

242nd ACS National Meeting, Denver, CO

Program Chair, Shana Sturla

Sunday, August 28, 2011

General Papers (08:00 AM - 12:00 PM) Room 207, Colorado Convention Center

08:00 AM

Carcinogenic nitrosamines in U.S. cigarettes: Three decades of remarkable neglect by the tobacco industry

Irina Stepanov PhD, Aleksandar Knezevich, Liqin Zhang PhD, Clifford H. Watson PhD, Dorothy K. Hatsukami PhD, Stephen S. Hecht PhD. Masonic Cancer Center and Tobacco Use Research Programs, University of Minnesota, Minneapolis, MN, United States; Centers for Disease Control and Prevention, Atlanta, GA, United States

08:25 AM

Progress towards personalized chemotherapy: Correlation of Pt-DNA adduct levels and clinical response in bladder and lung cancer patients undergoing platinum-based chemotherapy

Paul Henderson PhD. Department of Internal Medicine, Division of Hematology and Oncology, University of California Davis, Scaramento, CA, United States

08:45 AM

Quantitation of DNA adducts using high resolution mass spectrometry

Peter W Villalta PhD, Silvia Balbo PhD, Stephen S Hecht PhD. Cancer Center, University of Minnesota, Minneapolis, Minnesota, United States

09:05 AM

Protein targets of alkynyl analogs of 4-hydroxy-2-nonenal and 4-oxo-2-nonenal in a human monocyte cell line

Simona G Codreanu PhD, Daniel C Liebler PhD. Department of Biochemistry, Vanderbilt University, Nashville, TN, United States

09:25 AM

Hole injection and migration in nucleosomal DNA is different than in free DNA

Dr Yang Liu, Prof Nicholas E Geacintov, Prof Vladimir Shafirovich. Department of Chemistry, New York University, New York, New York, United States

09:45 AM

Identification of damage lesions derived from the 3'-deoxy-C3'-thymidiny radical

Amanda C Bryant-Friedrich PhD, Buthina Abdallah, Suaad Abdallah, Cheryl Ann Love, Kevin Trabbic. Department of Medicinal and Biological Chemistry, University of Toledo, Toledo, OH, United States; Department of Chemistry, Oakland University, Rochester, MI, United States

10:05 AM Intermission

10:20 AM

LC-MS/MS for assessing the formation, repair, and transcription mutagenesis of purine cyclonucleosides

Jin Wang, Changjun You, Jianshuang Wang, Candace Guerrero, Yinsheng Wang. Chemistry, University of California Riverside, Riverside, CA, United States

10:40 AM

DNA alkylation with quinolinium quinone methide: Mutagenic or suppressive?

Prof Qibing Zhou. College of Life Science and Technology, Huazhong University of Science and Technology, Wuhan, Hunang, China

11:40 AM

Conformational mapping of arylamine-DNA adducts: Structure-function-relationships

Bongsup Cho, Satyakam Patnaik, Vipin Jain, Vaidyanathan Ganesan. Department of Biomedical and Pharmaceutical Sciences, University of Rhode Island, Kingston, RI, United States

Founders Award (01:30 PM - 05:00 PM), Room 207 Colorado Convention Center

01:30 PM

Introductory Remarks. D. Liebler.

01:35 PM

Title: Award Presentation. F. Beland

01:40 PM

Control of cytochrome P450 catalysis by the proximal iron ligand

Santhosh Sivaramakrishnan PhD, Hugues Ouellet PhD, Paul R. Ortiz de Montellano PhD. Department of Pharmaceutical Chemistry, University of California, San Francisco, San Francisco, CA, United States

02:15 PM

Mechanism and protection against acetaminophen-induced hepatotoxicity

Andrew D Patterson, Yatrik M Shah, Frank J Gonzalez. Laboratory of Metabolism, National Cancer Institute, Bethesda, MD, United States

02:50 PM

Drug metabolism: A critical element of contemporary drug safety assessment

Dr. Thomas A Baillie PhD, DSc. School of Pharmacy, University of Washington, Seattle, WA, United States

