

CINF

Division of Chemical Information

E. Alvaro, Program Chair

OTHER SYMPOSIA OF INTEREST:

Crafting Chemical Communication
(see CHED, Tue)

Drug Discovery (see COMP, Sun, Tue, Wed, Thu)

New Directions in Chemometrics: Making Sense of Big & Small Chemical Data Sets (see ANYL, Thu)

Designing Chemical Libraries for Screening (see COMP, Sun)

SOCIAL EVENTS:

Reception, 6:30 PM: Sun

Luncheon, 12:00 PM: Tue

Skolnik Award Symposium Reception, 6:30 PM: Tue

BUSINESS MEETINGS:

Business Meeting, 1:00 PM: Sat

SUNDAY MORNING

Section A

Pennsylvania Convention Center
Room 112A

Effectively Harnessing the World's Literature to Inform Rational Compound Design

Cosponsored by MEDI

Financially supported by Genentech

D. F. Ortwine, Organizer, Presiding

8:25 Introductory Remarks.

8:30 CINF 1. PubChem's literature and patent information for drug discovery. S. Kim, P. Thiessen, T. Cheng, B. Yu, B.A. Shoemaker, J. Wang, E. Bolton, Y. Wang, S. Bryant

9:05 CINF 2. Harnessing the world's literature to provide a crystallographic perspective on compound design: federated pharmacophore searching as example. E. Davis, I. Bruno, P. Sanschagrin

9:40 CINF 3. GOSTAR and ChEMBL comparison – commercial vs. open chemogenomics databases. J.H. Voigt, U. Schmitz

10:15 Intermission.

10:30 CINF 4. Exploring available compound data with the open PHACTS discovery platform and KNIME. D. Digles, G.F. Ecker

11:05 CINF 5. NDEX, the Network Data Exchange: a resource for biological networks with application in informed compound design. D. Pratt

11:40 Concluding Remarks.

Technical program information known at press time.

The official technical program for the 252nd ACS National Meeting is available at:
www.acs.org/Philadelphia2016

Section B

Pennsylvania Convention Center
Room 112B

Bringing Cheminformatics into the College Chemistry Classroom

Cosponsored by CHED

R. E. Belford, S. Kim, Organizers, Presiding

8:15 Introductory Remarks.

8:20 CINF 6. Learning to find the right information: A survey of chemistry information literacy in the undergraduate classroom. T. Geoui

8:40 CINF 7. Co-developing chemical information management and laboratory safety skills. R. Stuart, L. McEwen

9:00 CINF 8. Introducing SIVVU, a web-based program for modeling spectrophotometric titration data. D.A. Vander Griend

9:20 Intermission.

9:30 CINF 9. Integration of cheminformatics material into the STEMWiki hyperlibrary. R.E. Belford, D.S. Larsen, A.P. Cornell

9:50 CINF 10. Holistic approach to cheminformatics in a liberal arts environment. P. Adler

10:10 CINF 11. Cheminformatics education and research at home: the best way to teach graduate chemistry in the professional community. H. Zhu

10:30 Intermission.

10:40 CINF 12. Fall 2015 cheminformatics OLCC project based learning: Validation of Wikipedia Chembox hazard information. R.E. Belford, B. Murphy

11:00 CINF 13. Cheminformatics in the chemistry classroom. D. Fourches

11:20 CINF 14. From textbook to computer: How computer-aided synthesis design (CASD) can support chemistry teachers and students in the future. V. Eigner Pitto, K. Borchardt, J. Eiblmair, M. Hutchings, F. Irlinger, H. Saller, P. Loew

11:40 CINF 15. Modern cheminformatics tools in the teaching laboratory: A practical exercise simulating a drug discovery project. C. Smith, T. Mansley

12:00 Concluding Remarks.

SUNDAY AFTERNOON

Section A

Pennsylvania Convention Center
Room 112A

Effectively Harnessing the World's Literature to Inform Rational Compound Design

Cosponsored by MEDI

Financially supported by Genentech

D. F. Ortwine, Organizer, Presiding

1:25 Introductory Remarks.

