

4:20 CHAS **32.** Establishing a sustainable safety culture in academic research labs. K.A. Miller

4:45 Concluding Remarks.

WEDNESDAY MORNING

Section A

Walter E. Washington Convention Center
Room 209C

Building a Safety Culture Across the Chemical Enterprise

Cosponsored by CCS[†] and PROF

J. Palmer, Organizer

J. M. Pickel, Organizer, Presiding

8:30 Introductory Remarks.

8:35 CHAS **33.** Safe operating cards (SOCs): Open communication helps best practices from industry move to academia. A.J. Miller, I. Tonks, C.L. Pitman

9:00 CHAS **34.** GHS information integration in PubChem. J. Zhang, P. Thiessen, A. Gindulyte, E. Bolton

9:25 CHAS **35.** Pharmaceutical industry best practices in lessons learned: ELN implementation of Merck's reaction review policy. R.A. Sayle, J.W. Mayfield

Section A

Walter E. Washington Convention Center
Room 209C

Emerging Trends in Research Operations

Cosponsored by CCS

J. M. Pickel, Organizer

C. D. Incarvito, Organizer, Presiding

10:00 Introductory Remarks.

10:05 CHAS **36.** Framingham State University: Science Building. J. Blount

10:30 CHAS **37.** Safe and appropriate application of filtered fume hoods. K. Crooks

10:55 CHAS **38.** iLab operating software materials management. C. Lopes

11:20 CHAS **39.** Monitoring VOCs within flammable liquid chemical storage cabinets for laboratory safety. A.E. Norton, K. Brown, W.B. Connick, A. Doepke, F. Nourain

11:45 Concluding Remarks.

Analytical, Environmental & Regulatory Challenges with Legalized Cannabis

Sponsored by AGRO, Cosponsored by CHAS[†]

WEDNESDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 209C

Emerging Trends in Research Operations

Cosponsored by CCS

J. M. Pickel, Organizer

C. D. Incarvito, Organizer, Presiding

1:30 Introductory Remarks.

1:35 CHAS **40.** Multidisciplinary research institutes and the challenges they bring. S. Elwood, R.M. Izzo, K. Angielo

2:00 CHAS **41.** Convergence of research operations and safety: A mutually beneficial partnership. K. Heard

2:25 CHAS **42.** Role of the EHS Professional in laboratory design. M.B. Koza

2:50 CHAS **43.** Taking safety management to the next level: Moving from assumptions to reality. S. Schwartz-Hinds, N. Watson

3:15 Intermission.

3:30 CHAS **44.** Designing and operating facilities to support the safe conduct of research activities. J.M. Pickel, K.B. Jeskie

3:55 CHAS **45.** Personal chemical exposure sensor with indoor positioning and robotics for laboratory safety. K. Brown, A. Brandes, A.E. Norton, P.B. Shaw, D.T. Neu, R. Voorhees

4:20 CHAS **46.** Hydrogen gas lab servers provide many advantages to laboratory operations. J. Speranza

4:45 CHAS **47.** Achieving a balance between expansion and cost control: Yale University West Campus Research Operations. C.D. Incarvito

CINF

Division of Chemical Information

E. Alvaro, Program Chair

OTHER SYMPOSIA OF INTEREST:

Advancing Graduate Education: Opportunities & Challenges
(see CHED, Sun)

Building a Safety Culture Across the Chemical Enterprise
(see CHAS, Tue, Wed)

Drug Design (see COMP, Wed, Thu)

SOCIAL EVENTS:

Luncheon, 12:00 PM: Tue

Reception, 6:30 PM: Sun

Skolnik Award Symposium Reception, 6:30 PM: Tue

BUSINESS MEETINGS:

Business Meetings, 12:30 PM & 3:00 PM: Sat

SUNDAY MORNING

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

Open Structures: Current Issues & Future Plans

Financially supported by CSA Trust, InChI Trust, IUPAC CPCDS, RDA CRDIG

M. G. Hicks, H. A. Lawlor, D. Martinsen, L. McEwen, Organizers, Presiding

8:15 Introductory Remarks.

8:20 CINF **1.** Caution! Normalization can be hazardous to your data health. E. Bolton

8:50 CINF **2.** Three degrees of interpretation: Why structure searches fail and how to maximize success. J.N. Curran

9:20 CINF **3.** Everything you know is wrong: The battle between e-chemists and 127 years of chemical structure drawing tradition. G.M. Banik, K. Nedwed, K. Kunitsky, M. D'Souza, T. Abshear

9:50 Intermission.