03:25 PM

Title: Intermission

03:40 PM

Insights into efficiency and specificity of bypass synthesis by Y-class DNA polymerases from X-ray crystallography

Professor Martin Egli PhD. Department of Biochemistry, Vanderbilt University, Nashville, Tennessee, United States

04:15 PM

Interactions of damaged DNA with DNA polymerases

Professor F. Peter Guengerich PhD. Department of Biochemistry and Center in Molecular Toxicology, Vanderbilt University School of Medicine, Nashville, Tennessee, United States

Monday, August 29, 2011

Young Investigator Symposium (08:00 AM - 11:40 AM), Room: 207

08:00 AM

Title: Introductory Remarks. S. Balbo

08:05 AM

Use of an aldehyde reactive probe to capture protein carbonyls

Charles G Knutson PhD, Ujjal Sarkar PhD, John S Wishnok PhD, Joshua R Korzenik MD, Steven R Tannenbaum PhD. Biological Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; Crohn's and Colitis Center, Massachusetts General Hospital, Boston, Massachusetts, United States

08:20 AM

Base structure and sequence factors influence DNA duplex stability of oligonucleotides containing O^6 -alkylguanosine-pairing synthetic nucleoside probes

Mr. Rahul R Lad, Prof. Shana J Sturla. Department of Medicinal Chemistry, University of Minnesota, Minneapolis, MN, United States; Institute of Food, Nutrition and Health, ETH Zurich, Zurich, Switzerland

08:35 AM

Oxygen-linked 8-phenoxy-deoxyguanosine nucleoside analogs

Heidi A. Dahmann, Prof. Shana J. Sturla PhD. ETH Zurich, Switzerland

08:50 AM

Unusual furanose "West" puckering of (5'S)-8,5'-cyclo-2'-deoxyguanosine in DNA

Dr. Hai Huang, Rajat S. Das, Prof. Ashis Basu, Prof. Michael P. Stone. Department of Chemistry, Vanderbilt University, Nashville, TN, United States; Center in Molecular Toxicology, Vanderbilt University, Nashville, TN, United States; Center for Structural Biology, Vanderbilt University, Nashville, TN, United States; Department of Chemistry, University of Connecticut, Storrs, CT, United States

09:05 AM

Structural investigation of exocyclic deoxyadenosine adducts induced by 1,2,3,4-diepoxybutane

Ewa A Kowal, Uthpala Seneviratne, Susith Wickramaratne, Natalia Tretyakova, Michael P Stone. Department of Chemistry, Center in Molecular Toxicology, Vanderbilt University, Nashville, TN, United States; Department of Medicinal Chemistry and Masonic Cancer Center and Department of Chemistry, University of Minnesota, Minneapolis, Minnesota, United States

09:20 AM Intermission

09:30 AM

Translesion synthesis across N^2 -3-ethenoguanine by microbial and human DNA polymerases

Linlin Zhao PhD, Plamen P Christov PhD, Ivan D Kozekov PhD, Alben Kozekova MS, Carmelo J Rizzo PhD, F. Peter Guengerich PhD. Department of Biochemistry and Center in Molecular Toxicology, Vanderbilt University, Nashville, TN, United States; Department of Chemistry and Center in Molecular Toxicology, Vanderbilt University, Nashville, TN, United States

09:45 AM

Human DNA polymerase κ utilizes a WMSA mechanism for the nucleotidyl transfer reaction

Lee Lior, Lihua Wang PhD, Shenglong Wang PhD, Suse Broyde PhD, Yingkai Zhang PhD. Department of Chemistry, New York University, New York, NY, United States; Department of Biology, New York University, New York, NY, United States

10:00 AM

Replication studies of carboxymethylated DNA lesions induced by *N*-nitroso compounds

Ashley L Swanson, Changjun You PhD, Jianshuang Wang PhD, Yinsheng Wang PhD. Environmental Toxicology Graduate Program, University of California, Riverside, Riverside, CA, United States; Department of Chemistry, University of California, Riverside, Riverside, CA, United States

10:15 AM

Stereochemical aspects of the conjugation of butadiene diepoxide with glutathione by glutathione transferases

