

## DIVISION OF CHEMICAL TOXICOLOGY T. Spratt, Program Chair

Location: [Marriott Marquis Washington, DC Georgetown University Room](#), except when notified

### SUNDAY MORNING

#### Chemical Research in Toxicology Young Investigators Award

H. Ai, *Organizer, Presiding*  
S. S. Hecht, T. M. Penning, *Presiding*

8:00 Introductory Remarks.

8:10 **1.** Targeted quantitative proteomic approaches for interrogating the human kinome. W. Miao, Y. Xiao, L. Guo, **Y. Wang**

8:55 **2.** Sequence-specific covalent capture for detection of disease-derived nucleic acid sequences. **K.S. Gates**, A. Gu, M. Imani Nejad, R. Shi, X. Zhang

9:40 Intermission.

9:55 **3.** Dynamic visualization of signaling molecules in living cells. **J. Zhang**

10:40 Award Presentation.

10:50 **4.** Seeing is believing: Fluorescent biosensors for redox signaling and oxidative stress. **H. Ai**

### SUNDAY AFTERNOON

#### Founders' Award

I. A. Blair, *Organizer, Presiding*

1:00 Founders' Award Presentation.

1:10 Introductory Remarks.

1:15 **5.** Biochemical and toxicological applications of mass spectrometry. **F.P. Guengerich**

1:55 **6.** Human aldo-keto reductases and aryl hydrocarbon activation. **T.M. Penning**

2:35 **7.** Chemical biology of DNA damage by  $\alpha,\beta$ -unsaturated aldehydes. **L.J. Marnett**

3:15 Intermission.

3:30 **8.** S-Nitrosation is a systems-wide regulatory process. **S.R. Tannenbaum**

4:10 **9.** Systems pharmacology approach to the study of mitochondrial dysfunction. **I.A. Blair**, Q. Wang, L. Guo, L. Weng, A. Salimatipour, W. Hwang, D. Lynch, C. Mesaros

### MONDAY MORNING

#### TOXI Young Investigators

Cosponsored by YCC  
T. Spratt, *Organizer*  
B. Ma, U. Sarkar, *Presiding*

8:00 **10.** Effect of statins on HMG-CoA reductase pathway and apolipoprotein A-I production in Friedreich's ataxia. **L. Guo**, Q. Wang, C.J. Strawser, L.A. Hauser, W. Hwang, D. Lynch, C. Mesaros, I.A. Blair

8:20 **11.** Mechanism of bioactivation of the cooked meat carcinogen 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) in human prostate. **M. Bellamri**, R.J. Turesky

8:40 **12.** Novel class of hydroxyl radical scavenging antioxidants prevents oxidative DNA damage in fibroblast cells exposed to trivalent arsenic. **S. Abdul Salam**, E.J. Merino, H. Zhu, P.N. Gurjar

9:00 **13.** Replicative bypass and mutagenic properties of alkylphosphotriester lesions in *Escherichia coli*. **J. Wu**, P. Wang, Y. Wang

9:20 **14.** Abasic and oxidized abasic lesion bypass by DNA polymerase theta yields one- and two-nucleotide deletions. **D.J. Lavery**, M.M. Greenberg

9:40 Intermission.

10:00 **15.** Characterization of the 2,6-diamino-4-hydroxy- $N^5$ -(methyl)-formamidopyrimidine DNA lesion. **S. Bamberger**, H. Pan, R. Bowen, C. Malik, T. Johnson-Salyard, C. Rizzo, M.P. Stone

10:20 **16.** Engineering a replicative DNA polymerase for specific damage bypass capability. **T.A. Coulther**, M.J. Ondrechen, P.J. Beuning

10:40 **17.** Mechanism of ribonucleotide incorporation by human DNA polymerase Eta. **Y. Su**, M. Egli, F.P. Guengerich

11:00 **18.** Independent generation of 2'-deoxyadenosine-N6-yl radical and its reactivity in DNA. **L. Zheng**, M. Griesser, D.A. Pratt, M.M. Greenberg

11:20 **19.** Investigation into the reactivity of a C5'-uridynyl radical. **M. Ellis**, A.C. Bryant-Friedrich

11:40 **20.** Arsenite binds to the RING finger domain of FANCL E3 ubiquitin ligase and inhibits DNA interstrand cross-link repair. Y. Wang, **J. Jiang**

### MONDAY AFTERNOON

#### Biological Targets of Botanical Supplements

Cosponsored by AGFD  
J. L. Bolton, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 **21.** Pharmacokinetic interactions between drugs and licorice botanical dietary supplements used by menopausal women. **R.B. Van Breemen**

2:15 **22.** Intestinal UGTs as targets for pharmacokinetic natural product-drug interactions. **M. Paine**

2:55 **23.** KEAP1 and done? Targeting the NRF2 pathway with sulforaphane. **T. Kensler**

3:35 Intermission.