1:30 CINF 16. Extracting and exploiting medicinal chemistry ADMET knowledge automatically from public and large pharma data. A. Dossetter, E.J. Griffen, A. Leach, S.T. Montague

2:05 CINF 17. Extracting knowledge from large in-vitro metabolic stability data sets using matched molecular pair analysis (MMPA). H. Zheng

2:40 CINF 18. Gravitational waves shaking the chemical universe: virtual chemistry 2.0. C. Detering

3:15 Intermission.

3:30 CINF 19. Network analytics of structured and unstructured data: an evolutionary solution. O. Lichtarge

4:05 CINF 20. Integrative data science, semantics, knowledge graphs, and evidence paths in the service of molecular discovery. J.J. Yang, T.I. Oprea, D.J. Wild

4:40 Concluding Remarks.

Section B

Pennsylvania Convention Center
Room 112B

Beyond Citations: Challenges & Opportunities in Altmetrics

E. Alvaro, R. Borchardt, Organizers, Presiding

M. R. Hartings, Presiding

1:30 Introductory Remarks.

1:35 CINF 21. Altmetrics in the library. A. Rauh

1:55 CINF 22. Trusting altmetrics: updates from NISO's recommended practices. T. Carpenter

2:15 CINF 23. Tell the full story of your research with altmetrics. W. Gunn

2:35 CINF 24. Is that a wart or a beauty mark? An altmetrics analysis of an assistant professor's scholarly activity. M.R. Hartings, R. Borchardt

2:55 CINF 25. Imperfect impact. S.J. Cantrill

3:15 Intermission.

3:30 CINF 26. Advanced Research Projects Agency – Energy (ARPA-E): The mechanism and metrics of funding transformational technology for energy innovation. D.W. Cunningham

3:50 CINF 27. Responsible usage of diverse research metrics. L. Colledge

4:10 CINF 28. Investigating impact metrics for performance for the US-EPA National Center for Computational Toxicology. A.J. Williams, M. Linnenbrink, K. Crofton, R. Thomas

4:30 CINF 29. Altmetrics: What has been the impact on ACS Publications? J. Lang

4:50 Concluding Remarks.

SUNDAY EVENING

Section A

Loews Philadelphia Downtown
Howe

CINF Scholarships for Scientific Excellence

S. J. Chalk, Organizer

6:30 - 8:30

CINF 30. Virtual nanoparticles. W. Wang, A. Sedykh, L. Zhao, B. Yan, H. Zhu

CINF 31. Experimental errors in QSAR modeling sets: What we can do and what we cannot do. L. Zhao, W. Wang, A. Sedykh, H. Zhu

CINF 32. Combining proprietary and published data in synthesis planning and reaction mining using Wiley ChemPlanner. O. Ravitz, D. Flannagan, J. Theisen

CINF 33. Modeling spectrophotometric titration data: tracking error from the measurement, through the model, and to the targeted output parameters. N. Kazmierczak, D.A. Vander Griend

CINF 34. Dark reactions project: A cheminformatics approach to hydrothermal synthesis. P. Adler, J. Schrier, A.J. Norquist, S. Friedler

CINF 35. Adverse drug reactions triggered by the common HLA-B*57:01 variant: A molecular docking study. G. Van Den Driessche, D. Fourches

CINF 36. ChemML: A machine learning and informatics program suite for the chemical and materials sciences. M. Haghightalari, J. Hachmann

MONDAY MORNING

Section A

Pennsylvania Convention Center
Room 112A

Chemistry Data for the People: From Policy to Practice

Value of Open for Chemists

Cosponsored by MPPG

E. Bolton, I. Bruno, Organizers

D. P. Henderson, L. McEwen, Organizers, Presiding

8:05 Introductory Remarks.