Sung-Hee Cho, F. Peter Guengerich. Department of Biochemistry and Center in Molecular Toxicology, Vanderbilt University School of Medicine, Nashville, Tennessee, United States

10:30 AM

Toward the understanding of benzo[a]pyrene (B[a]P) metabolism in human bronchial epithelial cells (HBEC) by a stable isotope dilution tandem mass spectrometry method

Ding Lu, Ronald Harvey, Ian Blair, Anil Vachani, James Kreindler, Trevor Penning. Center for Excellence in Environmental Toxicology, University of Pennsylvania, Philadelphia, PA, United States; Center for Cancer Pharmacology, University of Pennsylvania, Philadelphia, PA, United States; Department of Pharmacology, University of Pennsylvania, Philadelphia, PA, United States; Division of Pulmonary, Allergy and Critical Care, Department of Medicine, University of Pennsylvania, Philadelphia, PA, United States; The Ben May Department of Cancer Research, University of Chicago, Chicago, IL, United States

10:45 AM Intermission**10:55 AM**

QCI/DFT studies of metabolic pathways of hypoxia: Selective heterocyclic di-N-oxide antitumor agent tirapazamine (TPZ) and analogs

Jian Yin, Professor Rainer Glaser PhD, Professor Kent S Gates PhD. Chemistry, University of Missouri, Columbia, MO, United States; Biochemistry, University of Missouri, Columbia, MO, United States

11:10 AM

Examining the diabetogenic effects of trivalent arsenicals in cultured C2C12 myotubes

Samantha Attard, Jenna Currier, Felecia Walton, Christelle Douillet PhD, Zuzana Drobna PhD, Miroslav Styblo PhD. Department of Nutrition, UNC Chapel Hill, Chapel Hill, NC, United States; Department of Toxicology, UNC Chapel Hill, Chapel Hill, NC, United States

11:25 AM

Computational framework for characterizing biomarkers of organophosphorus insecticide mixture exposure

Mr. Jaime H Ivy, Jesse M Wright, Justin Rogers, Arthur N Mayeno, Michael A Lyons, Brad Reifeld. Chemical and Biological Engineering, Colorado State University, Fort Collins, CO, United States

Human Exposure and Responses to Toxins from the Air and Water (01:30 PM - 03:45 PM), Room 207 Colorado Convention Center**01:30 PM Introductory Remarks****01:35 PM**

Dose-response study of arsenic exposure, blood glutathione, and peripheral blood mononuclear cell DNA methylation in Bangladesh

Dr. Megan N Hall, Ms. Megan Niedzwiecki, Dr. Xinhua Liu, Ms. Julie Oka, Ms. Vesna Slavkovich, Ms. Vesna Ilievski, Ms. Diane Levy, Mr. A Siddique, Mr. Faruque Parvez, Dr. Joseph H Graziano, Dr. Mary V Gamble. Epidemiology, Columbia University, New York, NY, United States; Environmental Health Sciences, Columbia University, New York, NY, United States; Biostatistics, Columbia University, New York, NY, United States

02:15 PM

Biomarkers for the assessment of diabetes associated with chronic exposure to arsenic

Dana Loomis PhD, Luz Maria Del Razo PhD, Gonzalo García-Vargas, Zuzana Drobná PhD, Miroslav Stýblo PhD. Department of Epidemiology, University of Nebraska Medical Center, Omaha, NE, United States; Department of Toxicology, CINVESTAV-IPN, Mexico City, Mexico; Faculty of Medicine, Juarez University of Durango State, Gómez-Palacio, Mexico; Department of Nutrition, University of North Carolina at Chapel Hill, Chapel Hill, NC, United States

02:55 PM Intermission

03:05 PM

Linking arsenic metabolism and toxic effects

David J. Thomas. National Health and Environmental Effects Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, United States

Perspectives Lecture (04:00 PM - 05:45 PM) Room: 207 Colorado Convention Center

04:00 PM: Introductory Remarks

04:05 PM

ToxCast: Application of computational toxicology and high throughput screening to improve chemical safety assessment

Director, NCCT Robert Kavlock. Office of Research and Development, United States Environmental Protection Agency, United States