3:50 **24.** Comparing general and specific biological targets for assessing sufficient similarity of related botanical dietary supplements. **C.V. Rider**, S. Smith-Roe, S.S. Ferguson

4:30 **25.** Botanicals modulate estrogen metabolism through multiple targets. **J.L. Bolton**

### MONDAY EVENING

[Walter E. Washington Convention Center Halls D/E](#)

#### Sci-Mix

T. Spratt, *Organizer*

8:00 - 10:00

**18.** See Previous Listings. **41, 43, 45, 46, 48, 49, 50, 54, 55, 61, 63, 68, 70, 73, 74, 75, 77, 82, 84.** See Subsequent Listings.

## TUESDAY MORNING

### Crosslink DNA Repair

Cosponsored by BIOL

O. Scharer, Y. Wang, *Organizers, Presiding*

**8:00** Introductory Remarks.

**8:05 26.** Mechanisms of replication-coupled repair. **J.C. Walter**

**8:40 27.** Interstrand DNA cross-links derived from abasic sites in duplex DNA. **K.S. Gates**

**9:15 28.** Replication and repair of DNA interstrand cross-link lesions in human cells. N. Price, S. Liu, K.S. Gates, **Y. Wang**

**9:50** Intermission.

**10:05 29.** Lesion proximal FANCD2 is required for replication independent repair of interstrand crosslinks. M. Paramasivam, M. Bellani, J. Gichimu, H. Gali, **M. Seidman**

**10:40 30.** Hydrogen peroxide activated DNA cross-linking agents and their biomedical application. **X. Peng**, W. Chen, Y. Wang, H. Fan

**11:15 31.** Constitutive role of Fanconi anemia D2 gene in protecting cell from crosslinking DNA damage. **L. Li**

## TUESDAY AFTERNOON

### Toxicological Considerations in Antibody Drug Conjugate Design & Development

Cosponsored by MEDI

F. Guengerich, W. G. Humphreys, N. A. Meanwell, *Organizers, Presiding*

**1:00** Introductory Remarks.

**1:10 32.** Antibody drug conjugates: Design considerations for improving efficacy and safety. **P. Trail**

**1:55 33.** ADC linker immolation and cell killing activity. **D. Zhang**

**2:40** Intermission.

**2:55 34.** Development of next generation calicheamicin ADCs. **O.K. Ahmad**

**3:40 35.** Potent antibody-based conjugates for cancer therapy: From early stage research to a clinically approved drug. **P.D. Senter**

## TUESDAY EVENING

[Marriott Marquis Washington, DC](#)  
[Liberty Ballroom Salons N-P](#)

### Keynote Lecture

N. E. Geacintov, *Organizer, Presiding*

**5:00 92.** Understanding hepatotoxicity: Man to mouse to computer. **P.B. Watkins**

[Walter E. Washington Convention Center](#)  
[Ballroom C](#)

### General Posters

T. Spratt, *Organizer*

**7:00 - 9:00**

**36.** Pentachlorophenol alters secretion of interleukin 6 (IL-6) from human immune cells. **T. Martin**, M. Whalen

**37.** Analysis of methylated and ethylated peptides in human hemoglobin by liquid chromatography mass spectrometry: Association with cigarette smoking. **H.C. Chen**, S. Ip, F. Lin

**38.** Simultaneous determination of a major peroxidation-derived DNA adduct, M<sub>1</sub>dG and its oxidized metabolite 6-oxo-M<sub>1</sub>dG, in human leukocyte DNA by liquid chromatography nanoelectrospray-high resolution tandem mass spectrometry. **B. Ma**, C. Ruszczak, P.W. Villalta, O.R. Wauchope, L.J. Marnett, I. Stepanov

**39.** Pyridylhydroxybutyl, pyridyloxobutyl and methyl DNA phosphate adduct formation in rats treated chronically with enantiomers of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol. **B. Ma**, A.T. Zarth, E. Carlson, P.W. Villalta, P. Upadhyaya, I. Stepanov, S.S. Hecht