10:05 CINF **4.** InChI and standard for chemical structures. S.R. Heller

10:30 CINF **5.** Representing molecules with minimalism: A solution to the entropy of informatics. A. Clark

10:55 CINF **6.** Open semantic chemical structures: Ideas on the use of JSON-LD for representation of chemical entities. S.J. Chalk

11:20 CINF **7.** Enhancing scholarly literature with compound information. M. Cleeren, T. Hocht

11:45 Discussion.

Section B

Washington Marriott at Metro Center
Junior Ballroom 2

What do Synthetic Chemists Want from Their Reaction Systems?

Cosponsored by COMP, INOR, MEDI and ORGN

W. A. Warr, Organizer

D. Evans, Organizer, Presiding

8:40 Introductory Remarks.

8:45 CINF **8.** Applying machine learning to synthesis design: Prediction of organic reaction outcomes. C.W. Coley, R. Barzilay, T.S. Jaakkola, W.H. Green, K.F. Jensen

9:10 CINF **9.** Applications of machine learning methods for chemical reaction databases. V. Tkachenko, B. Sattarov, A. Korotcov, D.M. Lowe, R. Nugmanov, T.I. Madzhidov, A. Varnek

9:35 CINF **10.** Retrosynthesis and reaction prediction with deep neural networks. M. Segler, M. Waller

10:00 Intermission.

10:20 CINF **11.** International Chemical Identifier for Reactions (RInChI): What is RInChI and how does it revolutionize the handling of reaction databases? G. Blanke, J.M. Goodman, G. Grethe, H. Kraut

10:45 CINF **12.** Better synthesis for the next molecule. J.M. Goodman

11:10 CINF **13.** Pistachio: Search and faceting of large reaction databases. J.W. Mayfield, D.M. Lowe, R.A. Sayle

11:35 CINF **14.** Computational approach to the history of chemical reactivity: Exploring Reaxys database. E.J. Llanos, W. Leal, G. Restrepo, P. Stadler

SUNDAY AFTERNOON

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

Open Structures: Current Issues & Future Plans

Financially supported by CSA Trust, InChI Trust, IUPAC CPCDS, RDA CRDIG

M. G. Hicks, H. A. Lawlor, D. Martinsen, L. McEwen, Organizers, Presiding

1:20 Introductory Remarks.

1:25 CINF **15.** Experiences with chemical database merger and migration: The art to surviving detail hell (or the devil is in the details). G. Blanke

1:50 CINF **16.** Challenges representing the chemistry of crystal structures: How current initiatives could help. I. Bruno, S. Vyas

2:15 CINF **17.** Comparing CIP implementations: The need for an open CIP. J.W. Mayfield, D.M. Lowe, R.A. Sayle

2:40 CINF **18.** We need to talk about kekulization, aromaticity and SMILES. N. O'Boyle, J.W. Mayfield

3:05 Intermission.

3:20 CINF **19.** HELM: An open standard for biomolecule structure representation and exchange. T. Zhang, S.H. Rotstein

3:45 CINF **20.** Living in a world of federated knowledge: Challenges, principles, tools and solutions. R. Zakharov, V. Tkachenko

4:10 CINF **21.** Research in the chemical sciences as a global social machine. J.G. Frey

4:40 Discussion.

Section B

Washington Marriott at Metro Center
Junior Ballroom 2

What do Synthetic Chemists Want from Their Reaction Systems?

Cosponsored by COMP, INOR, MEDI and ORGN

D. Evans, Organizer

W. A. Warr, Organizer, Presiding

1:30 CINF **22.** From search tool to research partner: Changing the role of computers in chemical development. O. Ravitz, R. Threlfall, D.W. Flanagan

1:55 CINF **23.** Supporting synthetic research with SciFinder-n. J. Taylor, J. Schloss, K. Zielenbach

2:20 CINF **24.** Renaissance of reaction classification and visualization: History, definition and new use cases. V. Eigner Pitto, H. Kraut, Z. Meza-Renken, C. Oppawsky, A. Orta, H. Saller

2:45 CINF **25.** ReaxysTree for reactions. J. Swienty Busch

3:10 Intermission.