05:00 PM Reception

3. Tuesday, August 30, 2011

Drug Safety (01:30 PM - 04:50 PM) Room: 207 Colorado Convention Center

01:30 PM

Introductory Remarks. F. Guengerich

01:35 PM

Idiosyncratic drug induced liver injury: From man to mouse to computer

Director Paul Brent Watkins MD. Hamner – University of North Carolina Institute for Drug Safety Sciences, Research Triangle Park, North Carolina, United States

02:20 PM

Screening for drug induced liver injury potential

Dr J Gerry Kenna PhD. Safety Assessment UK, AstraZeneca, Alderley Park, Cheshire, United Kingdom

03:05 PM Intermission

03:20 PM

Kidney injury biomarkers in urine: From rats to regulatory approvals

David Gerhold, Frank Dieterle, Josef Ozer, Daniel Holder, Sean Troth, Warren Glaab, Wendy Bailey, Frank Sistare. NIH Chemical Genomics Center/National Center for Advancing Translational Sciences, present address: National Institutes of Health, Rockville, MD, United States; Safety Assessment/Molecular & Investigative Toxicology, Merck & Co. Inc., West Point, Pennsylvania, United States; Global Program Diagnostics, Novartis Pharma, Basel, Switzerland; Pharmacokinetics, Dynamics, and Metabolism, PGRD, present address: Pfizer, Andover, Massachusetts, United States; Department of Biometrics, Merck & Co. Inc., West Point, Pennsylvania, United States

04:05 PM

Role and influence of trans-membrane transporters in toxicity

William W Johnson. GlaxoSmithKline, United States

General Posters (07:30 PM - 09:30 PM)

Hall D, Colorado Convention Center

Selective monohydrolysis of (*E*)-1,1,4,4-tetramethoxybut-2-ene

Yahua Liu, Lawrence M Sayre. Department of Chemistry, Case Western Reserve University, Cleveland, OH, United States

Selective estrogen receptor modulators (SERMs) inhibit oxidative stress and malignant transformation in breast epithelial (MCF-10A) cells

L.P. Madhubhani P. Hemachandra, Judy L. Bolton, Gregory R. J. Thatcher. Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, College of Pharmacy, 833 S Wood Street, Chicago, Illinois, United States

Lesion topology and nucleotide excision repair: The mobile phenyl ring of C8-dG-PhIP allows NER susceptibility despite absence of a partner nucleotide in a deletion duplex

Hong Mu, Dara A. Reeves PhD, Konstantin Kropachev PhD, Yuqin Cai PhD, Shuang Ding PhD, Lihua Wang PhD, Alexander Kolbanovskiy, Marina Kolbanovkiy, Ying Chen, Assistant Professor Jacek Krzeminski PhD, Professor Shantu Amin PhD, Professor Suse Broyde PhD, Professor Nicholas E. Geacintov PhD. Department of Biology, New York University, New York, NY, United States; Department of Chemistry, New York University, New York, NY, United States; Department of Pharmacology, Pennsylvania State University College of Medicine, Hershey, PA, United States

Insights into the susceptibility of the 10*R* (+)-*cis-anti*-B[a]P-*N*²-dG adduct to human NER: Replacing the normal partner base C by an A mismatch dramatically decreases the efficiency of repair

Hong Mu, Hong Zhang, Shuang Ding PhD, Yuqin Cai PhD, Lihua Wang PhD, Dara A. Reeves PhD, Konstantin Kropachev PhD, Alexander Kolbanovskiy, Marina Kolbanovkiy, Ying Chen PhD, Professor Shantu Amin PhD, Professor Suse Broyde PhD, Professor Nicholas E. Geacintov PhD. Department of Biology, New York University, New York, NY, United States; Department of Chemistry, New York University, New York, NY, United States; Department of Pharmacology, Pennsylvania State University College of Medicine, Hershey, PA, United States

Generation of guanine-thymidine cross-links by peroxyxynitrite, a chemical mediator of inflammation

Dr Byeong Hwa Yun, Prof Nicholas E Geacintov, Prof Vladimir Shafirovich. Division of Environmental Health Sciences, Wadsworth Center, NYS Department of Health, Albany, New York, United States; Department of Chemistry, New York University, New York, New York, United States