**40.** Evidence for indole-3-methyl isothiocyanate formation upon human consumption of Brussels sprouts. **P. Upadhyaya**, A.T. Zarth, N. Fujioka, V. Fritz, S.S. Hecht

**41.** Qualitative analysis of the pyrolysis of cocaine and methamphetamine. **S. Raso**, O. Dodd, S. Bell

**42.** *Drosophila melanogaster* fatty acid amide production in the presence of Diminazene aceturate. **G. Suarez**, K.C. Prins, B.S. Meyer, R.L. Anderson, D.J. Merkler

**43.** Site-specific incorporation of *N*-(2'-deoxyguanosine-8-yl)-6-aminochrysene adduct in DNA and its replication in human cells. K.R. Rebello, **A. Chatterjee**, P. Pande, A.K. Basu

**44.** Absolute quantification of plasma fibulin-3 as a biomarker for asbestos exposure by immunoprecipitation-high resolution mass spectrometry. **Q. Wang**, L. Weng, C. Mesaros, I.A. Blair

**45.** Synthesis and *in vivo* quantitation of 2'-deoxyadenosine adducts resulting from bioactivation of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone and 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanol. **E.S. Carlson**, P. Upadhyaya, S.S. Hecht

**46.** Lesion recognition in nucleotide excision repair: Relationship between the structural properties of adducts and initial binding of XPC to the damaged site. **H. Mu**, N.E. Geacintov, Y. Zhang, S. Broyde

**47.** Accurate quantification of serum protein mesothelioma biomarkers. **L. Weng**, C. Mesaros, I. Blair

**48.** Nrf2-Keap1 signaling and implications for the metabolic activation of nitroarenes. **J. Murray**, M. Huang, C. Mesaros, V. Arlt, K. El Bayoumy, I.A. Blair, T.M. Penning

**49.** Toward genome-wide mapping of O(6)-methylguanine damage and repair in a human cell line. **M. McKeague**, I.A. Trantakis, J. Döhning, P. Steinberg, S.J. Sturla

**50.** Role of PARP-1 in the base excision repair of chromatin substates. **Y. Zeng**, D.R. Banerjee, C. Deckard, J.T. Sczepanski

**51.** DNA cross-linking by the anticancer prodrug PR-104A in oligonucleotides. **S. Danielli**, A. Stornetta, S.J. Sturla

**52.** Investigation of the presence in human urine of mercapturic acids derived from phenanthrene. **G. Cheng**, A.T. Zarth, P. Upadhyaya, P.W. Villalta, S. Balbo, S.S. Hecht

**53.** Arsenite binds to the zinc finger domains of TIP60 histone acetyltransferase and induces its degradation via the 26S proteasome. **L. Tam**, J. Jiang, P. Wang, L. Li, Y. Wang

**54.** Substituent effects of bifunctional agents on photo-induced DNA interstrand cross-link formation. **H. Fan**, X. Peng

**55.** Estrogenic activity of polycyclic aromatic hydrocarbon ortho-quinones in human endometrium. **I.G. Lee**, C. Mesaros, T.M. Penning

**56.** Deep learning methods applied to physicochemical and toxicological endpoints. **B. Sattarov**, A. Korotcov, V. Tkachenko, C. Grulke, A.J. Williams

