound 1 was a more potent component with IC₅₀ = 1.28 mM against α -glucosidase compared with deoxynorjirimycin (DNJ, IC₅₀ = 2.54 mM). Mechanistic analysis of their inhibition modes against α -glucosidase showed that compound 1 was noncompetitive. Furthermore, strong α -glucosidase inhibitors were proven to be present in the native seed in high quantities by an HPLC analysis chromatogram.

AGFD 93 Molecular properties and antioxidant activities of polysaccharide-protein complexes from medicinal mushrooms by ultrasound-assisted extraction

Jian-Yong Wu bcjywu@polyu.edu.hk, Hung Hom, Kowloon Hong Kong; Ka-Chai SIU; Yi-Ching CHEUNG Dept. of Applied Biology and Chem. Tech., The Hong Kong Polytechnic Univ., Hung Hom Kowloon, This study was to evaluate the effects of ultrasound-assisted extraction (UAE) on the total yield, molecular properties and antioxidant activities of polysaccharide-protein (PSP) complexes from mushrooms in comparison with boiling hot-water extraction (HWE). Three important edible/medicinal mushrooms were included in this study *Grifola frondosa* (Maitake), *Coriolus versicolor* (Yunzhi) and *Lentinus edodes* (Shiitake); UAE was performed with an ultrasonic probe at a fixed power in water at relatively low temperature (< 50 $^{\circ}$ C). Compared with HWE, the PSP yield from UAE was similar on *G. frondosa*, notably higher on *L. edodes* but notably lower on *C. versicolor*, while the average extraction rate (PSP yield per unit time) in UAE was notably higher for *G. frondosa* and *L. edodes*, but much lower on *C. versicolor*. All the PSPs from UAE had higher carbohydrate but lower protein contents than those from HWE. The molecular weight distribution (MWD) of all PSPs from UAE exhibited an overall shift to the lower MW side and a sharp peak at MW below 1.0 kDa, due probably to partial degradation of the PSPs under the ultrasound power. On SDS-page, all the PSPs from UAE exhibited several clear protein bands between 10-130 kDa but none from HWE. The results suggest that UAE was more selective and effective to retain specific and purer PSP fractions than HWE. The antioxidant activities of the PSPs attained by UAE from the three mushrooms were all higher than those by HWE as measured with three different activity assays due probably to the higher protein content and lower average MW. The results indicate that the UAE can only enhance the extraction of PSPs from certain mushroom materials and the PSPs from UAE can have significant differences in chemical properties and bioactivities from those from HWE.

AGFD 94 Antioxidative activity of organic versus conventional milk

Moushumi Paul, moushumi.paul@ars.usda.gov; Diane L. Van Hekken Dairy and Functional Foods Research Unit, USDA-ARS-NAA-ERRC,

Wyndmoor PA Some dairy proteins exhibit antioxidative activity, a property used for marketing foods as beneficial to American consumers. However, factors in milk production and processing that influence this activity are not fully understood. In this study, commercially available homogenized and pasteurized milk samples from conventional and organic dairies were assayed for antioxidative activity. Water-soluble protein mixtures were extracted and activities of samples were measured using the Oxygen Radical Absorbance Capacity (ORAC) assay. Values were compared to determine if the farming system under which the milk is produced exhibited any effect. Results show that activities of milk samples are comparable (58-67 $\mu\text{mol TE/oz}$) to other products marketed as antioxidant sources, e.g. vegetables and nuts (20-100 $\mu\text{mol TE/g}$). Additionally, commercially available homogenized and pasteurized milk produced conventionally and organically had similar activities. Assessing the effect of farming system on the activities of milk products will provide consumers information to select a healthy diet.

AGFD 95 Analysis of black raspberry polyphenols by high field NMR and HPLC-ESI-MS/MS Liladhar Paudel, lp20@zips.uakron.edu, Joseph C. Scheerens; Faith J. Wyzgoski; Peter L. Rinaldi; R. Neil Reese; M. Monica Giusti; Jodee Johnson; Noor W. Najjar; Joshua Bomser; James K. Hardy; Ann M. Chanon; Danijela Smiljanic; Chrys Wesdemiotis Univ. of Akron, Akron Ohio The Ohio State Univ., Wooster Ohio The Ohio State Univ.-Mansfield, Mansfield Dept. of Biology and Microbiology, South Dakota State Univ., Brookings South Dakota Dept. of Food Sci. and Technology, The Ohio State Univ., Columbus Ohio Dept. of Human Nutrition, The Ohio State Univ., Columbus Polyphenolic-rich black raspberry fruit extracts have shown chemoprotective activity against oral, esophageal, colonic and rectal forms of aerodigestive cancers. However, correlating individual components with the total activity of berry extracts requires the identification of these constituents on the molecular level. Our ^1H nuclear magnetic resonance (NMR) based metabolomic studies permitted quantitation of structure-activity relationships of black raspberry constituents to the inhibition of proliferation of HT-29 colon cancer cells. Our 1D and 2D NMR studies confirmed anthocyanin polyphenols, namely cyanidin 3-rutinoside, cyanidin 3-xylosylrutinoside, cyanidin 3-glucoside, and cyanidin 3-sambubioside to be important antiproliferative constituents of the extracts. However, additional phenolic components were also found to be significant. To unequivocally identify these compounds we collected black raspberry non-anthocyanin phenolic compounds fractions by semi-preparative HPLC then subjected them to HPLC-ESI-MS analysis. When NMR analyses of these fractions were combined with our metabolomic results, a variety of non-anthocyanin phenolic compounds were identified, including hydroxybenzoic acids, hydroxycinnamic acids, quercetin, myricetin, ellagic acid, resveratrols and their glycosylated and methoxylated derivatives. Our studies report the most complete analysis of black raspberry non-anthocyanin phenolics to date. Moreover, our research demonstrates how NMR and mass spectral techniques can be used to analyze highly variable fruit extracts and provide valuable information when assessing their phytomedicinal and nutraceutical benefits.

AGFD 96 Determination of the antioxidant capacity of plant parts of Psoralea esculenta (prairie turnip) and identification and quantitation of antioxidants Elizabeth Benjamin, paul.weber@briarcliff.edu; Eric Rohe; Paul L Weber Dept. of Chemistry, Briar Cliff Univ., Sioux City IA The root of *Psoralea esculenta* (prairie turnip) has been a staple of the diet of the Plains Indians. High concentrations of flavonoids were found to be present in various parts of the plant with stems/leaves containing large levels of genistein while the rind of the root was high in daidzein and exhibited a great variety of flavonoids. Since flavonoids are known to be potent antioxidants, the antioxidant capacity of extracts of plant parts was determined and antioxidant activity was used as a guide to purify these and other components by selective extraction and chromatography. Chemical characterization was accomplished using instrumental methods including HPLC, GC/MS, HPLC/MS and NMR. The significance of this work lies in the potential that the prairie turnip has as an important source of new and previously discovered antioxidants and attempts to underscore the importance of foods of cultural diets by revealing the nature of beneficial components.

AGFD 97 Preparation of carnosine-containing extracts from chicken and pork and their physiological activities Seung-Ki Kim, rla-tmdrl@hanmail.net, 72-1 Naeri, Daeduk-myun, Ansung Gyeonggi-do Republic of Korea ; Joong-Hyuck Auh, jhauh@cau.ac.kr, 72-1 Naeri, Daeduk-myun, Ansung Gyeonggi-do, Republic of Korea ; Cheon-Soek Park Dept. of Food Sci. and Technology, Chung-Ang Univ., Republic of Korea Dept. of Food Sci. and Biotechnology, KyungHee Univ., Republic of Korea L-carnosine, a natural dipeptide consisting of β -alanine and L-histidine, is widely found in vertebrate tissue. It has been known to play a role in some physiological activities as anti-glycation, anti-oxidation and free-radical scavenging activity. In this study, anti-glycation and DPPH radical scavenging activities were investigated with carnosine-containing extracts from chicken and pork prepared under optimum extraction conditions. The content of carnosine in pork was significantly higher than the in chicken. The yield of extraction was the highest at room temperature for 2 hours, and it was enhanced by increasing the hydrophilicity of the extraction solvent. The extract from pork loin showed highest anti-glycating activity (app. 60%) among all the samples and this implied that the physiological activities would depend on the relative ratio of carnosine instead of the sum of carnosine and anserine in the extracts.

AGFD 98 Effect of adding milk and sugar on various tea preparations Nixon Ogendi Mwebi, nmwebi@jsu.edu; Jennifer Brown Physical & Earth Sciences, Jacksonville State Univ., Jacksonville AL Tea, *camellia sinensis* consumption has

been linked to increased health benefits which are mainly attributed to the antioxidant potential of the various compounds such as polyphenols in the tea. In many parts of the world, tea is consumed with milk; and with substantial amounts of sugar added. A number of studies have addressed the effect of adding milk on tea. These studies have been inconclusive; with some studies indicating that addition of milk has minimal or no effect on the antioxidant potential of tea; other studies indicate that milk addition enhances the antioxidant potential of tea, yet others argue that the milk addition inhibits the antioxidant potential of tea. This controversy forms the basis of this study which methodically addresses the effect of adding milk on black and green tea under the optimized conditions used in other studies. On the other hand, little information is available regarding the effect of adding sugar on the antioxidant potential of teas. These arguments and considerations form the basis for our study. This study employs the FRAP technique which involves the reducing of the ferric complex to the ferrous complex by the reductant (antioxidant in the teas) as well as the DPPH method that quantify the ability of the antioxidant in the teas to reduce the free radical moiety. Our results indicate that milk and sugar addition has an effect on the antioxidant potential of teas and the effect depends on several factors including the fat content of the milk added and the type of sugar added.