8:15 CINF 37. Viewpoint on open access by an editor, author, reviewer, and reader. J.V. Sweedler

8:25 CINF 38. Data generation, publication and sharing. R. Kidd

8:35 CINF 39. Implementing a data sharing policy: A publisher perspective. R.J. Boucher, K. Sharples

8:45 CINF 40. Ten habits of happy data: An exploration of Elsevier's research data management program. A. De Waard, W. Gunn

8:55 CINF 41. Changing workflows and mindsets. M.G. Hicks

9:05 Panel Discussion.

9:35 Discussion.

9:45 Intermission.

10:00 CINF 42. NSF MPS Open Data workshop series: Taking the pulse of the research community on open data issues. M. Hildreth, L. McEwen

10:10 CINF 43. Open Data: What the reader wants to know rather than what the author wants to present. R.D. Rogers

10:20 CINF 44. Role of disciplinary data repositories in data publishing. I. Bruno, A. Sarjeant, E. Davis

10:30 CINF 45. Figshare data repository. D. Valen

10:40 CINF 46. Importance of open raw data in chemistry research. S. Dominguez Vivero, C. Cobas, A. Barba, F. Seoane, S. Fraga

10:50 CINF 47. Practical issues in chemistry data sharing in PubChem. S. Kim, E. Bolton, S. Bryant, Y. Wang

11:00 Panel Discussion.

11:30 Discussion.

11:40 CINF 48. Value of open data for chemists: Summary and perspectives. J.N. Currano

Section B

Pennsylvania Convention Center
Room 112B

Shedding Light on the Dark Genome: Methods, Tools & Case Studies

Cosponsored by BIOT, COMP and MEDI

R. Guha, T. I. Oprea, *Organizers, Presiding*

8:15 CINF 49. Illuminating the druggable genome: Linking diseases, targets and drugs. T.I. Oprea

8:40 CINF 50. Tracking biological targets in drug discovery using the ChEMBL and SureChEMBL databases. P. Mutowo

9:05 CINF 51. Formal ontologies and software tools to facilitate integration, classification and modeling of drug discovery data. S. Schürer, A. Lin, H. McGinty, Q. Cheng, A. Koleli, N. Zadeh, D. Vidovic

9:30 Intermission.

9:40 CINF 52. KEA2: Multiple views of the human kinome. N.F. Fernandez, A.D. Rouillard, K. Rikova, P. Hornbeck, A. Ma'ayan

10:05 CINF 53. Pharos - shining light on the druggable genome. D. Nguyen, T. Sheils, G. Mandava, A. Jadhav, N. Southall, R. Guha

10:30 CINF 54. From dark chemical matter to shedding light on the dark genome: How can chemistry and informatics enable biology? M. Glick

10:55 Intermission.

11:05 CINF 55. KinomeNet: accurate prediction of protein kinase inhibitors with deep convolutional neural networks. O. Isayev, A. Tropsha

11:30 CINF 56. Analogous phylogenetic analysis using protein length and protein disorder. H. Guo, G. Tuskan, X. Yang, H. Guo

11:55 Concluding Remarks.

MONDAY AFTERNOON

Section A

Pennsylvania Convention Center
Room 112A

Chemistry Data for the People: From Policy to Practice

Pain Points: Distilled, Analyzed & Next Steps

Cosponsored by MPPG

I. Bruno, D. P. Henderson, L. McEwen, *Organizers*

E. Bolton, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 57. Community forum for chemistry data and information. I. Bruno, L. McEwen, S.J. Chalk

1:55 CINF 58. Chemistry data pain points: distilled, analyzed, and next steps. E. Bolton, L. McEwen, I. Bruno

4:10 Concluding Remarks.

Section B

Pennsylvania Convention Center
Room 112B

Using New Media to Communicate Chemistry to the Public

Cosponsored by MPPG and PRES

S. R. Morrissey, *Organizer*

L. Wolf, *Organizer, Presiding*

M. Davenport, *Presiding*

1:30 Introductory Remarks.

1:40 CINF 59. Communicating chemistry on YouTube. A. Dylewski

2:00 CINF 60. Sound of science (and history and culture). M. Carr

2:20 CINF 61. Got something to say? Engaging with social media in the time you have. D.G. Oppenheimer, P. Grey

2:40 Intermission.