Inflammation-mediated nitrosative deamination of RNA: Resistance of adenosine and partition of guanosine to xanthosine and oxanine

Vasileios Dendroulakis, William M. Deen, Peter C. Dedon. Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, United States; Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA, United States

Quantitation of 7-ethylguanine in human leukocyte DNA by liquidchromatography-nanospray ionization-high resolution mass spectrometry

Silvia Balbo, Peter W Villalta, Stephen S Hecht. Masonic Cancer Center, University of Minnesota, Minneapolis, MN, United States

Investigation of cytotoxic and mutagenic effects of the minor groove adduct *O*²-methylthymine

Nisana Andersen, Jianshuang Wang, Yinsheng Wang. Department of Chemistry, University of California Riverside, Riverside, CA, United States

Structural and conformational insights into nucleotide excision repair of 2-acetylaminofluorene-dG adducts by UvrABC

Vipin Jain, Benjamin Hilton, Yue Zou, Paul Chiarelli, Bongsup Cho. Department of Biomedical and Pharmaceutical Sciences, University of Rhode Island, Kingston, RI, United States; Department of Biochemistry and Molecular Biology, East Tennessee State University, United States; Department of Chemistry, Loyola University, United States

Conformational mapping of DNA duplexes containing dG-acetylaminofluorene adduct

Satykam Patnaik, Paul Chiarelli, Bongsup Cho. Department of Biomedical and Pharmaceutical Sciences, University of Rhode Island, Kingston, RI, United States; Department of Chemistry, Loyola University, United States

Kinetics of O^6 -pyridyloxobutyl-2'-deoxyguanosine adduct repair by O^6 -alkylguanine DNA alkyltransferase using capillary HPLC-ESI MS/MS methodology

Delshanee Kotandeniya, Prof. Anthony E Pegg, Prof. Sreenivas Kanugula, Prof. Natalia Y Tretyakova. Department of Medicinal Chemistry and the Cancer Center, University of Minnesota, Minneapolis, Minnesota, United States; Department of Cellular and Molecular Physiology, Milton S. Hershey Medical Center, Pennsylvania State University College of Medicine, Hershey, Pennsylvania, United States

Solution structure studies of aminofluorene-DNA adduct complexed with Klenow fragment and DNA polymerase β

Vaidyanathan Ganesan, Fengting Liang, David Shock, William Beard, Samuel Wilson, Bongsup Cho. Department of Biomedical and Pharmaceutical Sciences, University of Rhode Island, Kingston, RI, United States; Laboratory of Structural Biology, NIEHS, National Institutes of Health, United States

Synthesis and biological evaluation of site-specific DNA lesions of 1,3-butadiene

Susith Wickramaratne, Srikanth Kotapati, Prof. Natalia Tretyakova PhD. The Masonic Cancer Center and the Departments of Medicinal Chemistry and Chemistry, University of Minnesota, Minneapolis, MN, United States

Conformational analysis of the effect of a single C8-arylguanine mutation on the B/Z-DNA equilibrium: An implication of arylhydrazine carcinogenesis

Brian C. Train, Vorasit Vongsutilers, Daniel J. Phillips, Peter M. Gannett. Department of Pharmaceutical and Pharmacological Sciences, West Virginia University, Morgantown, West Virginia, United States; Department of Chemistry, Bethany College, Bethany, West Virginia, United States

Effects of co-administration of γ -glutamylcysteine (GGC) and conjugated linoleic acid (CLA) on oxidative stress in human endothelial cells

Postdoctoral Fellow Yukiko K Nakamura Ph.D., Research Scientist Michael A Dubick Ph.D., Professor Stanley T Omaye Ph.D.. Department of Nutrition, University of Nevada, Reno, Reno, Nevada, United States; U.S. Army Institute of Surgical Research, San Antonio, Texas, United States

Species differences for the stereoselective carbonyl reduction of triadimefon to triadimenol and resulting stereoselective inhibition of cytochrome P450 enzymes