3:30 CINF **26.** Analyzing reaction pathways in Reaxys. M. Clark, F. van den Broek

3:55 CINF **27.** Any electron withdrawing group will do: Introducing specific ambiguity into reaction searches. J.N. Curran

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4:20 Panel Discussion.

4:45 Concluding Remarks.

Science Communications: The Art of Developing a Clear Message

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SUNDAY EVENING

Section A

Grand Hyatt Washington
Farragut Square/Lafayette Park

CINF Scholarships for Scientific Excellence: Student Poster Competition

S. J. Chalk, *Organizer*

6:30 - 8:30

CINF 28. Evaluation of three retention time prediction models: 1) logP, 2) ACD/ChromGenius, and 3) a quantitative structure retention relationship model. A.D. McEachran, K. Mansouri, S. Newton, B. Beverly, J.R. Sobus, A.J. Williams

CINF 29. REAL fragments: A database of synthetically accessible fragment-like molecules. O. Gavrylenko, A. Chupryna, T. Matviyuk, Y. Moroz

CINF 30. Analysis of X-Chem DNA-encoded chemical libraries. L. Xue, E.A. Sigel, Y. Zhang

CINF 31. Comparative cheminformatic analysis of DNA methyltransferase inhibitors. O. Palomino-Hernandez, J.L. Medina-Franco

CINF 32. Cheminformatic approach to identify antiviral components of mimic substances. A. Orlov, A.Y. Zhrebker, A.A. Eletskaia, L.I. Kozlovskaya, V.A. Palyulin, D.I. Osolodkin, I.V. Perminova

CINF 33. Cheminformatics approach to exploring and modeling trait-associated metabolic profiles. J. Ash, M.A. Kuenemann, D. Fourches

CINF 34. Performance improvements, new functionalities and applications of the 3D structure generator CORINA Classic. B. Bienfait, T. Kleinoeder, C. Schwab, A. Mostrag, A. Tarkhov, J. Rathman, C. Yang

CINF 35. Using publicly available resources to build a comprehensive knowledge-base of chemical information. B. Sattarov, R. Zakharov, V. Tkachenko

CINF 36. Predicting drug-target interactions by dual-network integrated logistic matrix factorization. M. Hao, S.H. Bryant, Y. Wang

CINF 37. Machine learning approach for fast and accurate prediction of optical properties of organic molecules. M.F. Afzal, J. Hachmann, C. Cheng

Technical program information known at press time.

The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

CINF 38. First-principles insight into catalytic process of iodotyrosine deiodinase: A thyroid hormone. S. Tah

CINF 39. Ascertaining binding constant error when modeling spectrophotometric titration data. N. Kazmierczak, D.A. Vander Griend

CINF 40. PKS enumerator to enumerate the chemical space of macrolides. P. Kyaw Zin, D. Fourches

MONDAY MORNING

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

Government(-Funded) Chemical Databases & Open Chemistry

L. McEwen, *Organizer*

E. Bolton, M. C. Nicklaus, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 41. Mining PubChem for solubility data. S.J. Chalk

9:00 CINF 42. COSMOS database as a tool for ontology-driven data mining, in silico modeling and read-across. C. Yang, J. Rathman, A. Mostrag, C. Schwab, A. Tarkhov, J. Liu, M. Cronin, J. Madden, A. Bassan, E. Fioravanzo

9:25 CINF 43. US FDA's chemical evaluation and risk estimation system. K. Arvidson, P. Volarath, L. Holt, M. Garg, D. Mehta

9:50 CINF 44. Globalizing FDA's Substance Registration System. F.L. Switzer, L. Callahan, Y. Borodina, T.A. Peryea

10:15 Intermission.

10:30 CINF 45. PubChem: An open chemistry database. J. Zhang, P. Thiessen, A. Gindulyte, E. Bolton

10:55 CINF 46. Hazardous Substances Data Bank: Recent features and enhancements. S. Jordan, G. Fonger, G.F. Hazard

11:20 CINF 47. Harmonization and exchange of government data on chemical(plus) substances. E. Schmid, S. Winfield, Y. Borodina, J. Harman

11:45 CINF 48. FDA/CDER Chemical Informatics Program's Chemical Dictionary. M.T. Kim, N. Kruhlak

Section B

Washington Marriott at Metro Center
Junior Ballroom 2

Collaborating for Success: Professional Skills Development for Undergraduates, Graduates & Post-Docs

Cosponsored by CHED, PROF and YCC

E. Alvaro, J. R. Garritano, *Organizers, Presiding*

8:20 CINF 49. Getting a grip on STEM: Conducting a needs assessment of graduate student needs through focus groups. D. Zwicky, N. Johnson

8:40 CINF 50. NSF Research Traineeship (NRT) Program: STEM graduate training and strong professional skill development. L. Regassa, N. Riddick

9:00 CINF 51. Advancing inclusive excellence for trainees on the top down. R. Hernandez, D. Stallings, S. Iyer

9:20 Intermission.