AGFD 99 Potential chemopreventive xanthenes and a new polyisoprenylated benzophenone derivative from *Garcinia humilis* Danniebelle N. Haase, dnhaase@gmail.com, Stacy-Ann Parker; Helen Jacobs; Simone Badal; Sheena Francis; Rupika Delgoda; George Huang; Tzuen-Rong J. Tzeng Univ. of the West Indies, Mona Kingston, Jamaica Dept. of Biological Science, Clemson Univ., Clemson South Carolina The Clusiaceae family, in particular the *Garcinia* genus, is a prolific producer of polyisoprenylated benzophenones and xanthenes. These oxygenated and prenylated phenol derivatives exhibit a wide range of biological activities, including anti-HIV, antioxidant, antibacterial, antimicrobial, antidepressant, antitumor, antihelminthic, insecticidal, and cytotoxic effects. As part of our continuing phytochemical survey of the Caribbean plants of Clusiaceae we report the isolation and structural elucidation of a new polyisoprenylated benzophenone 7-epi-aristophenone, the known simple benzophenone 4',6-dihydroxy-2,3', 4-trimethoxybenzophenone, four new xanthenes, three known xanthenes and several triterpenes and plant sterols from *Garcinia humilis*. The effect of the three known xanthenes, 1,5-dihydroxyxanthone, brasixanthone A and smeathxanthone B, on the activities of CYP1 enzymes and their cytotoxic potential using three cancerous cell lines from the colon, liver and breast will also be reported.

AGFD 100 Microwave-assisted extraction and isolation of red pigment from pitaya peel Ruqiang Huang, hruqiang@hotmail.com, Guangzhou Guangdong, China ; Bilian Huang, belinda_huang@163.com, Global Green Tech Industrial City, Changping, Tu Tang District, Dongguan Guangdong, China; Hongyue Huang, 1525800357@qq.com, Guangzhou Guangdong, China; Shuo Chen, chenshuo2012@yahoo.com.cn, Guangzhou Guangdong, China ; Xuewei Lu, joey_luxuev.student@sina.com, South China Univ. of Technolog, Guangzhou Higher Education Mega Center, Panyu, Guangzhou Guangdong , China ; Nianhui Li School of Life Science, South China Normal Univ., Guangzhou Guangdong, China Global Green Tech Group Ltd., Dongguan Guangdong, China School of Economics and Commerce, South China Univ. of Technology, Guangzhou Guangdong , China Pitaya (*Hyloereus*) is native to tropical desert areas of Central America, and also has distribution in tropical America, the West Indies and other tropical regions. In Asia, pitayas are mainly distributed in Taiwan and Vietnam. Presently in southern areas of China, such as in Guangdong, Hainan and Guangxi, pitaya is being cultivated. With pitaya peels as the raw material, this study focused on the microwave-assisted extraction and isolation of red pigment from pitaya peel. It was shown that the optimum conditions for extracting the natural pigment with water were as follows: 750 w (microwave power), 6 min (radiation time), 1:3 (solid:liquid ratio). After vacuum concentration, the crude pigment extract was applied to a polyamide tomography column, and the column contents were eluted with a water-ethanol gradient. The eluted fractions were collected and the value of R_f for each fraction determined using TLC. The developing solvent was a mixture of n-butanol: ethanol: 1 % ammonia (4:1:2). Combined components which had similar values of R_f were re-purified on the polyamide tomography column, and the similar components were combined. After vacuum freeze-drying, a highly purified red pigment of pitaya peel was obtained.

AGFD 101 Study on extraction of polysaccharides from longan seeds by cellulase Ruqiang Huang, hruqiang@hotmail.com, Guangzhou Guangdong, China ; Bilian Huan, belinda_huang@163.com, Global Green Tech Industrial City, Changping, Tutang District, Dongguan Guangdong, China ; Xuewei Lu, joey_luxuev.student@sina.com, ,South China Univ. of Technology, Guangzhou Higher Education Mega Center, Pan Yu, Guangzhou Guangdong, China ; Shuo Chen, chenshuo2012@yahoo.com.cn, Guangzhou Guangdong, China ; Hongyue Huang, 1525800357@qq.com, Guangzhou Guangdong, China ; Kewei Xu, soshore206@163.com, Guangzhou Guangdong, China School of Life Science, South China Normal Univ., Guangzhou Guangdong, China Administrative Division, Global Green Tech Group Ltd., Dongguan Guangdong, China School of Economics and Commerce, South China Univ. of Technology, Guangzhou Guangdong, China The study focused on extracting polysaccharides from longan seeds (LS) assisted by cellulase. Dry LS powder was weighed and stirred with deionized (DI) water (LS powder:DI water= 1:5 w/w). The mixture was adjusted to 40°C and pH 4.5, and then cellulase (700 EGU/g), 0.15% weight of LS powder, was added to the mixture. The mixture was incubated with the enzyme for 3.5 h. After inactivation of cellulase, the hydrolyzate was subsequently centrifuged at 4000 rpm and the supernatant was concentrated. The concentrate was treated with 85%/15% ethanol/water in a refrigerator for 12 hr to precipitate the crude LS polysaccharides (LSP). The LSP was re-dissolved in DI water and protein was precipitated with trichloroacetic acid. The

protein-free LSP solution was washed through Sephadex G-75 column using 0.1 mol/L NaCl as the eluent. Fractions were collected in different test tubes and measured by anthrone reagent assay. In addition, the fractions were accumulated and freeze-dried to obtain dry LSP.

AGFD 102 Enzymatic modification of a model homogalacturonan with a pectin methylesterase from papaya:

Effects of enzyme-substrate ratios on nanostructure and enzyme mode of action Yang Kim, yang.kim@ars.usda.gov, Randall G Cameron; Gary A Luzio; Brett J Savary; Prasanna Vasu; Martin A K Willams Citrus and Subtropical Products Lab., USDA / ARS, Winter Haven Florida Arkansas Biosciences Inst., Arkansas State Univ., State Univ. Arkansas Inst. of Fundamental Sciences, Massey Univ., Palmerston North, New Zealand Methyl ester distribution in pectin homogalacturonan has a major influence on functionality of pectin in food systems. A novel papaya pectin methylesterase was introduced to a homogalacturonan to characterize demethylesterified block nano-structure and to model enzyme mode of action at various enzyme-substrate (E-S) ratios. A controlled demethylesterification series was produced at the E-S ratio of 1:10, 1:25 and 1:50, respectively. Demethylesterified blocks were released as oligomers with a limited endopolygalacturonase digestion, separated and quantified by HPAEC. The results depicted that average demethylesterified block size (BS) and number of blocks per molecule (BN) differed depending on the degree of methylesterification (DM). Significant increase in BS and BN were observed in demethylesterified homogalacturonans with 50 DM, upon decreasing the E-S ratio ($P < 0.05$). Enzyme mode of action, modeled in silico, demonstrates a multiple attack mechanism. The results suggested the possibility of tailoring demethylesterified blocks by modifying E-S ratios of the papaya pectin methylesterase.

AGFD 103 Use of milled-rice co-products in value -added food products Fred Shih, fred.shih@ars.usda.gov; Kim Daigle; Sherwin Cheuk Southern Regional Research Center, New Orleans Louisiana Milled-rice co-products, particularly rice bran, are rich in antioxidants. A correlation was found to exist between the antioxidant activity and the total phenolic content of these rice ingredients. When added to ground beef, their methanol extracts inhibited the lipid oxidation, with relative effectiveness in the order of rice hull > rice bran > brown rice. When the ingredients were applied directly to the beef, both defatted brown rice flour and rice bran strongly retarded the lipid oxidation. Rice wax was used in combination with pullulan in the preparation of edible films. The films could be useful as carriers of flavor and nutritional additives or as barriers for separation and preservation purposes. Water vapor barrier properties were improved with increased addition of rice wax. Moisture sorption isotherms of the film were also studied, and the Brunauer-Emmet-Teller (BET) and Guggenheim-Anderson-de Boer (GAB) sorption models were tested to fit the experimental data. Changes in the sorption parameters, particularly such as the decrease in monolayer moisture content (Mo), reflect the trend of reduced hydration capacity with increase addition of rice wax, providing useful information on water activity conditions to achieve stability for the composite film.

AGFD 104 Isolation and structural characterization of eel type I collagen Masataka Saito, msaito@eiyo.ac.jp, 3-9-21, Chiyoda, Sakado Saitama, Japan; Tomoyuki Higuchi; Naoyuki Uchida; Hiramitsu Suzuki; Hiroshi Hayakawa; Chihiro Sato; Hikaru Go Laboratory of Food Sci. and Technology, Kagawa Nutrition Univ., Chiyoda, Sakado Saitama, Japan Dept. of Marine Science and Resources, Nihon Univ., Kameino, Fujisawa Kanagawa, Japan Type I collagen was extracted from skin of Japanese eel, *Anguilla japonica*, with the yield of 11.63% on the basis of wet weight. In the eel skin and muscle, type I collagens were estimated to contain 14.99% and 2.37%, respectively. Comparison of amino acid profiles with trout type I collagen showed differences in alanine, serine, hydroxyproline, and hydroxylysine contents. The denaturation temperature was 30.9 °C for the skin collagen and 31.7 °C for the muscle collagen, as determined by DSC. On the other hand, the $\alpha 1(I)$, $\alpha 2(I)$, and $\alpha 3(I)$ chains of eel type I collagen were isolated and also the cDNAs coding for proa1(I), proa2(I), and proa3(I) chains were cloned from eel muscle. Eel proa1(I) and proa3(I) showed only 85% and 76% amino acid sequence identities to trout proa1(I) and proa3(I), respectively, and eel proa2(I) had 79% identity to trout proa2(I). Thus, these results suggest that Japanese eel type I collagen may find a wide range of applications including functional foods, nutraceuticals, biomaterials, and pharmaceuticals.

AGFD 105 Effects of alcohol compounds on the growth and lipid accumulation of oleaginous yeast

Trichosporon fermentans Min-hua Zong, btmhzong@scut.edu.cn, Wushan RD., Tianhe District, Guangzhou, P.R. China, Guangzhou Guangdong, China; Chao Huang; Hong Wu State Key Laboratory of Pulp and Paper Engineering, South China Univ. of Technology, Guangzhou Guangdong, China Alcohol compounds are one kind of inhibitors in lignocellulosic hydrolysates. In this work, the effects of alcohol compounds commonly found in lignocellulosic hydrolysates, including catechol, hydroquinone, furfuryl alcohol, and vanillyl alcohol, on the cell growth and lipid accumulation of *Trichosporon fermentans* were systematically investigated for the first time. Among them, catechol proved to be the most toxic and vanillyl alcohol the least toxic to the cells. Interestingly, vanillyl alcohol could even stimulate the lipid accumulation and sugar consumption at its low concentrations. Additionally, the inhibition on cell growth by the alcohols was generally more sensitive to the variation of inoculum size, temperature, and initial pH than that on lipid synthesis. The fatty acid composition of lipids, however, was not influenced clearly by these alcohol compounds. Comparative study demonstrated that the examined alcohols exerted less inhibition than their aldehyde analogues but more inhibition than their acid counterparts on the cells.