- 57.** Total synthesis of site-specific oligonucleotides containing 2'-deoxyadenosine adduct formed by 6-nitrochrysene and their biological studies. **B.V. Powell**, A.K. Basu
- 58.** Determination of heavy metal acceptable concentration using fixed monitoring benchmarks in river system and soil pore-water in S.Korea. **B. Jeong**, J. An, G. Yu, K. Nam
- 59.** Determination of the ecotoxicological threshold concentration of Cu in soil pore water in Korea with biotic ligand model and species sensitivity distribution. **G. Yu**, B. Jeong, K. Nam
- 60.** Versatile method to construct model DNA-protein cross-links (DPCs). **S. Pujari**, M. Zhang, S. Ji, M.D. Distefano, N.Y. Tretyakova
- 61.** Modified deaza-adenosine mimics ad DNA minor groove alkylation probes. **L.J. Weselinski**, V. Begoyan, S. Xia, A. Ferrier, M. Tanasova
- 62.** Development of rapid, high throughput labeling methods for measuring aldehydes from P450 reactions. **A.M. Hanson**, D.A. Barnette, G.P. Miller
- 63.** Bypass efficiency and mutagenesis assays of site-specific arylamine DNA adducts in cell. **K. Bian**, F. Chen, Q. Tang, D. Li
- 64.** Comprehensive kinetic study of ALKBH2 and related family enzymes. **M. Vittori**, **K. Bian**, F. Chen, Q. Tang, D. Li
- 65.** Expression of a fragment of DNA polymerase zeta from *Dictyostelium discoideum*. **S.K. Mauldin**, D. He
- 66.** Replication and repair of 8-methoxypsoralen-derived DNA-DNA interstrand cross-links in human cells. **N.E. Price**, Y. Wang, K.S. Gates
- 67.** Polymerase bypass of DNA-protein and DNA-peptide cross-links. **S. Ji**, O. Scharer, N.Y. Tretyakova
- 68.** Conformational and configurational equilibria of a 2'-deoxyribosylurea adduct in single strand and duplex DNA. **A.H. Kellum**, M.P. Stone, A.K. Basu, J. Vijay
- 69.** Terbinafine bioactivation pathways to liver toxicity assessed using predictive modeling and experimental approaches. **D.A. Barnette**, L. Dang, T. Hughes, S. Swamidass, G.P. Miller
- 70.** Sequence-dependent repair of 1, N6-ethenoadenine by the AlkB family DNA repair enzymes. **Q. Tang**, F. Chen, K. Bian, D. Li
- 71.** Independent generation of neutral purine radicals involved in DNA damage. **L. Zheng**, M.M. Greenberg
- 72.** Importance of the glutathione and its degradation by  $\gamma$ -glutamyl transferase in lung tumor development. R.B. Penney, N.S. Kowalkowski, E.R. Siegel, **G. Boysen**
- 73.** Mitochondrial M1dG levels linked to oxidative stress and mitochondrial dysfunction in disease. O.R. Wauchope, **M.M. Mitchener**, W.N. Beavers, J. Galligan, P. Kingsley, H. Shim, T. Blackwell, T. Luong, M. deCaestecker, J.P. Fessel, L.J. Marnett
- 74.** Mechanisms of recognition of bulky DNA lesions by the DNA damaging sensor XPC. **K.M. Feher**, K.D. Walsh, N.E. Geacintov
- 75.** Mitochondrial DNA adducts of lipid peroxidation products with rotenone. **K.P. Gillespie**, I.A. Blair
- 76.** Temporal impact of toxic exposures on cellular recovery. **J.A. Mouch**, A. Han, J.V. Miller, N. Prince, M.S. Prediger, J.W. Boyd
- 77.** Withdrawn
- 78.** Characterization of a domoic acid-producing diatom. **M. Wang**, S. Lai, P. Lin, H. Lai
- 79.** Withdrawn
- 80.** Development of a threshold of toxicological concern framework based on chemoinformatics. **M. Cheeseman**
- 81.** Evidence of bioactivation of the anti-HIV drug etravirine to reactive metabolites *in vitro* and *in vivo*. A.L. Godinho, C.C. Jacob, S.A. Pereira, **M.S. Marques**, A. Antunes
- 82.** Chemistry of independently generated thymidine radical cation: DNA hole transfer and other competing processes. **H. Sun**, M.M. Greenberg
- 83.** Histone protein tails inhibit depurination of N7-methylated deoxyguanosine and form DNA-protein crosslinks with alkylated DNA in nucleosome core particles. **K. Yang**, M.M. Greenberg
- 84.** Degradation from C5' oxidation and its adducts as potential biomarkers. **S.H. Cho**, A.C. Bryant-Friedrich
- 85.** Functional characterization of glutathione S-transferases by photoreactive and mechanism-based activity-based probes. **E. Stoddard**, B. Killinger, R.N. Nair, N. Sadler, J. Smith, R. Corley, A.T. Wright
- 86.** Using medaka embryos coupled with a whole sediment exposure strategy to assess copper bioavailability and toxicity in sediment. **W. Li**, P. Chen
- 87.** Histones are targets for modification by the glycolytic by-product methylglyoxal. **J. Galligan**, J.A. Wepy, M. Streeter, P. Kingsley, M.M. Mitchener, O.R. Wauchope, W.N. Beavers, K. Rose, T. Wang, D.A. Spiegel, L.J. Marnett
- 88.** Wide selected ion monitoring (SIM)/MS<sup>2</sup> data independent acquisition method for DNA adduct omics analysis. **J. Guo**, P.W. Villalta, R.J. Turesky
- 89.** Investigation of environmental fate and toxic mechanisms of monovalent and trivalent thallium. **C. Yang**, P. Chen
- 90.** Biological uptake, distribution and depuration of radio-labeled graphene in adult zebrafish. **L. Mao**
- 91.** Bringing it all together: A web-based database for chemical and biological data to support environmental toxicology. **A.J. Williams**, C. Grulke, J. Smith, S. Watford, R. Jolley, J. Dunne, E. Edmiston, J. Edwards