9:30 CINF 52. Expand career support for STEM graduate students with the Graduate Career Consortium. A. Clobes, N. Lundsteen

9:50 CINF 53. Career pathways and resources for professional development. S. Nichols

10:10 CINF 54. Professional development and career resources: The past, present, and future of ACS on Campus. S. O'Reilly, M. Qiu

10:30 CINF 55. Science communication and education network (SCeNe) professional development workshops. C.B. Monroe, S. Rodriguez Martinez, D.J. Steinberg

10:50 Intermission.

11:00 CINF 56. Data carpentry in the Caltech libraries. D. Wrublewski, G. Clement, T. Morrell

11:20 CINF 57. Case studies in patent information. R.M. Kaminecki

11:40 CINF 58. Professional skill set development: Research operations management. J.M. Pickel

Building a Safety Culture across the Chemistry Enterprise

Institutional & Enterprise Level Efforts to Developing a Safety Culture

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CCS, CEI, CELL, CEPA, CHAS, CINF, COLL, CPRC, CTA, DAC, ETHX, I&EC, INOR, ORGN, PROF, SCHB and YCC

Chemistry in an Evolving Political Climate: Research Priorities & Career Pathways in Public Policy

Sponsored by YCC, Cosponsored by BIOL, CARB, CCPA, CEI, CELL, CEPA, CHED+, CINF, COLL, COMSCI, CPRC, DAC, GEOC, IAC, PRES and SCHB

MONDAY AFTERNOON

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

Government(-Funded) Chemical Databases & Open Chemistry

L. McEwen, *Organizer*

E. Bolton, M. C. Nicklaus, *Organizers, Presiding*

1:35 Introductory Remarks.

1:40 CINF 59. Building a model organism metabolome database. C. Steinbeck, M.R. Viant

2:05 CINF 60. Pharos: Putting targets in context. D. Nguyen, T. Sheils, G. Mandava, N. Southall, R. Guha

2:30 CINF 61. Chemical databases and other open-chemistry resources provided by the NCI CADD Group. H. Patel, Y. Pevzner, D. Dhaked, M.L. Peach, M.C. Nicklaus

2:55 CINF 62. Jmol: The evolution of a powerful molecular visualization tool enhanced by US public databases. O.S. Rothenberger, R.M. Hanson

3:20 Intermission.

3:35 CINF 63. ZINC: A free database of commercially available compounds for virtual screening and ligand discovery. J.J. Irwin

4:00 CINF 64. Chemistry Development Kit v2.0. J.W. Mayfield, E.L. Willighagen

4:25 CINF 65. Open Chemistry: Rich, open source tools for chemical data on the web and desktop. M.D. Hanwell

4:50 CINF 66. Open chemistry registry and mapping platform based on open source cheminformatics toolkits. V. Tkachenko, D. Slenker, N. Jeilazkova, A. Gaulton, A.J. Williams, C. Steinbeck, C. Evelo, E.L. Willighagen

Section B

Washington Marriott at Metro Center
Junior Ballroom 2

Collaborating for Success: Professional Skills Development for Undergraduates, Graduates & Post-Docs

Cosponsored by CHED, PROF and YCC

E. Alvaro, J. R. Garritano, *Organizers, Presiding*

1:20 CINF 67. Importance of skills development in the ACS certified bachelor's degree in chemistry. T.J. Wenzel

1:40 CINF 68. Fostering collaboration for success: How NSF CCIs train students for STEM leadership. D. Watt

2:00 CINF 69. Facilitating broader impacts: Disseminating knowledge to facilitate new and traditional careers in chemistry. K. Deards

2:20 Intermission.

2:30 CINF 70. Assessment of information literacy skills of students in large undergraduate chemistry courses. S.P. Baykoucheva, M. Koppel, S. Rastogi

2:50 CINF 71. Connecting organic chemistry to the real world with Chemistry Class Advantage™. M. Pozenel

3:10 CINF 72. Withdrawn.