AGFD 106 Application of high pressure homogenizer for the preparation of chlorella vulgaris nano-suspension Ri Yu, ohno1984@hanmail.net, Chung-Ang Univ. 2nd Campus, Daedeok-myeon, Anseong-si, Gyeonggi-do, Anseong Gyeonggi-do, Republic of Korea ; Han-Cheol Park; Dong-Un Lee Dept. of Food Sci., Chung-Ang Univ., Anseong Republic of Korea Chlorella is known as a rich source of lutein, and the lutein is located within the cell membrane of chlorella. However, the rigid structure of chlorella inhibits the effective extraction of lutein. The objection of research was to disrupt the chlorella cells into nanometer scale and thereby increases the extractability of lutein from the broken cells. The disruption of chlorella based on use of the microfluidizer (MF) technique was used to prepare nano-suspensions of chlorella. The effects of processing parameters including pressure, number of cycle, and dilution on the size reductions of chlorella were investigated. Average mean diameters of 300 nm – 600 nm were obtained by applying pressures of 80 MPa or higher. Luteins from MF-treated chlorella were then extracted and analyzed by HPLC. Up to six-fold increases in lutein extractability were observed by breaking of chlorella cells and preparing a nano-suspension.

AGFD 107 Preparation of smoked Bissaria (Atherina boyeri) and utilization of its powder in different popular food products Hany A Abou Gharbia, samehmawad@gmail.com, Aflaton St, Alexandria Alexandria, Egypt ; El Sayed Abou Tour; Aly Abdelnaby Food Sci., Alexandria Univ., Alexandria Egypt The fish called "Bissaria" used in the present investigation has no industrial use up to now. Bissaria deteriorates rapidly because of its small size, fragile body and high activity of gut enzymes. The study aimed to prepare different products of bissaria fish, mainly hot smoked bissaria as a snack and powdered smoked bissaria (PSB). This powder (PSB) was incorporated as a natural flavouring agent into different popular food products such as fish fingers (kofta), pizza, paste, mayonnaise, tahina and potato chips. Data on different changes that affects the quality and shelf life of different products during storage were determined. The degree of consumer acceptability for these products was evaluated. Most of the products were highly accepted because of the pleasant flavor of the smoked bissaria. The optimum conditions required to prepare each of these products were described. The influence of processing and storage conditions on the oxidative stability and the microbial count was also conducted.

AGFD 108 Extraction of zein from DDGS for commercial applications Emily Thayer, abeard@benedictine.edu; Sarah Laskares, abeard@benedictine.edu, Aileen Beard, Dept. of Chemistry and Biochemistry, Benedictine College, Atchison KS The increasing use of ethanol as a fuel source has led to a corresponding increase in the generation of distillers dried grain with solubles (DDGS). Current uses of DDGS are mainly limited to food and feed applications. Corn-based DDGS contain a relatively large concentration of proteins. Zein, the predominant protein found in corn, has many potential commercial uses, particularly in bio-based polymers. Current methods of zein extraction from DDGS involve flammable solvents and high temperature (70% ethanol and 70 °C is typical), which limit their application on a large, commercial scale. The purpose of our research was to investigate safer and more cost-effective methods of zein extraction. We tested a variety of organic and inorganic solvents to determine the maximum solubility of zein. We then investigated the effects of concentration, pH, temperature and grain pulverization on the extraction of zein from DDGS. The results of this research will be presented.

AGFD 109 Characterization of jet-milled rice flour and the effect on resistant starch (type 3 & 4) formation Jiwon Park, pjw114@gmail.com; Joong-Hyuck Auh, jhauh@cau.ac.kr, 72-1 Naeri, Daeduk-myun, Ansong Gyeonggi-do, Republic of Korea ; Dong-Un Lee Dept. of Food Sci. and Technology, Chung-Ang Univ., Ansong, Republic of Korea The physicochemical properties of jet-milled rice flour (JMRF) were evaluated compared to the conventional rice flour and the resistant starch from JMRF was prepared & characterized for the application as dietary fiber. The average particle size distribution of JMRF (11 µm) was 1/10 of the control while the damaged starch increased by 3 times by jet milling. Molecular weight and side chain distribution of starch fraction was not affected by jet-milling, but water solubility index and in vitro digestibility significantly increased compared to the control. Resistant starches (RS) of type 3 & 4 were prepared by thermal cycling and chemical treatment, respectively. Although higher content of damaged starch in JMRF than the control, no differences were observed in the levels of RS formation. RS type 4 exhibited lower in vitro digestibility than RS type 3, which were comparable with the commercial RS prepared from corn.

AGFD 110 Delivering omega-3 lipids into food beverages through a nano-clear o/w emulsion Dongming Tang, dtang@ocean-nutrition.com, Dept. of Research and Development, Ocean Nutrition Canada Ltd., Dartmouth Nova Scotia Canada The cloudiness of traditional omega-3 lipids in water emulsion makes it unsuitable vehicle to deliver polyunsaturated fatty acids into food beverages. A nano-clear omega-3 lipids in water emulsion that will remain clear upon dilution has been successfully developed and shows promise in the application of food beverages. In addition to various emulsifiers with different HLB value, some co-emulsifiers and co-solvents were used to reduce the emulsion droplet size and the amount of emulsifiers used in the clear emulsion. The tri-angle phase diagram of omega-3 lipids, emulsifier, and co-solvent showed that additional solvents (i.e., co-solvents) can be present in the continuous phase and in many cases are preferred. Finally, antioxidants in both dispersed phase and continuous phase and appropriate masking agent are necessary to prevent the oxidation of omega-3 lipids or mask off-notes.

AGFD 111 Nano-encapsulation of coenzyme Q10 with octenyl succinic anhydride modified starch Sherwin Cheuk, sherwin.cheuk@ars.usda.gov Kim Daigle; Fredrick Shih; Elaine Champagne; James Patindol Dept. of Food

Processing & Sensory Quality, USDA-ARS-SRRC, New Orleans Louisiana Octenyl succinic acid/ester modified starch (OSE-ST) was used to encapsulate coenzyme Q10 (CoQ10). CoQ10 was dissolved in rice bran oil (RBO) and incorporated into an aqueous OSE-ST solution. High pressure homogenization (HPH) of the mixture (OSE-CoQ10) was conducted at 170 kPa for 5-6 cycles. The resulting emulsion had particle size (Z-average) range of 250-300 nm (PDI range of 0.100 to 0.250) and the absolute zeta (ζ) potential varied between 8.4 to 10.6 mV. CoQ10 retention of the emulsion and freeze dried products, determined by a hexane rinse, was >98%. There was a notable increase in the ζ potential from 10 mV of the freshly homogenized solution to 25 mV after freeze drying and redispersion in water. Reconstitution of the freeze dried product in buffers with pH values of 3 to 7 at 4°C and 25°C had no effect on the range and distribution of the nanoparticles' size in the limits of pH tested. However, the ζ potential decreased with decreasing pH. At higher pH values, the zeta potential peaked at eight days of storage for both temperatures.

AGFD 112 HPMC reinforced with different cellulose nano-particles Cristina Bilbao-Sainz, cristina.bilbao@ars.usda.gov, Julien Bras; Tina Williams; Tangi Sénechal; William Orts USDA-ARS-WRRC, Albany CA Ecole internationale du papier de la communication imprimée et des biomatériaux, Grenoble, France Three different types of cellulose nanoparticles : (i) nano-fibrils cellulose (NFC), (ii) nano-fibrils cellulose oxidized using the tempo reaction (NFCt) and (iii) cellulose whiskers, were incorporated into HPMC edible films at different concentrations. The films were examined for mechanical and moisture barrier properties verifying how the addition of cellulose nano-particles affected the water affinities and the diffusion coefficients. The reinforcing effect of the cellulose particles was observed when whiskers were used as the filling material; an increase of 22% in tensile strength and 55% in Young's modulus were achieved while the elongation at break of the films was preserved. Addition of whiskers also improved the water barrier properties of the films. This effect was attributed to the lower water affinity of the films. Furthermore, the whiskers only decreased 3-6% the transparency of the HPMC films showing 86-89 % visible light transmission values, allowing application as edible barrier and transparent film.

AGFD 113 Quality attributes and chemical composition of wheat germ subjected to different heat treatments Hany A Abogharbia, m_m_youssef@yahoo.com, Food Sci. and Technology, Alexandria Univ., Alexandria, Egypt Wheat germ (WG) was analyzed for its chemical composition, amino acids, and minerals contents. Results showed that WG contains high levels of protein (34.57%). The moisture, ether extract, fibre and ash contents were 1.12, 9.40, 2.00 and 4.52%, respectively. Also it was found that WG was a good source of most essential amino acids, and that the protein was of high quality. Moreover, WG contains sufficient amounts of some important minerals. Wheat germ was also subjected to different heat treatments in order to inactivate lipase enzyme, and it was found that using 100°C for 15 min was sufficient to inactivate the enzyme. Also the lipid classes for wheat germ oil was studied as well as fatty acid composition

AGFD 114 Transferring GC carrier gas from helium (He) to hydrogen (H₂) for the determination of fatty acids Hui Zhao, h.zhao@eplbas.com, Henry D Scobell; Keith J Duff Method Development, EPL BioAnalytical Services, Niantic IL This study aimed at replacing conventional helium (He) carrier gas with hydrogen (H₂) gas for fatty acid analysis. The chromatography was optimized for baseline separation using H₂ as the carrier gas obtained from a H₂ generator in combination with a small bore DB-wax column (20m x 0.18mm x 0.18 μ m). The total GC run time decreased by 53% from 36 minutes to 17 minutes. The resolution was improved and higher number of theoretical plate was achieved. Switching from He to H₂ is also cost-effective. Helium is a non-renewable resource, the supply of which is shrinking and the price is expensive. When a hydrogen gas generator is utilized, a stable, low volume stream of H₂ gas (>99.9999% pure) is produced on demand via the electrolysis of DI water at low pressure and safety issues due to the risk of explosion are minimized.