John F Kenneke PhD, Christopher S Mazur, Megan R Holton, Thomas J Sack. National Exposure Research Laboratory, U.S. Environmental Protection Agency, Athens, GA, United States; Region 4, U.S. Environmental Protection Agency, United States; Senior Service America Incorporated, United States

O⁶-alkyl-guanine hybridization probes: Mono- and bi-cyclic3-deazacytosine analogs

Dr. Todor Angelov, Prof. Shana Sturla. Institute of Food, Nutrition and Health, ETH Zürich, Zürich, Switzerland

Ethnic differences in metabolism and DNA adduct formation by 1,3-butadiene

Mr. Srikanth Kotapati, Mr. Dewakar Sangaraju, Dr. Loic Le Marchand MD, PhD, Dr. Natalia Y Tretyakova PhD. Masonic Cancer Center, University of Minnesota, Minneapolis, Minnesota, United States; Cancer Centre, University of Hawai'i, Honolulu, Hawai'i, United States

N⁶-Formylation of lysine: A pathological secondary modification of histone proteins

Bahar Edrissi, Koli Taghizadeh, Peter C. Dedon. Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA, United States; Center for Environmental Health Sciences, Massachusetts Institute of Technology, Cambridge, MA, United States

Redox reactions between cysteines of tubulin and glyceraldehyde-3-phosphate dehydrogenase: Implications for oxidative stress and neurodegeneration

Lisa M Landino PhD, Tara D Hagedorn. Department of Chemistry, The College of William and Mary, Williamsburg, Virginia, United States

Detoxification of Benzo[a]pyrene-7,8-dione by human recombinant SULTs via sulfation of B[a]P-7,8-catechol

Dr. Li Zhang, Prof. Trevor M Penning, Prof. Ian A Blair. Centers of Excellence in Environmental Toxicology and Cancer Pharmacology, Department of Pharmacology, University of Pennsylvania, Philadelphia, PA, United States

Oxidation of furan to a reactive metabolite by human cytochrome P450 enzymes

Leah A Brus, Ding Lu PhD, Lisa A Peterson PhD. Division of Environmental Health Sciences, School of Public Health, & Masonic Cancer Center, University of Minnesota, Minneapolis, MN, United States

Natural antioxidants act synergistically to inhibit lipid peroxidation

Martha A. Hass PhD, Alaa M. Hammad. Arts & Sciences, Albany College of Pharmacy and Health Sciences, Albany, NY, United States

Pyridyloxobutyl DNA adducts and their relationship to tumor formation in the A/J mouse lung model

Anna M Urban MPH, Pramod Upadhyaya PhD, Lisa A Peterson PhD. Division of Environmental Health Sciences, University of Minnesota, Minneapolis, MN, United States; School of Public Health, University of Minnesota, Minneapolis, MN, United States; Masonic Cancer Center, University of Minnesota, Minneapolis, MN, United States

Protein targets of lipid electrophiles from alkynyl linoleic acid

Hye-Young H. Kim PhD, Keri A. Tallman PhD, Ned A. Porter, Daniel C. Liebler PhD. Chemistry, Vanderbilt University, Nashville, TN, United States; Biochemistry, Vanderbilt University, Nashville, TN, United States

Sequence-dependent structural perturbations induced by the β -anomer of the aflatoxin B₁ formamidopyrimidine (FAPY) adduct in DNA

Grad Student Liang Li, Dr. Kyle L Brown, Michelle Y Wang, Amanda Meyers, Professor Michael P Stone. Department of Chemistry and Center in Molecular Toxicology, Vanderbilt University, Nashville, TN, United States; Department of Chemistry, Augustana College, Rock Island, IL, United States

Inhibition and mechanism based inactivation of human cytochrome P450 2A6 and 2A13

Valerie M Kramlinger, Linda B von Weymarn PhD, Sharon E Murphy PhD. Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Twin cities, Minnesota, United States; Masonic Cancer Center, University of Minnesota, Minneapolis, Minnesota, United States

Nevirapine metabolism to 4-formyl-nevirapine: Possible role in nevirapine toxicity