3:30 CINF 73. Collaborative efforts between faculty and embedded safety professionals to improve critical thinking skills of undergraduates. S.B. Sigmann

3:50 Intermission.

4:00 CINF 74. Data management: A skill for all chemists. M. Sheffield, M. Savidakis-Dunn

4:20 CINF 75. Tell your story your way: Why chemistry professionals should understand bibliometrics and altmetrics. R. Borchardt

4:40 CINF 76. Five years of helping chemists to create an online presence using freely available resources. A.J. Williams

Building a Safety Culture across the Chemistry Enterprise

Grassroots Approaches to Developing a Safety Culture

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CCS, CEI, CELL, CEPA, CHAS, CINF, COLL, CPRC, CTA, DAC, ETHX, I&EC, INOR, ORGN, PROF, SCHB and YCC

Chemistry in an Evolving Political Climate: Research Priorities & Career Pathways in Public Policy

Sponsored by YCC, Cosponsored by BIOL, CARB, CCPA, CEI, CELL, CEPA, CHED+, CINF, COLL, COMSCI, CPRC, DAC, GEOC, IAC, PRES and SCHB

MONDAY EVENING

Section A

Walter E. Washington Convention Center
Halls D/E

Sci-Mix

E. Alvaro, *Organizer*

8:00 - 10:00

8, 14, 17, 29-35, 39-40. See previous listings.

CINF 77. Keeping up and keeping organized: Alerting services and personal bibliographic databases. C.F. Huber

80, 113, 142. See subsequent listings.

TUESDAY MORNING

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

Informatics & Chemical Biology: Identifying Targets & Biological Pathways

Cosponsored by BIOL and MEDI

R. J. Bienstock, *Organizer, Presiding*

8:00 CINF 78. Data harmonization and quality assurance in metabolomics for biological pathway identification. D.A. Sheen, W. Fortunado de Carvalho Rocha, D. Bearden, K.A. Lipka

8:25 CINF 79. Withdrawn.

8:50 CINF 80. Exploring opioid receptor-ligand binding patterns, as a fingerprint to identify potential biased agonists. K. Martinez Mayorga, A. Madariaga-Mazon, C.R. Garcia-Jacas

9:15 Intermission.

9:25 CINF 81. Development of a search engine for chemical biology and drug discovery. D.W. Selinger, A.P. Sukharevsky

9:50 CINF 82. Design and analysis of biologically annotated libraries for phenotypic screening deconvolution. A.M. Wassermann

10:15 CINF 83. Way2drug cheminformatics platform for drug repurposing. V. Poroikov, D. Druzhilovskiy, A. Rudik, P. Pogodin, D. Filimonov, A. Lagunin, G. Sastry

10:40 Intermission.

10:50 CINF 84. Towards the use of bioassays as predictors of adverse events in clinical trials. M. Clark, M. Shkrob, A. Yuryev

11:15 CINF 85. Mechanism-of-action elucidation using deep convolutional neural networks. A. Heifets, I. Wallach, K.T. Nguyen

11:40 CINF 86. Using deep neural networks with heterogeneous chemical data to support phenotypic assay campaigns. A. de la Vega de Leon, V.J. Gillet

Section B

Washington Marriott at Metro Center
Junior Ballroom 2

Markush 360: Current & Future of Generic Structures in Chemical Patent Creation, Search & Analysis

Á. Figyelmes, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 CINF 87. Understanding linguistic Markush expressions in chemical patents. L. Weber, M. Irmer, C. Bobach

8:40 CINF 88. Everlasting challenge: Markush indexing, searching and display in modern retrieval systems. V. Eigner Pitto, H. Kraut, H. Matuszczyk, F. Ailer

9:10 CINF 89. Advanced Markush technologies: Automatic generation, non-hit visualization and overlap analysis. P. Kovács, Á. Figyelmes, G. Botka, J. Kendi

9:40 CINF 90. Challenges and successes in machine interpretation of Markush descriptions. D.M. Lowe, J.W. Mayfield, R.A. Sayle

10:10 Intermission.

10:25 CINF 91. Challenges in extracting Markush structure data from structure depictions and related text. A.T. Valko, P. Johnson

10:55 CINF 92. MARPAT: CAS's database of Markush structures. P. Blasi

11:25 CINF 93. Markush enumeration to manage, mesh and manipulate substances of unknown or variable composition. A.J. Williams, C. Grulke, A.D. McEachran, E. Schymanski

11:55 Concluding Remarks.