AGFD 115 Cholesterol is a glycoalkaloid precursor in potato plants Erik V Petersson, erik.petersson@slu.se, Nurun Nahar; Paresh Dutta; Anders Broberg; Rikard Åslund-Tröger; Lisbeth Jonsson; Folke Sitbon Dept. of Plant Biology and Forest Genetics, Swedish Univ. of Agricultural Sciences, Uppsala, Sweden Dept. of Food Sci., Swedish Univ. of Agricultural Sciences, Uppsala, Sweden Dept. of Chemistry, Swedish Univ. of Agricultural Sciences, Uppsala, Sweden Science Dept., National Food Administration, Uppsala, Sweden Dept. of Botany, Stockholm Univ., Stockholm, Sweden Steroidal glycoalkaloids (SGA) are toxic secondary metabolites naturally occurring in potato. Cholesterol is commonly considered as an important precursor of SGA, however, firm analytical evidence for this view is presently lacking. To confirm the hypothesis, potato plants (cv. 'King Edward' and 'Bintje') were fed with deuterium-labeled cholesterol (D₅-cholesterol) and incubated for three weeks. Analyses showed that D₅-cholesterol had been taken up by the plants, mainly in the older parts. D₅-labeled SGA (α -solanine and α -chaconine) were identified in extracts from plants fed with D₅-cholesterol, but not from plants fed with water, or with D₆₋₂₇ hydroxycholesterol. The ratio of D₅-SGA compared to D₅-cholesterol was greater in young parts of the plant than in the older ones, likely reflecting a higher metabolic activity in developing tissues. In conclusion, our work unequivocally demonstrates that cholesterol is a SGA precursor in the potato.

AGFD 116 Determination of degree of substitution in carboxymethyl cellulose by Fourier transform infrared (FTIR) spectroscopy Jian Xiong, lcjxiong@scut.edu.cn, Wushan, Guangzhou Guangdong, China ; Jun Ye; Yanxing Zhang College of Light Chemistry and Food Sci., South China Univ. of Technology, China State Key Laboratory of Pulp and Paper Engineering, South China Univ. of Technology, Guangzhou, China Guangdong Paper Industrial Research Inst., China

This paper reports a Fourier transform infrared (FTIR) spectroscopic technique for the determination of degree of substitution (DS) in sodium carboxymethyl cellulose (CMC). Based on the analysis of the spectra from FTIR spectroscopic measurements, it was found that the marker bands selected at 1420 and 1735 cm⁻¹, attributed to C=O carbonyl stretching vibration of CMC and CMC-H, respectively, are related to the DS in CMC. The results showed that there is a linear relationship between the ratios of intensities and DS, and thus calibration curves were established.

AGFD 117 Allenes in asymmetric catalysis: Rhodium(I)-catalyzed enantioselective addition of arylboronic acids to α -ketoesters Feng Cai, feng.cai@utsouthwestern.edu; Xiaotao Pu; Xiangbin Qi; Monika I Antczak; Joseph M Ready Biochemistry, Univ. of Texas Southwestern Medical Center, Dallas Asymmetric catalysis to prepare pure enantiomer is among the most important technologies in pharmaceutical and pesticide industry. Many drugs and pesticides need to be enantiomerically pure. Using chiral transition metal complexes to produce enantiomerically pure drugs and pesticides is a primarily choice. Effective chiral ligands play a pivotal role in this process. Allene is chiral too, but to date, they have made few contributions to asymmetric catalysis since it is difficult to be manipulated. In this work, the first time, a chiral allene ligand is adopted into a Rhodium transition metal complex and this complex could catalyze an asymmetric addition of arylboronic acids to α -ketoesters to afford high enantiomerically pure tertiary alcohols. These tertiary alcohols are very common in drug molecules, pesticide and natural products, such as: Lexapro® and Dermacozine D.

AGFD 118 Organocatalytic methods to transform glycerin into glycerol carbonate Britni A Hervert, hervertba@lopers.unk.edu; Palencia Hector Chemistry, Univ. of Nebraska at Kearney Vegetable oils are renewable resources for biopolymers, chemical intermediates, and biofuels. Glycerin is a cheap byproduct of the biodiesel synthesis from the transesterification between vegetable oils, such as soybean oil and methanol. Glycerol carbonate is seeing as a promising green solvent that can be synthesized from glycerin and dimethylcarbonate. We had developed a method that use new non-symmetrical N-heterocyclic carbenes (NHCs) for the transesterification of dimethylcarbonate and glycerol at room temperature and under solventless conditions. One of the most active catalysts yielded glycerol carbonate with 4 mol % at room temperature in less than an hour. Several catalysts were synthesized and screen for the reaction. The new catalysts were compared with other known NHCs and they were more active under the same conditions

AGFD 119 Production of activated carbon from hemp by-products by carbon dioxide and steam activation Seung-Soo Kim, sskim2008@kangwon.ac.kr, Jinsoo Kim, jkim21@khu.ac.kr, 1 Seocheon-dong, Giheung-gu, Yongin Gyeonggi-do, Republic of Korea ; Gyeong-Ho Choi Dept. of Chemical Engineering, Kangwon National Univ., Samcheok Gangwon-do, Republic of Korea Dept. of Chemical Engineering, Kyung Hee Univ., Yongin Gyeonggi-do, Republic of Korea Dept. of Chemical Engineering, Kangwon National Univ., Samcheok Gangwon-do, Republic of Korea Hemp is known as one of the most productive and useful plants, which grows quickly in a moderate climates with only moderate water and fertilizer. Traditionally in Korea, hemp bast is used for natural fibers, and the other parts such as stem and root are treated as wastes. These hemp by-products can be transformed to activated carbon using a thermal treatment of pyrolysis. To understand pyrolysis characteristics, thermogravimetric analysis was carried out using TGA, in which hemp by-products were mostly decomposed at the temperature range of 270~370°. The effect of process variables such as carbonization temperature, activation temperature, activation time and activation agents was investigated to optimize the preparation conditions. First, hemp by-products were carbonized under the N₂ flow at the temperature from 400° to 600° for 120 min, followed by CO₂ or H₂O activation. After carbonization, the BET surface area of the solid products was in the range of 33-37 m²/g depending on carbonization temperature from 400 to 600°. The BET surface area of activated carbon increased to 460-900 m²/g, depending on activation temperature and activation agents.

AGFD 120 Antioxidant properties of polysaccharide-protein complex isolated from mycelium of a medicinal fungus Cordyceps Cs -HK1 Jian-Yong Wu, bcjywu@polyu.edu.hk Yi-Ching CHEUNG; Ka -Chai SIU Dept. of Applied Biology and Chem. Tech., The Hong Kong Polytechnic Univ., Hung Hom Kowloon, Cordyceps sinensis (Berk.) Sacc., generally called Cordyceps or the Chinese caterpillar fungus, is a precious medicinal fungus. Polysaccharides are the major bioactive constituents of Cordyceps with anticancer, immunomodulating and antioxidant activities. Because natural Cordyceps is rare and expensive, fermentation is widely applied for production of Cordyceps fungal mycelium and polysaccharides. Cs -HK1 is a fungus isolated from a wild Cordyceps fruiting body in our lab and its mycelial culture has been established, and applied to liquid fermentation. In this study, a protein-bound polysaccharide or PSP was isolated from the hot water extract of Cs -HK1 mycelial biomass by ethanol precipitation. The antioxidant activities of PSP were determined with the Trolox equivalent antioxidant capacity (TEAC), reducing ability of plasma (FRAP) and ferric ion chelating assay methods. Removal of the protein constituent from the PSPs led to a notable drop (15-32%) in antioxidant activities. When the PSPs were degraded into different molecular weight fractions by acidic hydrolysis, the lower molecular weight fractions exhibited higher antioxidant activities. The results suggest that the protein content and molecular weight are important factors on antioxidant properties of the protein-bound polysaccharides.

AGFD 121 Characterisation of carnauba and other Copernicia sp waxes from Brazil Edy S Brito, edy@cnpat.embrapa.br, R Dra Sara Mesquita, Amanda Rayssa F. Batista; Nagila M. P. S. Ricardo; Elaine C Cabral; Marcos N

Eberlin; Eduardo J Pilau; Fabio C Gozzo Embrapa Tropical Agroindustry, Fortaleza CE, Brazil Dept. of Organic and Inorganic Chemistry, Universidade Federal do Ceara, Fortaleza CE, Brazil Inst. of Chemistry, Universidade Estadual de Campinas, Campinas SP, Brazil Carnauba wax (*Copernicia prunifera*) is widely applied in cosmetic, food, and pharmaceutical industries. It has unique physical properties due to its composition based on esters of long chain alcohols and fatty acids. In this work we evaluated carnauba wax and other six waxes of different *Copernicia* palms (*C. alba*, *C. bayleana*, *C. glabrescens*, *C. textilis*, *C. hospita* and *C. yarei*) by GC-MS, DSC and NIR. Surprisingly, a wide similarity was observed amongst samples. DSC revealed a fusion temperature range of 79.2 to 84.2 °C, with an eutectic behavior. NIR bandwidths were observed at wavenumbers of 2957 cm⁻¹ –2945 cm⁻¹ (C-H stretch). MALDI-TOF highlighted a series of high molecular weight compounds (500 Da to 900 Da). The spectrum base peak, C₅₆H₁₁₂O₂Li (m/z -823.8822) corresponded to a fatty acid esterified with a long chain alcohol. Analysis with GC-MS after wax transesterification confirmed tetracosanoic acid and docotriacontanol as the major compounds.

AGFD 122 Evaluation of the safety of crop products produced through biotechnology Wayne Parrott, wparrott@uga.edu, Univ. of Georgia, Athens GA Products produced through biotechnology are the most highly scrutinized food products on the market. The safety assessment of such food crops involves a multi-pronged approach. The newly introduced gene, its source and its product (the protein it encodes) together with the performance of the plant as well as the impact of the plant on the environment are all examined in great detail. Both the intended change and possible unintended effects are examined. In the greater than 15 years that biotech products have been grown commercially no safety issues have been attributed to the newly introduced gene. On the other hand, benefits from the technology included reduced pesticide application; less soil erosion because of the more widespread adoption of no or low-till practices; decreased petroleum costs because of the reduced need to enter the field; increased diversity in the field; reduced mycotoxin levels in grain; among others.