2:55 CINF 62. Compound interest: Communicating chemistry using infographics. A. Brunning

3:15 CINF 63. Pop culture chemistry. R. Burks

3:35 Panel Discussion.

Kavli Symposium on Chemical Neurotransmission: What Are We Thinking?

Sponsored by ANYL, Cosponsored by BIOL, BMGT, CHED, CINF, MEDI, PMSE and SCHB

MONDAY EVENING

Section A

Pennsylvania Convention Center
Halls D/E

Sci-Mix

E. Alvaro, *Organizer*

8:00 - 10:00

3-4, 8-10, 15-16, 30-31, 35-36, 51-52, 55. See previous listings.

86, 92-95. See subsequent listings.

TUESDAY MORNING

Section A

Pennsylvania Convention Center
Room 112A/B

Herman Skolnik Award Symposium

E. Alvaro, L. McEwen, *Organizers*

E. Bolton, *Organizer, Presiding*

8:45 Introductory Remarks.

8:50 CINF 64. Developing databases and standards in chemistry. S.R. Heller

9:15 CINF 65. Two decades of open chemical data at DTP/NCI. D. Zaharevitz

9:40 CINF 66. Using InChI to manage data. P. Linstrom

10:05 CINF 67. Open chemistry resources provided by the NCI CADD group. M.C. Nicklaus

10:30 Intermission.

10:45 CINF 68. Evolution of open chemical information. V. Tkachenko

11:10 CINF 69. Open chemical information at the European Bioinformatics Institute. C. Steinbeck

11:35 CINF 70. History and the future of tools and software components for working with public chemistry data. W. Ihlenfeldt

Connectivity & the Global Reach of Chemistry: Honoring the Life & Scientific Contributions of Ernest L. Eliel

Sponsored by ORGN, Cosponsored by BMGT, CHED, CINF, HIST, INOR, MEDI, MPPG, PMSE and SCHB

TUESDAY AFTERNOON

Section A

Pennsylvania Convention Center
Room 112A/B

Herman Skolnik Award Symposium

E. Alvaro, L. McEwen, *Organizers*

E. Bolton, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 CINF 71. PubChem a resource for cognitive computing. S. Boyer

2:30 CINF 72. SPL and openFDA resources of open substance data. Y. Borodina

2:55 CINF 73. Building a network of interoperable and independently produced linked and open biomedical data. M. Dumontier

3:20 Intermission.

3:35 CINF 74. Chemical structure representation in PubChem. R.A. Sayle

4:00 CINF 75. iRAMP & PubChem: Of the people, for the people. L. McEwen

4:25 CINF 76. Open chemical information: Where now and how? E. Bolton

4:50 Concluding Remarks.

4:55 Award Presentation.

WEDNESDAY MORNING

Section A

Pennsylvania Convention Center
Room 112A

Using Public Information to Support a Chemical Safety Culture

Cosponsored by CHAS†

E. Bolton, L. McEwen, R. Stuart, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 CINF 77. Users roundtable: Laboratory use cases for chemical safety information. R. Stuart, L. McEwen, E. Bolton

8:45 CINF 78. Risk assessment and crisis management in the research laboratory using online resources: A EH&S perspective. S. Singh, N. Bharti

9:10 CINF 79. Institutional use of chemical safety data streams. C.A. Jakober

9:35 CINF 80. Chemical safety and hazard information in PubChem. J. Zhang, P. Thiessen, A. Gindulyte, L. McEwen, R. Stuart, E. Bolton, S. Bryant

10:00 Intermission.