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

Sponsored by AGFD, Cosponsored by AGRO, CINF and PROF

Understanding the Chemistry of Our Planet

Chemistry's Role in our Earth System

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CEI, CELL, CEPA, CINF, COLL, CPAC, DAC, GEOC, I&EC, INOR, ORGN, SCHB and YCC

TUESDAY AFTERNOON

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

Herman Skolnik Award Symposium

E. Alvaro, D. Winkler, *Organizers*

E. Davis, *Presiding*

1:45 Introductory Remarks.

1:50 CINF 94. Approaching reality: Simulating electronic devices. T.R. Clark

2:15 CINF 95. Applications of machine learning to materials and chemical property prediction. A. Tropsha

2:40 CINF 96. Nanoinformatics platform for environmental impact assessment of manufactured nanomaterials. Y. Cohen, M. Bilal, P. Church, H. Liu, R. Liu

3:05 CINF 97. Accurate and interpretable nanoQSAR models from genetic programming-based decision tree construction approaches. C. Oksel

3:30 Intermission.

3:45 CINF 98. Self-organizing neural networks in chemistry. J. Gasteiger

4:10 CINF 99. Understudied proteins: Time to shift the paradigm. T.I. Oprea

4:35 CINF 100. Sparse QSAR modelling methods for therapeutic and regenerative medicine. D.A. Winkler, F.R. Burden, H. Autefage, M. Stevens, E. Gentleman, A. Hook, P. Williams, M. Alexander

5:10 Award Presentation.

Section B

Washington Marriott at Metro Center
Junior Ballroom 2

Why Open Data? Effective Use Cases & Exemplars for Open Data & Citizen Science

T. Hanna, D. P. Henderson, L. McEwen, *Organizers, Presiding*

1:45 Introductory Remarks.

1:50 CINF 101. Benefits of making data from the EPA National Center for Computational Toxicology available for reuse. A.J. Williams, K. Mansouri, V. Tkachenko, K. Blinov, C. Grulke

2:15 CINF 102. Environmental protection belongs to the public: Citizen science at EPA. A. Parker

2:40 CINF 103. Solar Army: Incorporating real-time research into outreach efforts. J.D. Schuttefield Christus, M. DeBoever

3:05 CINF 104. Hunting for people: Building public engagement with your science. J. Ranganathan

3:30 Intermission.

3:45 CINF 105. Solving biomolecular puzzles with citizen science. S. Cooper

4:10 CINF 106. Reliability of data: A meaningful and comprehensive assessment. A. Kazakov, A. Bazyleva, E. Paulechka, V. Diky, K. Kroenlein

4:35 CINF 107. For reproducibility, we need the methods behind the open data. L. Teytelman

5:00 CINF 108. PubChem and open data. S. Kim, E. Bolton

Understanding the Chemistry of Our Planet

Human Impacts to our Planet

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CEI, CELL, CEPA, CINF, COLL, CPAC, DAC, GEOC, I&EC, INOR, ORGN, SCHB and YCC

WEDNESDAY MORNING

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

Government(-Funded) Chemical Databases & Open Chemistry

L. McEwen, *Organizer*

E. Bolton, M. C. Nicklaus, *Organizers, Presiding*

9:05 Introductory Remarks.

9:10 CINF 109. ViralChEMBL: Purification and enhancement of antiviral activity data from ChEMBL. D.I. Osolodkin, A.A. Nikitina, A. Orlov

9:35 CINF 110. ChemDB: A database of structure and biological activity data for pre-clinical compounds tested against HIV, *Mycobacterium tuberculosis*, and opportunistic infections. L. Sumner, M. Rush, M. Whiting, G. Noble, D. Huffman, M. Nasr

10:00 CINF 111. ChemIDplus at NLM: History and capabilities. S. Jordan, G.F. Hazard, M. Miller

10:25 Intermission.

10:40 CINF 112. PubChem as a biologics database. N. O'Boyle, R.A. Sayle, E. Bolton

11:05 CINF 113. ScrubChem: Cleaning of PubChem BioAssay data to create diverse and massive bioactivity datasets for use in modeling applications. J.B. Harris, J.C. Harris, O. Isayev, A. Tropsha, R. Judson

11:30 CINF 114. Adding value to public data using the BioAssay Express: Using semantic web axioms and machine learning to support annotation. H. Kucuk-McGinty, J.E. Kranz, B.A. Bunin, A. Clark

Section B

Washington Marriott at Metro Center
Junior Ballroom 2

Drug Discovery: Cheminformatic Approaches

Cosponsored by COMP

E. Davis, *Organizer, Presiding*

9:15 Introductory Remarks.