Alexandra M.M. Antunes PhD, Ana L.A. Godinho MSc, Sofia A. Pereira PhD, Gordon Surratt, Gonalo Gamboa da Costa PhD, Frederick A. Beland PhD, M. Matilde Marques PhD. Centro de Química Estrutural, Instituto Superior Técnico; Universidade Técnica de Lisboa, Lisboa, Portugal; Departamento de Farmacologia, Faculdade de Ciências Médicas, Universidade Nova de Lisboa, Lisboa, Portugal; Division of Biochemical Toxicology, National Center for Toxicological Research, Jefferson, AR, United States

Selective enrichment and profiling of low-abundance serum serine hydrolases using click chemistry

Ujjal Sarkar PhD, postdoc associate Charles G. Knutson PhD, John S. Wishnok Ph.D, Professor Steven R. Tannenbaum PhD. Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, United States; Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA, United States

Identification of myeloperoxidase-catalyzed oxidation of tyrosine residues in human serum proteins for a potential inflammatory disease biomarker

Pilsoo Kang, Yu Zeng, John S Wishnok, Steven R Tannenbaum. Department of Biological Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States

Synthesis of modified uridine as a radical precursor for the study of oxidative damage to RNA

Raziya Shaik, Amanda Bryant Friedrich PhD. Department of Chemistry, University of Toledo, Toledo, Ohio, United States

Styrene and its metabolites exhibit potential for multiple-site interaction with CYP2E1

Jessica H Hartman, Gunnar Boysen PhD, Grover P Miller PhD. Department of Biochemistry and Molecular Biology, University of Arkansas for Medical Sciences, Little Rock, AR, United States; Department of Chemistry, University of Arkansas at Little Rock, Little Rock, AR, United States

Non-competitive inhibition of UDP-glucose dehydrogenase by 6-thiopurine and 6-thiouric acid and quantification of the enzymatic formation of UDP-glucuronic acid by UDP-glucose dehydrogenase

Richard M Hyslop PhD, Ryan J. Rafferty. Chemistry and Biochemistry, University of Northern Colorado, Greeley, CO, United States

Thiol-mediated reactivation of oxidatively-inactivated protein tyrosine phosphatase 1B: Kinetics studies

Zachary D. Parsons, Kent S. Gates. Department of Chemistry, University of Missouri, Columbia, Missouri, United States; Department of Biochemistry, University of Missouri, Columbia, Missouri, United States

Optical properties of amylose-encapsulated chromophores

Adjunct professor Sung-Jae Chung Ph.D, student Suk-Won Chung, student Kevin D Ko, student Kim Hyunsoo. School of Arts & Sciences, Marymount University, Arlington, VA, United States; Centreville High School, Centreville High School, Clifton, VA, United States; science and Technology, Thomas Jefferson High School, Alexandria, VA, United States; Department of Biomedical Engineering, Johns Hopkins University, Baltimore, MD, United States

Inflammation induced changes to the serum metabolome

Erin G. Prestwich, I. Ramesh Babu, Koli Taghizadeh, Peter C. Dedon. Biological Engineering, Massachusetts Institute of Technology, Cambridge, MA, United States; Center for Environmental Health Sciences, Massachusetts Institute of Technology, Cambridge, MA, United States

Determination of p53 mutation pattern and spectrum due to B[a]P radical cations in a yeast based reporter system

Sushmita Sen PhD, Zahidur Abedin PhD, Jeffrey Field PhD. Department of Pharmacology, University of Pennsylvania, Philadelphia, PA, United States

Occurrence of algal toxin *Microcystin-LR* in source waters and its removal by *Moringa oleifera* seed extract

Pinar Omur-Ozbek PhD, Victor Sam. Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, CO, United States

Rapid estimation of activation enthalpies for cytochrome-P450-mediated hydroxylations

Dr. Arthur N. Mayeno PhD, Jonathan L. Robinson, Dr. Brad Reisfeld PhD. Department of Chemical & Biological Engineering, Colorado State University, Fort Collins, Colorado, United States; Department of Chemical & Biological Engineering, Princeton University, Princeton, New Jersey, United States

Lack of estrogenic potential of monomers utilized in Eastman Tritan™ Copolyester

James Deyo DVM, PhD, Emmett O'Brien PhD, Steve Green PhD. Product Safety and Health, Eastman Chemical Company, Kingsport, TN, United States; Specialty Plastics Technology, Eastman Chemical Company, Kingsport, TN, United States