10:15 CINF 81. Semantic annotation of the laboratory chemical safety summary in PubChem. G. Fu, J. Zhang, E. Bolton, J.G. Frey, S.J. Chalk, M.I. Borkum, L. McEwen

10:40 CINF 82. GHS and NFPA diamonds: Where they come from and how they can be useful. R.A. Sayle

11:05 CINF 83. Critical cases for information identifiers in chemical asset management. L. McEwen

11:30 CINF 84. Surveying the academic laboratory population: Project updates from the iRAMP collaboration. L. McEwen, R. Stuart

11:45 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Pennsylvania Convention Center
Room 112A

General Papers

Informatics for Medicinal Chemistry

E. Alvaro, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 85. Active machine learning perspective on hit identification and optimization. D. Reker, G. Schneider

2:00 CINF 86. Binding affinity prediction using frequency of protein-ligand interactions: method validation and application to bromodomain inhibitors. J. Meslamani, A. Vincek, E. Russinova, A. Plotnikov, R. Sanchez, M. Zhou

2:25 CINF 87. MOARF, an integrated workflow for multiobjective optimization: Implementation, synthesis, and biological evaluation. N. Brown

2:50 CINF 88. Systematic generation of analog relationships of bioactive compounds and promiscuity analysis. D. Stumpfe, D. Dimova, J. Bajorath

3:15 Intermission.

3:30 CINF 89. SAR characteristics of matching molecular series and exploration of structural relationships. D. Dimova, J. Bajorath

3:55 CINF 90. How frequent are your clusters in hierarchical cluster analysis? Quantifying their frequencies considering ties in proximity. G. Restrepo, W. Leal, E. Llanos, C. Suarez, M. Patarroyo

4:20 CINF 91. Line notations for nucleic acids (both natural and therapeutic). R.A. Sayle

4:45 Concluding Remarks.

THURSDAY MORNING

Section A

Pennsylvania Convention Center
Room 112A

General Papers

E. Alvaro, *Organizer, Presiding*

8:45 Introductory Remarks.

8:50 CINF 92. VSViewer3D: An open source tool for interactive data mining of 3D virtual screening data. D.J. Diller, K. Diller

9:15 CINF 93. Strategies to improve PubChem data quality and search effectiveness through data analysis. L. Zaslavsky, G. Fu, A. Gindulyte, P. Thiessen, S. Kim, E. Bolton

9:40 CINF 94. Sketchy sketches: Hiding chemistry in plain sight. D.M. Lowe, J.W. May, R.A. Sayle

10:05 Intermission.

10:20 CINF 95. Hybrid search engine for chemical information in PubChem. J. Chen, S. He, A. Gindulyte, E. Bolton, S. Bryant

10:45 CINF 96. Amoeba-inspired heuristic search dynamics for semi-quantitative estimation of unknown chemical kinetics. M. Aono

11:10 CINF 97. Database searching and rediscovering the wheel in scientific research. C.S. Gilpin, R.K. Gilpin

11:35 Concluding Remarks.

New Directions in Chemometrics: Making Sense of Big & Small Chemical Data Sets

Sponsored by ANYL, Cosponsored by CINF

THURSDAY AFTERNOON

New Directions in Chemometrics: Making Sense of Big & Small Chemical Data Sets

Sponsored by ANYL, Cosponsored by CINF

TOXI

Division of Chemical Toxicology

A. Bryant-Friedrich, Program Chair

OTHER SYMPOSIA OF INTEREST:

Bioanalytical Tools for Chemicals of Emerging Concern in the Environment (see ENVR, Thu)

Medicinal Chemistry of Chemical Biology (see MEDI, Mon)

Nucleic Acid Therapeutics (see MEDI, Mon)

Epigenetics (see MEDI, Wed)

Chemistry of the People, by the People, for the People Plenary Session (see MPPG, Sun)

Biologically-Related Molecules & Processes (see ORGN, Tue, Wed)

SOCIAL EVENTS:

Dinner, 6:30 PM: Sat

BUSINESS MEETINGS:

Business Meeting, 6:30 PM: Tue

SUNDAY MORNING

Section A

Philadelphia Downtown Courtyard by Marriott Juniper's Ballroom

Chemical Research in Toxicology Young Investigator Award

Y. Aye, Organizer, Presiding

8:30 Introductory Remarks.