9:20 CINF 115. Assay Central: A new approach to compiling big data and preparing machine learning models for drug repurposing. K.M. Zorn, M.A. Lingerfelt, A. Clark, S. Ekins

9:45 CINF 116. Integrated cheminformatics to guide drug discovery. M.D. Segall, E. Champness, P. Hunt, T. Mansley

10:10 CINF 117. CSD-driven conformer generation: Finding missing rings and a large-scale validation. P. Sanschagrin, M.G. Read, P. McCabe, J. Cole, O. Korb, R. Taylor

10:35 Intermission.

10:50 CINF 118. Autonomous model building with a preponderance of well annotated assay protocols. A. Clark

11:15 CINF 119. Meeting the ever changing demands of synthetic chemistry: A chemical workbench for biopolymers. J. Bishop

11:40 CINF 120. *In silico* pharmacology: Predicting pharmacokinetic and toxic properties. P. Schyman, R. Liu, V. Desai, A. Wallqvist

Drug Design

Sponsored by COMP, Cosponsored by CINF

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WEDNESDAY AFTERNOON

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

Government-(Funded) Chemical Databases & Open Chemistry

L. McEwen, *Organizer*

E. Bolton, M. C. Nicklaus, *Organizers, Presiding*

1:20 Introductory Remarks.

1:25 CINF 121. EPA Comptox Chemistry Dashboard: Web-based data integration hub for environmental chemistry and toxicology data. A.J. Williams, C. Grulke, A.D. McEachran, A. Richard, J. Smith, R. Jolley, J. Dunne, E. Edmiston, J. Edwards

1:50 CINF 122. Need and benefits for structure standardization to facilitate integration and connectivity between government databases. V. Tkachenko, C. Grulke, A.J. Williams

2:15 CINF 123. Materials project: Milestones, challenges, and opportunities in high-throughput computational chemistry. J. Montoya, K. Persson

2:40 CINF 124. WebFF: Ontology based force-field repository for organic and soft materials. F.R. Phelan, H. Sun

3:05 Intermission.

3:20 CINF 125. Management and distribution of chemical data in the PDB. J. Young

3:45 CINF 126. PDB-Chem: A sub-atomic resolution database and resolution extension tool. R.E. Cachau, I.A. Topol, J. Zhu, A. Podjarny, M.L. Peach, M.C. Nicklaus

4:10 CINF 127. Publishing reference data on the Internet. P. Linstrom

4:35 CINF 128. Building a high quality reference tandem mass spectral library for comprehensive compound identification. X. Yang, P. Neta, S. Stein

Section B

Washington Marriott at Metro Center
Junior Ballroom 2

Drug Discovery: Cheminformatic Approaches

Cosponsored by COMP

E. Davis, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 129. Characterizing the chemical space of kinase inhibitors using molecular descriptors computed from molecular dynamics trajectories. J. Ash, D. Fourches

2:00 CINF 130. Splitting the difference - with confidence. R.D. Clark, M. Waldman

2:25 CINF 131. Development and comparison of deep learning toolkit with other machine learning methods. A. Mitrofanov, A. Korotcov, V. Tkachenko, S. Ekins

2:50 Intermission.

3:05 CINF 132. Stopping Zika virus: Computational search for deactivating agents. N. Sizochenko, J.R. Leszczynski

3:30 CINF 133. Fragment promiscuity and binding mode variability. M.N. Drwal, G. Bret, J. Desaphy, C. Perez, E. Kellenberger

3:55 CINF 134. Chemical-biological space exploration for discovery of novel anti-HIV agents. V. Poroikov, D. Filimonov, D. Druzilovskiy, Y. Pevzner, M.C. Nicklaus

4:20 CINF 135. Ensemble machine learning to improve scoring functions. X.S. Wang

Drug Design

Sponsored by COMP, Cosponsored by CINF

THURSDAY MORNING

Section A

Washington Marriott at Metro Center
Junior Ballroom 1

General Papers

E. Alvaro, *Organizer, Presiding*

8:45 CINF 136. Towards linking chemical-disease and chemical-gene/protein information in PubChem. L. Zaslavsky, D.M. Lowe, E. Bolton