Estimation of dermal permeability in untested vehicles based on measured permeability in a reference vehicle

Heather J. Avens, Ken M. Unice, Jennifer Sahmel. ChemRisk, Boulder, CO, United States; ChemRisk, Pittsburgh, PA, United States

"Just in Time" derivatization workflow for GC-MS metabolomics studies

Colleen McNaney, Dr. Serhiy Hnatyshyn PhD, Dr. Michael Reilly PhD, Dr. Dieter Drexler PhD. Department of Applied and Investigative Metabolomics and Department of Discovery Analytical Science, Bristol-Myers Squibb, Wallingford, CT, United States; Department of Applied Investigative Metabolomics and Department of Discovery Analytical Science, Bristol-Myers Squibb, Princeton, NJ, United States

Tailoring microsensor-array composition and operation for biomarkers in simulated exhaled breath

Dr Phillip H Rogers PhD, Dr. Kurt D Benkstein PhD, Dr. Steve Semancik PhD. Materials Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland, United States

Wednesday, August 31, 2011

Human Exposure and Responses to Toxins from the Air and Water (08:30 AM - 11:50 AM), Room: 207 Colorado Convention Center

08:30 AM

State-of-the-Art in Research on Endocrine-Active Chemicals and Perspectives. K. Thayer

08:35 AM

Introduction of Speakers. D. Doerge

08:40 AM

Reproductive and chronic toxicity testing of endocrine-active compounds in rodents

PHARMACOLOGIST Barry K. Delclos Ph.D.. Division of Biochemical Toxicology, National Center for Toxicological Research, Jefferson, AR, United States

09:15 AM

Perinatal PCB exposure and deficits in cognitive function: Parallels between animals and humans

Professor Susan L. Schantz Ph.D.. Department of Comparative Biosciences and Neuroscience Program, University of Illinois at Urbana-Champaign, Urbana, IL, United States

09:50 AM

Human biomonitoring of environmental chemicals

Dr. Antonia M. Calafat Ph.D.. Division of Laboratory Sciences, Centers for Disease Control and Prevention, Atlanta, GA, United States

10:25 AM Intermission

10:40 AM

PBPK modeling of endocrine active chemicals: Linking animal toxicity studies with human exposures

TOXICOLOGIST Jeffrey W. Fisher Ph.D.. Division of Biochemical Toxicology, National Center for Toxicological Research, Jefferson, AR, United States

11:15 AM

U.S. safety assessment of food contact substances

TOXICOLOGIST Michelle L. Twaroski Ph.D.. Center for Food Safety and Applied Nutrition, U.S. Food and Drug Administration, College Park, MD, United States

Bioanalytical Platforms in Biomarker Discovery and Development (01:00 PM - 05:30 PM) Room: 207 Colorado Convention Center

01:00 PM: Introductory Remarks

01:05 PM

Metabolomics techniques for biomarker discovery

Professor Chris Beecher PhD. Pathology, University of Michigan Medical School, Ann Arbor, MI, United States

01:55 PM

Emerging field of lipidomics

Oswald Quehenberger PhD. Departments of Medicine and Pharmacology, University of California, San Diego, La Jolla, CA, United States

02:45 PM

Biomarkers of toxicity: Discovery through NMR-based biochemical profiling

Nelly Aranibar. Bioanalytical and Discovery Analytical Sciences, Bristol-Myers Squibb, Princeton, NJ, United States

03:50 PM

Steroid analysis by LC-MS to monitor toxicity and support toxicological model development

Kara Pearson, Thomas Griffiths II, Yi Yang, Louise Saldutti, Neetesh Bhandari, Alema Galijatovic-Idrizbegovic, William Schaefer. Safety Assessment and Laboratory Animal Research, Merck & Co. Inc., West Point, PA, United States

04:40 PM

Lipid tracing and metabolic flux for translatable biomarker development in drug discovery

Director Thomas P Roddy PhD. Discovery and Preclinical Sciences, Merck & Co., Rahway, NJ, United States