AGFD 123 Addressing the Safety of Crop Protection Products in a Global Market Wendelyn Jones, wjones@croplifeamerica.org, Washington DC; Ray McAllister; Barbara Glenn Feeding an estimated 9 billion people worldwide by 2050 will require a doubling of food production. This will necessitate more sophisticated technologies within modern agriculture. Products that protect America's food crops are subject to 170 health, safety and environmental tests to ensure safety and effectiveness prior to pesticide registration by the EPA. Development, testing and registration of a new pesticide active ingredient typically takes 9 to 10 years and cost the pesticide manufacturer in excess of \$250 million. On average, only one in 139,000 chemicals screened for pesticide activity successfully makes it through the regulatory process from the discovery laboratory to the farmer's field. Additionally, global trade is dominated by the transfer of agricultural products. It follows that the regulatory process for agricultural chemicals, global harmonization efforts and emerging technical challenges faced by this sector of the chemical industry are key drivers to the global challenge to feed the world.

AGFD 124 Toxicological Safety Assessment of Biotech Crops Carey A Mathesius carey.mathesius@pioneer.com, DuPont Agricultural Biotechnology, Pioneer Hi-Bred International, Inc., Ankeny IA The safety assessment process including toxicology will be reviewed for the commercialization of crops derived from biotechnology, which have been modified to express agronomic (including herbicide resistance and insect tolerance) or nutritional traits. The safety assessment pathway for biotech crops is similar to that for individual food ingredients, however the complexities associated with crops as a food or feed lend more to a qualitative assessment between the biotech crop and its non-biotech comparator. The presentation will focus on the mammalian safety assessment principles and discuss specific toxicology studies conducted to ensure the safety of the transgenic proteins and food and feed products derived from biotech crops.

AGFD 125 Allergenicity Evaluations of Proteins Introduced into Crop Products using Biotechnology Laura S Privalle, laura.privalle@basf.com, Research Triangle Park North Carolina, The allergenicity potential of proteins introduced through biotechnology is evaluated as part of the safety assessment of transgenic crop products. Since no single specific parameter can be attributed to a food allergen, the assessment is based on a weight of evidence approach. Characteristics that are considered include sequence homology to known allergenic proteins by applying bioinformatics analyses using an allergen database; resistance to pepsin digestion using simulated mammalian gastric fluid; heat stability measuring loss of functional activity; and exposure as determined by expression levels. Impact on the levels of endogenous allergens by the transformation event is also considered. These may be monitored by immunoblotting techniques using sera from patients allergic to the food. Two dimensional gel electrophoresis followed by mass spectral analysis and gel-free quantitative proteomics methods are being developed as alternative approaches to immunoblots. While the use of animal models have been proposed as a screening tool, to date, none has not been successfully developed and validated to support these safety evaluations.

AGFD 126 Analytical Methods for Testing Biotechnology Products Jingwen Chen, jingwen.chen@syngenta.com, Durham North Carolina; Patrick Doyle Since the introduction of genetically modified (GM) crops in the early 1990s, there are about 30 commercial events that are currently cultivated around the world. With the increase in the number of commercial GM events, there will be increased demand for testing agricultural commodities for the presence of products derived from modern biotechnology (GMO's). As major trait providers, biotechnology companies develop, validate, and implement various analytical methodologies in their R&D programs as well as in their stewardship programs. These GMO detection methods are

provided to authorities for product registration as part of the regulatory submission. This presentation will provide an overview of analytical methods and applications implemented throughout a product life cycle. The characteristics of both protein- and DNA-based methodologies for analyzing samples from seed/grain and processed food will be discussed. The presentation will also cover regulatory requirements for detection methods and reference materials, and stewardship of Biotechnology products.

AGFD 127 Formulation of the Total Western Diet (TWD) as Basal Diet for Rodent Cancer Studies Korry J Hintze, korry.hintze@usu.edu, Robert E Ward; Abby D Benninghoff Nutrition, Dietetics and Food Sci., Utah State Univ., Logan Animal, Dairy and Veterinary Sciences, Utah State Univ., Logan Rodent cancer studies typically use diets based on nutrient profiles optimized for growth and fertility; dietary components are often modulated to investigate cancer outcome. A rodent diet that more closely represents American diets may be warranted for cancer studies. We have formulated the TWD to emulate the average American intake (50th % from NHANES) for micro and macro-nutrients based on nutrient density. Compared to the AIN-93G diet, the TWD contains fewer calories from protein and carbohydrate, and twice that from fat as well as more saturated and monounsaturated fats, but less polyunsaturates. The TWD contains half the complex carbohydrates and twice the level of simple sugars. The TWD contains significantly less calcium and copper, and significantly more sodium. Several vitamins are at least 1-fold lower in the TWD (B6, thiamine, folate, B12, and vitamins D and E). An in-depth discussion of the diet and preliminary results will be presented.

AGFD 128 Pleiotropic Beneficial Effects of 3,3'-Diindolylmethane Leonard F Bjeldanes, lbjel@berkeley.edu Dept. of Nutritional Sciences and Toxicology, Univ. of California, Berkeley 3,3'-Diindolylmethane (DIM) is a natural autolytic product present in food plants of the Brassica genus. The anticarcinogenic effects of DIM are well established in rodent models and the compound is currently in several clinical trials. Studies of the modes of action of DIM indicate that this indole can affect several signaling pathways that are associated with cancer and other diseases. Included in the group of DIM-modulated pathways are those involving the Ah receptor, estrogen receptors, the androgen receptor, reactive oxygen release, and the innate immune response. Our studies of the selective effects of DIM on the activities of steroid hormone receptors and reactive oxygen release will be summarized and the immune modulating effects of DIM will be discussed in more detail. Taken together, our studies show that DIM can affect several signaling pathways involved in disease defense, including a stimulation of immune function.

AGFD 129 Antioxidant and Anti-inflammatory Activity Correlate for Specific Maillard Reaction Products David Kitts, david.kitts@ubc.ca; Xiumin Chen Univ. of British Columbia, Vancouver BC, Canada Crude Maillard reaction products (MRPs) together with isolated fractions recovered by ultrafiltration from sugar-amino acid model systems comprising fructose (Fru), glucose (Glc) or ribose (Rib) reacted with glycine (Gly) or lysine (Lys) at 121°C for 60 min were examined for antioxidant (ORACFL assay and a cell-based intracellular oxidation assay) and anti-inflammatory activities (differentiated Caco-2 cells). α -dicarbonyl compounds generated in the hexose models were predominantly glucosone and 3-deoxyglucosone (3-DG), with 3-deoxypentosone (3-DP) and pentosone being the major α -dicarbonyls produced in the pentose models. MRPs derived from Glu-Lys showed the highest inhibitory capacity ($P < 0.05$) among the six model systems against IFN- γ and phorbol ester (PMA)-induced nitric oxide (NO) and IL-8 production in 21 day cultured Caco2 cells. A concentration of 1.25 mg/mL produced a percentage of inhibition that was 52.4% and 35.0%, respectively. A low molecular weight fraction (MW < 1kDa) produced from Glu-Lys MRPs displayed high ($P < 0.05$) affinity to inhibit NO and IL-8 in inflamed Caco-2 cells. iNOS transcription and translation in these same cells was also inhibited, thus influencing production of reactive nitrogen species (RNS). The efficacy of crude MRPs to inhibit intracellular oxidation ($P < 0.05$) was correlated with capacities to inhibit NO and IL-8, thus indicating that MRPs that have anti-inflammatory activity also function as antioxidants. In conclusion, we have demonstrated that pre-exposure of low molecular weight MRPs derived from a heated Glu-Lys mixture can attenuate disrupted intestinal RNS metabolism associated with intestinal inflammation in Caco-2 cells. The novel anti-inflammatory capacity of MRPs in inflamed intestinal Caco-2 cells was correlated with its antioxidant activity and not the composition of α -dicarbonyl compounds.

AGFD 130 Food goes omics – State of the art in curation of chemical data and prospects for epidemiological research Augustin Scalbert, scalberta@iarc.fr, Isabelle Romieu; Nadia Slimani; Joseph Rothwell Claudine Manach; Cristina Andres-Lacueva; Mireia Urpi-Sarda Nutrition and Metabolism Section, International Agency for Research on Cancer, Lyon, France Unite de Nutrition Humaine, INRA, Saint-Genès-Champanelle, France Nutrition and Food Sci. Dept., Pharmacy School, Univ. of Barcelona, Spain Foods are extremely complex and contain about 20,000 compounds, either natural constituents, additives or contaminants, that can be toxic or may exert beneficial effects on health. Understanding their role in nutrition requires full knowledge on their chemistry, occurrence in foods, metabolism and bioavailability, biological properties, and effects on health. Much information exists, largely scattered in thousands of papers and therefore not easily analysed. Proper databases are eagerly needed to allow to process this complex data at high speed and to analyse interactions between exposure and health in a more global and comprehensive way. Around the example of Phenol-Explorer, a recently developed database on content in foods and metabolism of dietary polyphenols (<http://www.phenol-explorer.eu/>), we will illustrate how a comprehensive open-access information system on food bioactives may radically change our understanding of diet and health relationships, just as other databases have fundamentally changed molecular biology during the last 20 years.

AGFD 131 Structure-/activity relationships of coffee compounds and their implications for optimizing the

health benefits of coffee beverages Veronika Somoza, veronika.somoza@univie.ac.at, Dept. of Nutritional and Physiological Chemistry, Univ. of Vienna, Austria Epidemiological studies provide evidence that moderate coffee consumption is associated with the prevention or the delay of degenerative diseases such as diabetes type 2, cardiovascular Alzheimer's or Parkinson's disease, and several types of cancer. These beneficial effects have been attributed in part to the antioxidant activity of coffee. Harmful effects of an increased coffee consumption are mostly associated with caffeine, which is a mild stimulant of the CNS, increasing heartbeat, blood pressure and the basal metabolic rate (BMR). Regular intake of caffeine may lead to habituation which is followed by increasing doses, resulting in, e.g., headaches, cardiac arrhythmias or gastric acid reflux ("heartburn"). In cell culture studies, animal and human intervention trials, we identified the most potent coffee components that (a) stimulate/inhibit gastric acid secretion, (b) act as key chemopreventive and antioxidant compounds, (c) affect the BMR and energy metabolism, and (d) stimulate craving-associated dopamine secretion in neuronal cells.