8:45 TOXI 1. Protein modification by lipid electrophiles and its consequences. L.J. Marnett, J. Camarillo, W.N. Beavers, J. Galligan

9:15 TOXI 2. Reactivity of damaged DNA in nucleosomes. M.M. Greenberg

9:45 TOXI 3. Succinylation and SIRT5 as important regulators of heart function. H. Lin

10:15 Intermission.

10:30 TOXI 4. T-REX™ on-demand redox targeting: A toolset for functional discoveries and validations. S. Parvez, M.J. Long, H. Lin, Y. Zhao, J. Haeghele, V. Pham, D. Lee, Y. Aye

11:00 TOXI 5. Master and commander of the cellular antioxidant response. J.R. Poganik, Y. Aye

11:30 TOXI 6. Switching gears: ribonucleotide reductase antagonizes cell proliferation. Y. Aye

SUNDAY AFTERNOON

Section A

Philadelphia Downtown Courtyard by Marriott Juniper's Ballroom

Founders Award Lecture & Symposium

S. Brody, N. E. Geacintov, Organizers, Presiding

1:30 Introductory Remarks.

1:40 TOXI 7. Regulation of dual incision and repair synthesis in human nucleotide excision repair. O.D. Schärer, F. Adebakke, J. Rageul

2:15 TOXI 8. Impact of structural features of DNA lesions on their recognition and repair by the human nucleotide excision repair system. N.E. Geacintov

2:50 TOXI 9. Elucidating structure-function relationships in lesion containing DNA: Insights from molecular modeling. S. Brody

3:25 Intermission.

3:45 TOXI 10. Insights into the DNA damage recognition by the Rad4/XPC nucleotide excision repair complex. J. Min, A. Ansari, X. Chen, Y. Velmurugu

4:20 TOXI 11. DNA damage and repair in chromatin: Finding the keys to get in. P. Mao, M. Duan, J. Wyrick, M. Smerdon

Increasing the Value of Water Monitoring Data for Pesticide Fate & Effects Evaluations

Sponsored by AGRO, Cosponsored by ENVR and TOXI

MONDAY MORNING

Section A

Philadelphia Downtown Courtyard by Marriott Juniper's Ballroom

Young Investigators Symposium

U. Sarkar, Organizer, Presiding

8:00 TOXI 12. Parsing the conformational and configurational equilibria of a 2'-deoxyribosylurea DNA adduct. A.H. Kellum, V. Jasti, A.K. Basu, M.P. Stone

8:20 TOXI 13. Mutagenic and cytotoxic properties of the O²-alkylthymidine lesions in human cells. J. Wu, P. Wang, L. Li, Y. Wang

8:40 TOXI 14. Investigation of RNA oxidation via selective generation of a C5'-uridyl radical. M. Ellis, A.C. Bryant-Friedrich

9:00 TOXI 15. Quantitative assessment of the biological consequences and repair of carboxymethylated and ethylated DNA adducts. C. You, P. Wang, S. Nay, J. Wang, X. Dai, T. O'Connor, Y. Wang

9:20 TOXI 16. Sequencing of 8-oxo-7,8-dihydro-2'-deoxyguanosine in the genome by next-generation sequencing methods. Y. Ding, A.M. Fleming, C.J. Burrows

9:40 Intermission.

9:50 TOXI 17. Transcriptional bypass of O²-alkylthymidine lesions by T7 RNA polymerase and human RNA polymerase II. N. Williams, P. Wang, Y. Wang

10:10 TOXI 18. Tracing androgen metabolism with inhibition of aromatase in breast cancer: in vitro studies, clinical correlates and implications for acquired resistance. L. Bottalico, L. Gil de Gomez, Q. Wang, A. Frey, N. Snyder, I.A. Blair

10:30 TOXI 19. Metatranscriptomics reveals functional effects of diazinon exposure on gut microbiome. B. Gao, X. Bian, L. Chi, P. Tu, K. Lu

10:50 TOXI 20. Toxicological study of quinone-protein adducts by molecular modeling and spectroscopic analysis. M.S. Elgawish

11:10 TOXI 21. Cadmium inactivates a zinc-dependent endonuclease of the human mismatch repair pathway. S.M. Sherrer, P.L. Modrich