9:00 CINF 137. Platform for unified molecular analysis (PUMA). M. González-Medina, J.L. Medina-Franco

9:15 CINF 138. Structural isosteres of phosphate groups in the protein data bank. A. Borrel, Y. Zhang, L. Ghemto, L. Regad, G. Boije af Gennas, A. Camproux, J.T. Yli-Kauhaluoma, H. Xhaard

9:30 CINF 139. Exploration of REAL arrays for initial hit finding. O. Savich, O. Vasylychenko, A. Chupryna, M. Platonov, Y. Moroz

9:45 CINF 140. Optimization of dangerous parameters in global analysis of spectrophotometric titration data: Information beyond the binding constant. D.A. Vander Griend, N. Kazmierczak

10:00 CINF 141. Pesticide quantitative biodegradability-structure relationships. D. Girovic, M. Hastings, K. Lynn, R. Rasoulpour, S. Gehen, D. Tomandl

10:15 Intermission.

10:30 CINF 142. Activity landscape plotter: An open web-based server to assess structure activity relationships. M. González-Medina, O. Méndez-Lucio, J.L. Medina-Franco

10:45 CINF 143. Practical and effective: Strategies to engage chemistry undergraduate students into library information literacy training. S. Guo

11:00 CINF 144. CAS Registry: A unique identifier of chemical substances. E.N. Cheeseman

11:15 CINF 145. Search for highly strained disulfide bonds in the Protein Databank. D. Riccardi

11:30 CINF 146. Intentional diversification of molecular library. Y. Kwon, S. Kang, I. Kim, K. Kim, J. Yoo, H. Lee, J. Shin

11:45 CINF 147. Integrated *in silico* approaches to design power conversion efficient solar cells: Renewable energy for future. S. Kar, J.R. Leszczynski

Drug Design

Sponsored by COMP, Cosponsored by CINF

TOXI

Division of Chemical Toxicology

T. Spratt, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Analytical Toxicology in the 21st Century (see ANYL, Sun)

Pfizer Award in Enzyme Chemistry (see BIOL, Tue)

Off Targets No More: CYP450 Enzymes as Drug Discovery Targets (see MEDI, Mon)

Ecological & Human Health Impacts of Emerging Environmental Contaminants (see ENVIR, Sun, Mon, Wed)

Food-Borne Toxicants: Formation, Analysis & Toxicology (see AGRO, Wed, Thu)

Arthur C. Cope Award Symposium (see ORGN, Tue)

SOCIAL EVENTS:

Dinner, 6:30 PM: Tue

Award Ceremony, 9:00 PM: Tue

BUSINESS MEETINGS:

Business Meeting, 8:30 PM: Tue

SUNDAY MORNING

Section A

Marriott Marquis Washington, DC
Georgetown University

Chemical Research in Toxicology Young Investigators Award

H. Ai, *Organizer, Presiding*

S. S. Hecht, T. M. Penning, *Presiding*

8:00 Introductory Remarks.

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

8:55 TOXI 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 TOXI 3. Dynamic visualization of signaling molecules in living cells. J. Zhang

10:40 Award Presentation.

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

Analytical Toxicology in the 21st Century

Sponsored by ANYL, Cosponsored by TOXI

SUNDAY AFTERNOON

Section A

Marriott Marquis Washington, DC
Georgetown University

Founders' Award

I. A. Blair, *Organizer, Presiding*

1:00 Founders' Award Presentation.

1:10 Introductory Remarks.

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

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

2:35 TOXI 7. Chemical biology of DNA damage by α,β -unsaturated aldehydes. L.J. Marnett

3:15 Intermission.

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

4:10 TOXI 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

Section A

Marriott Marquis Washington, DC
Georgetown University

TOXI Young Investigators

Cosponsored by YCC

T. Spratt, *Organizer*

B. Ma, U. Sarkar, *Presiding*

8:00 TOXI 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 TOXI 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 TOXI 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 TOXI 13. Replicative bypass and mutagenic properties of alkylphosphotriester lesions in *Escherichia coli*. J. Wu, P. Wang, Y. Wang

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

9:40 Intermission.

10:00 TOXI 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 TOXI 16. Engineering a replicative DNA polymerase for specific damage bypass capability. T.A. Coulther, M.J. Ondrechen, P.J. Beuning

Technical program information known at press time. The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017