AGFD 132 Hypoglycemic effect of stilbene glycoside from *Polygonum multiflorum* in KK CgAy/j type 2

diabetic mouse model and its mechanisms Wenping Tang, wenpingt@eden.rutgers.edu, Yue Liu; Shiming Li; Henryk Daun; Mou-Tuan Huang; Chi-Tang Ho Dept. of Food Sci., Rutgers Univ., New Brunswick New Jersey Dept. of Chemical Biology, Rutgers Univ., Piscataway New Jersey *Polygonum multiflorum* (PM) has long been used as a tonic and anti-aging agent in traditional Chinese medicine. Its major active compound, 2,3,5,4'-tetrahydroxystilbene 2-O- β -glucopyranoside (stilbene glycoside, SG) with strong antioxidant and anti-inflammatory activities, is hypothesized to have antidiabetic effect. Recent results show that SG does not alter hyperglycemia in type 1 diabetic rodent model, therefore in this study we evaluated its hypoglycemic effect in type 2 diabetes with KK CgAy/j transgenic mouse model. At the end of the 7-week study, mice feeding on 0.075% PM-SG extract had a blood glucose level of 121.6 mg/dl, compared to 233.6 mg/dl in control mice, indicating a remarkable hypoglycemic effect of SG in type 2 diabetes ($p < 0.003$). We explored possible mechanisms by evaluating the effect of SG on proinflammatory cytokines which are closely associated with insulin resistance. The levels of plasma insulin, insulin-like growth factor and AMP-activated protein kinase in the liver were also investigated.

AGFD 133 Pesticide residues in food: The role of dietary risk assessment Mary G. Panek, mary.panek@basf.com,

Crop Protection Division, BASF Corporation, Research Triangle Park North Carolina The media often highlights pesticide residues found in fruits and vegetables. How do scientists outside the agricultural industry interpret this information? Section 408 of the Federal Food, Drug, and Cosmetic Act (FFDCA) authorizes EPA to set tolerances for pesticide residues on foods. The agency can set a tolerance only if EPA scientists determine the tolerance is "safe", i.e. "there is a reasonable certainty that no harm will result from aggregate exposure to the pesticide chemical residue including all anticipated dietary exposure and all other exposures for which there is reliable information" (FFDCA definition). The EPA and industry use U. S. food consumption data and residues measured in field trials and monitoring programs to determine exposure. The exposure for the total population or subpopulation such as children is combined with acute or chronic toxicological endpoints to determine safety levels. This presentation gives a basic overview of dietary risk assessment as performed in the U. S.

AGFD 134 Secondary standards – barrier or benefit? Jane M Stewart, jane.stewart@basf.com Environmental and

Consumer Safety, BASF, Research Triangle Park NC The increasing demands of consumers and the influence of non-governmental organizations have driven food retailers to set their own private standards concerning not only food quality, but also pesticide residues in food, and social and environmental issues along the production chain. These private or commercial standards, known as secondary standards, are generally more restrictive (e.g. requiring lower levels of pesticide residues) than official regulatory or import requirements. Secondary standards based on pesticide residue levels are generally based on emotive or hazard-based criteria and not associated to dietary risk evaluations. Some retailers believe that these standards can help suppliers improve the quality of their products and provide a competitive edge. Other stakeholders believe that the costs of complying with these additional standards create an excessive burden for small-scale producers and developing countries, and thus a trade barrier in the market.

AGFD 135 Remediation of fungicide residues on fresh produce using gaseous ozone Spencer S Walse,

spencer.walse@ars.usda.gov, San Joaquin Valley Agricultural Sciences Center, USDA-ARS, Parlier CA Ozone fumigation was explored as a means for degrading organic fungicide residues on fresh produce. Fungicides sorbed onto model abiotic glass surfaces or onto grape berries were fumigated separately in a flow-through chamber. The relative degradation of fungicides on berries at gaseous ozone concentrations of 900 ± 12 ppmv (mLL⁻¹) over 2 h was similar to that on glass; reductions were observed for only fenhexamid (~ 64%), cyprodinil (~ 38%), and pyrimethanil (~ 40%). Boscalid and iprodione levels did not change significantly based on a single factor analysis of variance (ANOVA) at the 95% level of confidence ($p = 0.05$). The kinetics and mechanism of gaseous ozonation, supported by gas chromatography- and liquid chromatography-mass spectrometry product analyses, is discussed in the context of facilitating compliance with maximum residue level (MRL) tolerances. AGFD 136 Creating and Marketing More Sustainable Food Consumer Goods Cristian Barcan(1), cristian.barcan@partners.basf.com, 16050 Northcliff Sq, Elbert Colorado 80106, US . (1) Most global predictions indicate that there will be at least 9 billion people in the world by year 2050. This will create additional challenges for the food industry on

producing consumer goods that are safe, affordable, socially responsible, and without additional burden on the environment and its resources. To address this challenge, consumer goods/brands have to become more sustainable over time in areas such as safety, environmental impact, social aspects, and costs of ownership. We will explain how a set of traceability and sustainability measurements and self-improvement tools - combined with an independent product sustainability standard and certification program - can help food manufacturers and brand owners create and market more sustainable goods. The S.E.T.® toolset also helps brand owners comply with the vertical product sustainability standard ProSustain® currently held by Det Norske Veritas (DNV).

AGFD 137 Phytochemical absorption and metabolism in food based cancer prevention studies Steven Schwartz, SCHWARTZ.177@OSU.EDU, Columbus, Ohio Several research investigations at Ohio State Univ. are focused on food based interventions targeted toward cancer prevention. Collaborations among investigators in various disciplines contribute to a “Crops to the Clinic” theme to develop functional food products for these studies. Research in our laboratory involves LC/MS/MS measurement of potentially bioactive phytochemicals and their metabolites as markers of intake in pre-clinical and human pilot food based interventions. Identification of metabolites may also assist in an understanding of biological mechanisms and additionally the bioavailability of phytochemical compounds that might previously be considered poorly absorbed from the diet. Results to be discussed include pre-clinical and human trials that incorporate phytochemicals present in tomatoes, soy, berries and cruciferous vegetables.

AGFD 138 The Evolution of Food Polyphenolics from Color and flavor problems to Health Benefits John W Finley, jfinley@agcenter.lsu.edu; Jack Losso; Zhimin Xu Dept. of Food Sci., Louisiana State Univ. The Journal of Agricultural and Food Chemistry has been a leading source of papers in the evolution of the study of the importance of polyphenolics in foods. Early studies focused on the negative effects on color and flavour of foods. Then for several years it has been hypothesized that the protective mechanism of the antioxidants was that they quenched free radicals or broke oxidative chain reactions. The prevention or removal of the oxidized compounds and or radicals would lead to better health outcomes. There is a growing body of evidence suggesting that plant based polyphenolic antioxidants may help prevent or delay onset of a multiplicity of disease. For several years it has been hypothesized that the protective mechanism of the antioxidants was that they quenched free radicals or broke oxidative chain reactions. The prevention or removal of the oxidized compounds and or radicals would lead to better health outcomes. Newer work suggests that a variety of polyphenolics can alter expression of genes in the inflammatory pathway. This is a very compelling hypothesis which is supported by studies in cell cultures of various tissues where addition of polyphenolic significantly alters inflammatory gene expression as well as frequently promoting apoptosis in cancer cells. The concern with many of these studies is that the polyphenolics are delivered directly to the cells. Data also show that the absorption of the polyphenolics is very limited. In addition there is only limited data on the possible metabolites of the polyphenolics and the bound materials or metabolites interact in various tissues

AGFD 139 Agricultural Chemistry's Toolset for the 21th Century J. Bruce German, jbgerman@ucdavis.edu, Univ. of California, Davis The field of Chemistry revolutionized science in the 20th century and its applications transformed the human condition. Analytical chemistry defined the principles of molecular and mechanistic experimentation and was central to the discoveries of biochemical pathways, essential nutrients and commodity compositions. Now, life sciences are shifting emphasis towards understanding human health in literally individual detail as agriculture strives to maximize the potential health and performance of each individual while minimizing their impact on the environment. This new era of sustainability, genetic diversity and the prevention of disease will challenge life science research's basic principles, our toolsets and their applications. Research must move from strategies where reductionist experiments identified single targets to integrative models capable of providing complex solutions of entire systems. Similarly, the analytical power of chemistry is guiding research and development into the complex mechanisms underlying chronic diseases, the multi-factor diagnostics to identify those at risk from them, to dietary solutions to resolve and prevent them. The goal of bringing this chemistry to personalizing health is challenging the scientific community to continuously innovate with instrumentation platforms of unprecedented analytical power, efficiency, sensitivity and diversity. Agriculture in the next 3 decades must itself rise to the challenge of providing the means to nourish 9 billion people as a sustainable system that simultaneously improves the environment. This challenge will also require the tools of life sciences that reveal evolution in molecular detail and provide insights into behaviour of individual organisms and entire ecosystems. In this future, chemistry will continue to be the core of Agriculture and Life Sciences.

AGFD 140 Translating the Basic Science of Sulforaphane Action into a Healthy Broccoli Meal Elizabeth H Jeffery, ejeffery@uiuc.edu, Univ. of Illinois, Cell culture studies show us the complexity of sulforaphane action in preventing carcinogenesis, inflammation, cardiovascular disease and more. Animal studies have been used to confirm these mechanisms. Yet epidemiological studies do not consistently show these health benefits in humans. Causes of this lack of reproducibility include differences in content of bioactives with plant genotype and the growing environment, loss of bioactives during processing and food preparation as well as variation in human response due to genotype. A key concern is the need to release the sulforaphane from its thioglycoside form, glucoraphanin. The plant contains the thiohydrolase myrosinase, with a relatively stable form present in broccoli seed, but a heat sensitive form present in the mature vegetable, which can be lost during processing. Sulforaphane bioavailability from a broccoli meal can be improved by an external thiohydrolase source. Bioactivity

of broccoli depends not only upon release of sulforaphane from glucoraphanin, but also upon enhancing effects of other components within broccoli.