11:30 TOXI 22. Replication studies of C3'-epimeric lesions of 2'-deoxyribonucleosides in E. coli cells. P. Wang, N.J. Amato, Y. Wang

11:50 TOXI 23. Mass spectrometry based studies of DNA-protein cross-linking. A. Groehler, C. Campbell, P.W. Villalta, P. Jacobson, M. Garry, N.Y. Tretyakova

Increasing the Value of Water Monitoring Data for Pesticide Fate & Effects Evaluations

Sponsored by AGRO, Cosponsored by ENVR and TOXI

MONDAY AFTERNOON

Section A

Philadelphia Downtown Courtyard by Marriott Juniper's Ballroom

Asbestos Fate, Exposure, Remediation & Adverse Health Effects

I. A. Blair, Organizer, Presiding

1:30 TOXI 24. Overview: Penn Superfund Research and Training Program Center: Asbestos, fate, transport, remediation and adverse health effects. T.M. Penning

2:10 TOXI 25. Fate of asbestos in soil: remediation prospects and paradigm. J. Willenbring, S. Mohanty, A. Salamattipour, C. Gonneau, D. Jerolmack, B. Casper

2:40 TOXI 26. Aggregate dynamics and their control on the mobility of asbestos in the environment. D. Jerolmack, L. Wu, C. Ortiz, J. Willenbring

3:10 TOXI 27. Historic cohort study to identify effects of chrysotile asbestos exposure on past residents of Ambler, PA. E. Emmett, A. Agawu, S. Elahi, F. Barg, D. Wiebe

3:40 Intermission.

3:55 TOXI 28. Mouse models of malignant mesothelioma. J. Testa, C. Menges, M. Cheung, Y. Kadariya, J. Talarckek, R.A. Pietrofesa, R. Simmons, M. Christofidou-Solomidou, S. Albelda

4:25 TOXI 29. Chemopreventive properties of LGM2605. M. Christofidou-Solomidou, R.A. Pietrofesa, A. Velalopoulou, S. Albelda

4:55 TOXI 30. Biomarkers of asbestos exposure. I.A. Blair, L. Weng, C. Mesaros, N. Snyder, W. Hwang, A. Vachani

Increasing the Value of Water Monitoring Data for Pesticide Fate & Effects Evaluations

Sponsored by AGRO, Cosponsored by ENVR and TOXI

Pollinators: Agrochemicals, Behavior & Disease

Sponsored by AGRO, Cosponsored by AGFD, ENVR and TOXI

TUESDAY MORNING

Section A

Philadelphia Downtown Courtyard by Marriott Juniper's Ballroom

Chemical Toxicology in the Study of Health Disparities among Ethnic/Racial Groups

S. Balbo, S. S. Hecht, Organizers, Presiding

8:30 Introductory Remarks.

8:35 TOXI 31. Differing frequencies of clinically relevant genomic alterations (CRGA) in colorectal cancers of patients to define disparities in outcomes. E.P. Mitchell

9:15 TOXI 32. Relationships between body burden of contaminants, biomarkers of effects and health outcomes among Inuit in the Canadian Arctic. L.H. Chan

9:55 TOXI 33. Unconventional gas and oil drilling operations (UGOD) in the Marcellus Shale and health disparities. T.M. Penning

10:35 Intermission.

10:50 TOXI 34. Individual variation in human arsenic biotransformation: Intuitive and puzzling determinants drive variability. W. Klimecki

11:30 TOXI 35. Analysis of nicotine and tobacco smoke toxicant and carcinogen metabolites in relation to ethnic differences in lung cancer susceptibility in cigarette smokers. S.S. Hecht, S. Park, S. Carmella, D.O. Stram, C.A. Haiman, L. Le Marchand, S.E. Murphy

12:10 Concluding Remarks.

Agrochemicals & Pollinators: Current Science & Risk Assessment Approaches

Sponsored by AGRO, Cosponsored by AGFD, ENVR and TOXI