## WEDNESDAY MORNING

### General Papers

T. Spratt, *Organizer*

G. P. Miller, L. Zhao, *Presiding*

**8:00 93.** Chemistry and biology of N<sup>5</sup>-alkyl-fapy-dG damage in DNA. **M.P. Stone**, M. Egli, R.S. Lloyd, A. Mc Cullough, C. Rizzo, R.J. Turesky

**8:20 94.** Aldehydes increase the tumorigenic properties of tobacco specific nitrosamines in rodent tumor models. **L.A. Peterson**, M.K. Oram, M. Flavin, D. Seabloom, W.E. Smith, I. Cornax, M. O'Sullivan, P. Upadhyaya, L. Zhang, S.S. Hecht, S. Balbo, T.S. Wiedmann

**8:40 95.** Unwinding kinetics of carcinogenic adducts: Correlation with processing by nucleotide excision repair machinery. **V. Shafirovich**, A.Y. Epie, V. Zheng, M. Kolbanovskiy, N.E. Geacintov

**9:00** Intermission.

**9:10 96.** Structural insights into the post-chemistry steps of nucleotide incorporation catalyzed by a DNA polymerase. **Z. Suo**

**9:30 97.** Central role of PCNA in promoting replication of damaged DNA. **G. Moldovan**

**9:50 98.** Lucidin-derived N<sup>2</sup>-guanine DNA lesion is not a major contributor to the mutagenicity of lucidin. **L. Zhao**

**10:10 99.** Spore photoproduct within DNA is a surprisingly poor substrate for its designated repair enzyme: The spore photoproduct lyase. **L. Li, L. Yang, S. Peter**

**10:30** Intermission.

**10:40 100.** Real-time prediction of physicochemical and toxicological endpoints using the web-based CompTox Chemistry Dashboard. **A.J. Williams, T. Martin, V. Tkachenko, C. Grulke, K. Mansouri**

**11:00 101.** Reaction of the antiepileptic drug carbamazepine with bionucleophiles: Bioactivation is not required. **I.L. Martins, J.P. Telo, M.S. Marques, A. Antunes**

**11:20 102.** Programed release of nitric oxide, via oxidative metabolism, in animals and humans from clinical candidate MK-8150. **K. Mitra**

**11:40 103.** Can pipe tobaccos be characterized for regulatory purposes without a puff of pipe smoke?. **J.H. Lauterbach**

### **WEDNESDAY AFTERNOON**

#### **Advanced Mass Spectrometric Techniques in Toxicology**

S. Balbo, P. Villalta, *Organizer, Presiding*

**1:00** Introductory Remarks.

**1:05 104.** Advances in mass spectrometry techniques for metabolism, pharmacology and toxicology. **J. Josephs**

**1:45 105.** Capillary electrophoresis for trace-level detection: Metabolites and proteins. **P. Nemes, R.M. Onjiko, C. Lombard-Banek**

**2:25 106.** Exposing the exposome: Utilizing global metabolomics to characterize toxicant exposure and effect. **B. Warth**

**3:05** Intermission.

**3:20 107.** Probing stress-induced effects on RNA and posttranscriptional modifications by LC-MS. **B. Addepalli, C. Sun, P. Limbach**

**4:00 108.** Advances in human biomonitoring of heterocyclic aromatic amines by high resolution accurate mass spectrometry. **J. Guo, S. Xiao, Y. Wang, B. Yun, P. Murugan, C.J. Weight, K.K. White, L.R. Wilkens, L. Le Marchand, K. Dingley, M.A. Malfatti, K. Turteltaub, P.W. Villalta, R.J. Turesky**

**4:40** Concluding Remarks.