AGFD 141 High antioxidant potatoes: Acute in vivo antioxidant source and hypotensive agent in humans

after supplementation to hypotensive subjects Joe A Vinson, vinson@scranton.edu, Cheryl A Demkosky; Duroy A Navarre Dept. of Chemistry, Univ. of Scranton, PA Vegetable and Forage Crops Research Laboratory, USDA -Agricultural Research Service, Prosser WA Potatoes are the most consumed vegetable in the US diet. Pigmented potatoes have high concentrations of antioxidants including phenolic acids, anthocyanins and carotenoids. In a single dose study we gave normal fasting subjects 6-8 small microwaved purple potatoes or an equivalent amount of potato starch in the form of biscuits. Post-prandial plasma and 24-hour urine antioxidant capacity was increased by the potatoes and decreased by the starch, i.e. potatoes were in vivo antioxidants and starch was a prooxidant. In a crossover study 18 hypertensive subjects, average BMI 29, consumed either 6-8 purple potatoes twice daily or no potatoes in their normal diet for 4 weeks and then crossed over to the other regimen. Potatoes did not change body weight, lipids or HbA1c. Diastolic blood pressure was significantly decreased by potatoes, -4.3%, a 4 mm decrease. Systolic blood pressure decreased 3.5%. This blood pressure drop occurred in spite of the fact that 14/18 subjects were concomitantly taking blood pressure medication. Thus purple potatoes are an effective hypotensive agent and lower the risk of heart disease and stroke in hypertensive subjects without a weight gain.

AGFD 142 Role of dietary factors and phytochemicals in colon cancer risk Ruth S MacDonald,

ruthmacd@iastate.edu, Dept. of Food Sci. and Human Nutrition, Iowa State Univ., Ames Among the common forms of cancer, colon cancer incidence is the most highly correlated with diet and lifestyle factors. Many foods and food components have been implicated as mediators of colon cancer risk. These include dietary proteins, fiber and lipids and several classes of plant derived compounds. The colonic environment is mediated by the microbial population which is, in part, influenced by dietary factors. Recent evidence suggests that specific dietary components and phytochemicals may influence the colonic environment in ways that may impact colon cancer progression. By examining cellular events that are influenced by dietary components, potential mechanisms that are involved in the carcinogenic pathway may be defined. These include altering the colonic microbial population, affecting mucosal barrier function, moderating inflammatory systems and interacting with hormonal pathways. Using mouse models, the influence of food-derived compounds have been investigated with the goal of identifying protective components and their mechanisms of action.

AGFD 143 Lemon oil solubilization in mixed surfactant solutions: Rationalizing microemulsion and

nanoemulsion formation Jijia Rao, jiajiaor@foodsci.umass.edu, Davis Julian McClements Dept. of Food Sci., University of Massachusetts, Amherst Massachusetts Lipophilic functional ingredients are usually incorporated into aqueous-based foods in the form of colloidal dispersions. In this study, we investigated the rate and extent of solubilization of emulsified lemon oil in mixed non-ionic surfactant solutions: sucrose monopalmitate (SMP) and/or Tween 80 (T80). The influence of surfactant concentration, type, and mixing ratio on lemon oil solubilization was investigated. The lemon oil solubilization process was rapid (< few minutes), with the rate increasing with increasing surfactant concentration. For a particular surfactant type and concentration, lemon oil was transferred from emulsion droplets into microemulsion droplets until a critical lemon oil concentration (C_{sat}) was reached, after which it remained as emulsion droplets. The value of C_{sat} increased with increasing surfactant concentration and was higher for SMP than for T80. This study provides important information for the rational design of food grade colloidal delivery systems for delivering functional lipids for food and beverage applications.

AGFD 144 Computationally modeled self-assembly of higher order structure of collagen peptides Fei Xu,

feixu@cabm.rutgers.edu, Vikas Nanda Dept. of Biochemistry, Univ. of Medicine and Dentistry of New Jersey, Piscataway Center for Advanced Biotechnology and Medicine, Rutgers Univ., Piscataway New Jersey Collagen organized into fibers and matrices has been widely utilized as biomaterial in encapsulation of drug and nutritional supplements due to its high biocompatibility and low toxicity. Self-assembly of synthetic collagen peptides into higher order structures is an important step toward construction of collagen matrices. We use computational de novo design to develop self-assembling collagen-like peptides. The resulting peptides form nano-scale structures with multiple phases, i.e. cold-induced aggregates corresponding to well-ordered fibers at low concentrations and hydrogels at high concentrations. The hydrogels show a spectrum of morphology and gelation properties depending on peptide composition. Computational models predict that this process is well controlled self-assembly induced by sticky-ended intermediates. This prediction is supported by structural and biophysical characterizations, i.e. Circular Dichroism, Small-Angle X-ray diffraction, Electron Microscopy. Micro-rheology characterization and morphology studies with Scanning Electron Microscopy help us understand the relationship between the gelation properties and the primary sequences of peptides.

AGFD 145 Metabolic study on reducing effect of functional milk formula on lead exposure in mice Jingjing

Jiao, jingjing_jiao@yahoo.com. Zhejiang Univ., Hangzhou Zhejiang, China Lead poisoning is presently the most common disease of environmental origin throughout the world. Many researches discussed harmful effects of excess lead exposure. Nevertheless, few studies focused on finding effective ways to reduce lead exposure. ICR male mice were administered an intra-peritoneal injection of 7 mg Pb/kg-bw each day in two continuous weeks. Mice under high lead exposure were orally

administered with functional milk (10 mL/kg), which was made of powdered milk with addition of Vc, calcium lactate, ZnSO₄, FeSO₄ and polyphenols. The addition levels were according to China National Standard of Food Enrichment. The blood of mice in each group was collected periodically by retroorbital bleeding. Finally, mice were killed by dislocation and their brains, livers, kidneys and femurs in each group were collected. Pb, Ca, Fe and Zn levels in all of collected samples were determined. Blood kinetic study indicated that Pb level was significantly reduced by averagely 69.5% compared to the control group during the whole feeding process. Metabolic study suggested that Pb is preferably absorbed in the blood and excreted via the urine after its metabolism in enterohepatic cycle. Pb levels in liver and kidney administered with functional milk were also reduced by 61.2% and 37.9% respectively while Pb levels in brains and femurs were not significantly reduced ($P > 0.05$). Meanwhile, Ca, Fe and Zn levels in all of samples were not significant difference compared to the control group ($P > 0.05$). This metabolic study found that the functional milk accompanying with addition of selected food enrichments has a great potential on reducing lead exposure and such recipe doesn't affect the absorption of essential trace elements in mice. This study has important significance for the researches on preventing excess lead exposure in vivo.

AGFD 146 Complete structural elucidation of isomeric forms of malonylglucoside isoflavones Vamsidhar Yerramsetty, yerra005@umn.edu, Baraem Ismail Food Sci., Univ. of Minnesota, St Paul MN Malonylglucosides undergo interconversions when subjected to thermal processing. In addition to nonconjugated glucosides, interconversion to isomeric forms of malonylglucosides in heated buffer and soymilk systems was reported. Complete structural elucidation of the isomers is important to determine their biological significance. Malonylglucoside isomers were isolated from soy grits and subjected to nuclear magnetic resonance analysis. Upon comparison of the proton spectra of malonylglucosides and their isomers, minor differences were observed in the glucose region. Heteronuclear multiple-bond correlation spectroscopy experiments indicated a downfield shift of the H-4'' proton of the glucose ($\delta\text{H-4}'' = 4.90$) in the isomers spectra, whereas, a similar effect was observed for H-6'' protons in malonylglucosides ($\delta\text{H-6}'' = 4.27; 4.55$). This indicates that the malonate group is present on the 4th carbon of the glucose moiety of the isomers (4''-O-malonylglucoside) as compared to 6th carbon of that of the malonylglucosides (6''-O-malonylglucoside).

AGFD 147 Probing rearrangements occurring in casein micelles during concentration: Addition of soluble caseins Pulari Krishnankutty Nair pkrishna@uoguelph.ca, Milena Corredig Dept. of Food Sci., Univ. of Guelph, Ontario Canada Dept. of Dairy Development, Guelph Ontario Canada This research aimed at determining if rearrangements occur in casein micelles during concentration. Milk was concentrated using osmotic stressing and soluble caseins (sodium caseinate) were added at 0.2% before or after concentration. Rennet induced sol gel transitions were then studied, as rennet specifically hydrolyzes k-casein, present on the surface of the casein micelles, imparting steric stability. The formation of the rennet-induced gel was followed using rheology and diffusing wave spectroscopy. After 120 minutes of gelation, the gels showed the highest elastic modulus for concentrated milk, and 382 ± 41 and 5 ± 5 Pa for the milk with sodium caseinate added before and after, respectively. Soluble caseins inhibited rennet-induced aggregation, but when added after concentration. This confirmed the hypothesis that rearrangements occur during concentration. These results bring a better understanding of the effects of concentration of milk processing functionality, and of the possible use of casein micelles as functional delivery systems.

AGFD 148 Assessment of Groundwater Contamination in Agriculture areas through lysimetric studies Tanu - Jindal, tjanujindal@gmail.com, Amity Inst. of Environmental Toxicology, Safety and Management, Noida Uttar Pradesh, India Unlined drains and excessive use of agrochemicals are the major threat for surface water and groundwater through leaching. Contamination in groundwater lasts for several years irreversibly. To know the point source of groundwater contamination lysimetric studies were undertaken in the agriculture area. The leachate from the lysimetric experiment showed calcium hardness 3878.4 mg/l, total hardness 5161.1mg/l, total dissolved solids 10920 mg/l, nitrite 21.3 mg/l, nitrate 1153.9 mg/l, electrical conductivity 16014 $\mu\text{mhos/cm}$ against the WHO permissible limits of 100mg/l, 500mg/l, 1000mg/l 0.1mg/l, 45 mg/l and 1400 $\mu\text{mhos/cm}$ respectively. However BOD was almost near and COD was much below the WHO permissible limits. Heavy metals organochlorines, organophosphates, synthetic pyrethroids, PCB's and PAHs were not detectable and were under the safe limits. Study reveals that contamination increases the hardness, nitrate, nitrite concentration, electrical conductivity and COD of groundwater at alarming levels and makes it unfit for drinking posing health risks.

AGFD 149 Composition of the essential oil from *Artemisia vulgaris* L. grown in Pennsylvania, USA and its apoptosis-dependent antitumor activity in promyelocytic leukemia cell line HL-60 Jack D. Williams, jwilliams@mercyhurst.edu; Ayman Saleh; Dom N. Acharya Chemistry and Biochemistry, Mercyhurst College, Erie PA Dept. of Biochemistry, Lake Erie College of Medicine and School of Pharmacy, Erie PA Extracts from the aerial parts of *Artemisia vulgaris* L. grown in Erie Pennsylvania USA, were obtained by hydro-distillation of the fresh leaves and buds. The major volatiles present in the oils were identified using GC-MS and compared to those from *Artemisia vulgaris* L. originating outside of the US. Leaf oil was rich in Germacrene D (25%), Caryophyllene (20%), α -Zingiberene (15%), and α -Humulene(5%). Bud oil contained 1,8-Cineole (32%), Camphor (16%), Borneol (9%), and Caryophyllene (5%). A trace amount of trans-2-hexenal, which has not been reported previously, was also found. The extracts induced apoptosis in HL60-cells. AGFD 150 Detection of Shiga toxin-producing *E. coli* in Environmental samples by Immune-PCR Xiaohua He(1), xiaohua.he@ars.usda.gov, 800 Buchanan St, Albany California 94710, US ; Baetrix Quinones(1); Stephanie McMahon(1);

Michael Cooley(1); Robert E. Mandrell(1). (1) Detection of Shiga toxin producing Escherichia coli (STEC) in the environment remains difficult because the numbers of bacteria in samples often are below the detection threshold of the method. We developed an immuno-polymerase chain reaction (IPCR) assay for the detection of Shiga toxin 2 (Stx2). The qualitative detection limit of the assay is 0.1 pg/mL in phosphate buffered saline (PBS) with a quantification range of 10 to 100,000 pg/mL. The IPCR method was 10,000-fold more sensitive than an analogue conventional enzyme-linked immunosorbent assay in PBS. Application of the IPCR assay to 23 enriched cultures of feces, feral swine colon, soil and watershed samples collected from the environment revealed that the IPCR detected Stx2 in all 15 samples that were shown to be STEC-positive by real-time PCR and culture methods. The modification of the IPCR will be useful for evaluating the occurrence of STEC in the environment.

AGFD 151 Comparative analysis of over the counter milk thistle commercial herbal extracts Mahmoud A. Saleh, saleh_ma@tsu.edu, Houston Texas 77004, US Comparative analysis of over the counter milk thistle commercial herbal extracts Milk thistle has been used for centuries to treat acute and chronic liver diseases and, even today, is one of the most widely used herbal medications. Its active ingredients consist of several closely related flavinoids, collectively known as silymarin. 24 different commercial brands of milk thistle extracts were purchased from local markets and analyzed for their chemical constituents using HPTLC, HPLC and LCMS. All products showed great variation in their contents of the silymarin isomers. Identification of the chemical constituents were done based on their chromatographic motilities (Rf & tR) and confirmed by mass spectrometry. Antioxidant activities were also evaluated for all of the products using radical scavenging assay with DPPH reagent

AGFD 152 Nutritional and nutraceutical properties of strawberry guava and common guava Kayanne McCook-Russell, kayanne.mccook02@uwimona.edu.jm, UWI, Mona, Kingston West Indies Kingston 7, Jamaica . In our ongoing quest to phytochemically characterize and discover the nutraceutical properties of exotic Jamaican fruits, we undertook research on strawberry guavas (*Psidium cattleianum*), and compared them to the popularly known *Psidium guajava* (guava). Strawberry guavas demonstrated three times the antioxidant activity (1130 trolox equivalence/100g FW) and twice the levels of total polyphenols and vitamin C exhibited by their counterpart. Triterpenoids (ursolic and oleanolic acids, and their 2a-hydroxy analogues), citric acid and other compounds were isolated from the fruit extracts of *P. cattleianum* for the first time. Their hexane and ethyl acetate extracts showed low anti-inflammatory activity, as determined by COX enzyme inhibitory assay, while a mixture of 2a-hydroxyursolic and 2a-hydroxyoleanolic acids showed moderate activity. The ethyl acetate and methanol extracts of *P. guajava* also demonstrated anti-inflammatory activity. Our results demonstrate that *Psidium cattleianum* is superior to *Psidium guajava* in several ways, and should be exploited for its health-beneficial properties.

AGFD 153 Mood and mood disorders: Current the rapies, alternative medicine and computational studies Karina Martinez-Mayorga, kmartinez@tpims.org, Fabian H. Lopez-Vallejo; Jose L. Medina-Franco; Terry L. Peppard. Torrey Pines Inst. for Molecular Studies, Port St Lucie FL Robertet Flavors, Inc., Piscataway NJ Mood is an emotional state in constant change. Mood disturbances include depression and bipolar disorder. According to WHO, 13-20% of the world's population exhibit depressive symptoms (lower quality of life, disability, etc.). We examined reports of mood and mood disorder published since 2000, focusing on three aspects: current treatments, complementary and alternative medicine (CAM) and computational studies. The primary database was SciFinder, complemented by Web of Science, PubMed, Cochrane Library and Google Scholar. Keywords searched (alone or combined) yielded the following frequencies: Mood disorder (53), bipolar disorder (45), depression (153), antidepressant (134), CAM (17), aromatherapy (22), aromachology (10), computational chemistry (3), molecular modeling (28), chemoinformatics (4), virtual screening (14), docking (25) and QSAR (16). We obtained >170 original articles and reviews. Analysis of this information is presented. Overall, systematic and comparative studies are required. The use of computational methods and data mining will be invaluable.

AGFD 154 Screening of small molecules and pectin present on the rind of bacuri (*Platonia insignis*) an Amazonian fruit. Edy S Brito, edy@cnpq.embrapa.br; Williams P Batista; Kirley M Canuto; Rosa V. S. Mamede Embrapa Tropical Agroindustry, Fortaleza, Brazil Bacuri (*Platonia insignis*) is an amazonian fruit with a pleasant scented pulp. However, its yield is in the range of 15 to 20% and 65% of rind. Therefore, in this work we screened the bacuri rind in such a way to propose further use of this material. The apolar extract (11.7% d.w.) composed of a yellow oleoresin was analyzed by GC-MS and revealed isoprenoid derived compounds. The polar extract (3.8% d.w.) was fractionated yielding a major compound, which was identified by NMR and MSn, as the biflavonoid morelloflavone. Finally, the residue was extracted with ammonium oxalate to obtain pectin (37.6% d.w.), which rheological properties were measured indicating a similar pattern to citrus pectin.

AGFD 155 Acidic polysaccharide analysis by high performance liquid chromatography Xun Yan, xun.yan@amway.com, Access Business Group LLC, Ada MI Hyaluronic acid and chondroitin are two common acidic polysaccharides that distribute widely in connective, epithelial and neural tissues. Commercially, hyaluronic acid and chondroitin are used as nutrition supplements, food additives and medical treatments. Hyaluronic acid is a copolymer of glucuronic acid and glucosamine. Chondroitin is comprised of glucuronic acid and galactosamine with various levels of

sulfation. The direct analysis of acidic polysaccharides is difficult due to the wide distribution in the degree of polymerization. Several analytical methods have been studied in the past, including capillary electrophoresis and size-exclusive chromatography. However, these methods lack satisfactory selectivity. This paper will discuss our studies on analyzing hyaluronic acid and chondroitin. Specifically, the method will use acidic hydrolysis, pre-column derivatization and reverse phase HPLC to quantitate these components.

AGFD 156 Diterpenes profile in coffee: Influence of roasting process Rafael C E Dias, rafael.rafaeltam@gmail.com, Adelia F Faria; Adriana Z Mercadante; Neura Bragagnolo; Marta T Benassi Dept. of Chemistry, Instituto Federal Catarinense, Araquari Santa Catarina, Brazil Dept. of Food Sci., Universidade Estadual de Campinas, Campinas São Paulo, Brazil Dept. of Food Sci. and Technology, Universidade Estadual de Londrina, Londrina Paraná, Brazil *Coffea arabica* (Arabica) and *Coffea canephora* (Robusta) are the main commercial species of coffee. Arabica coffee has superior quality and is highly commercially valued. Kahweol and cafestol are diterpenes with physiological effects and potential to discriminate species. These compounds are partially stable during roasting, but dehydroderivatives can be formed. Both diterpenes were quantified in Arabica and Robusta coffees with different roasting degrees. The amount of diterpenes and their structures were verified (HPLC-PDA-APCI/MS/MS). In dark roast samples dehydroderivatives were identified. The roasting process influenced the levels of diterpenes similarly in both species, but the effect was dependent on the intensity of process. Cafestol and kahweol were degraded in dehydrocafestol and dehydrokahweol, respectively, after 8 min (commercial roasting). However, the amounts of diterpenes remained stable during the roasting due to relative increase of lipid concentration. This enhances the potential of using the diterpenes as discriminant between Arabica and Robusta in blends roasted in different degrees.

AGFD 157 Synthesis and evaluation of molecularly imprinted polymer microspheres used as detection for Erythromycin Ethylsuccinate in food Jiandu Lei, jiandul@stanford.edu, No.1, 2st North Street, Zhongguancun, Haidian District, Beijing Beijing, China National Key Laboratory of Biochemical Engineering, Inst. of process engineering, CAS, Beijing Beijing China The preparation and evaluation of molecularly imprinted polymer (MIP) microspheres for Erythromycin Ethylsuccinate (EEs) by aqueous suspension polymerization is reported for the first time in this study. The MIPs were prepared by using EEs as template molecule, methacrylic acid (MAA) as functional monomer, ethylene glycol dimethacrylate (EDMA) as cross-linker. The morphological of MIPs was characterized by scanning electron microscopy. The analysis showed that the diameter of the prepared MIPs can be controlled within about 60 μ m. The binding behavior of the template EEs on the MIPs was evaluated by UV-Vis spectrophotometric analysis. The selectivity analysis indicated that MIPs had a good selectively adsorption ability to EEs. In addition, the imprinted microspheres were used to detect EEs in milk, the good selectivity and high recovery were obtained.



International Year of
CHEMISTRY
2011

Mark your calendar for the
243rd ACS National Meeting
in San Diego
March 25 - 29, 2012



International Year of
CHEMISTRY
2011

from -
DIVISION OF AGRICULTURAL & FOOD CHEMISTRY
AMERICAN CHEMICAL SOCIETY
1155 16TH STREET, NW
WASHINGTON DC 20036



t
h
e

CORNUCOPIA

AGFD