CINF

Division of Chemical Information

R. Bienstock*, Program Chair*

SOCIAL EVENTS:
Reception & Poster Session, 6:30 PM: Sun
Luncheon, 12:00 PM: Tue
BUSINESS MEETINGS:
Committee Meetings, 12:30 PM: Sat

SUNDAY MORNING

Section A

Westin Boston Waterfront
Harbor Ballroom II

Chemoinformatic Approaches to Enhance Drug Discovery Based on Natural Products

J. L. Medina-Franco, *Organizer, Presiding*
N. Sánchez-Cruz, *Presiding*

8:30 Introductory Remarks.

8:35 CINF 1. Exploiting PubChem for drug discovery based on natural products. **S. Kim**, E. Bolton

9:00 CINF 2. Connecting traditional with evidence-based medicine. **T. Polgar**

9:25 CINF 3. Development of a "drug-like" natural product library from the East African flora. C. Simoben, **F. Ntie-Kang**, W. Sippl

9:50 Intermission.

10:05 CINF 4. Development of an innovative database to uncover chemical and biological information from Brazilian biodiversity. **A.D. Andricopulo**, M. Valli, A. Pilon, I. Castro-Gamboa, A. Dametto, M. Pinto, R. Freire, V.D. Bolzani

10:30 CINF 5. Search of biased mu-opioid receptor ligands from nature. **A. Madariaga**, A.F. Marmolejo, K. Martinez Mayorga

10:55 CINF 6. Predicting blood-brain barrier permeability of marine-derived kinase inhibitors. **F. Plisson**, A.M. Piggott, N. Hamilton, R.J. Capon

11:20 CINF 7. Template-free 3D structure generation and conformer search: Complex natural products and macrocycles. **A.N. Jain**, A.E. Cleves

Section B

Westin Boston Waterfront
Lewis

Reporting & Reproducibility of Chemistry Research Data

Cosponsored by ETHX and ORGN
Financially supported by Chemical Structure Association Trust; IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)
M. G. Hicks, H. A. Lawlor, L. R. McEwen, V. F. Scalfani, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 8. The internet of molecules. **S. Boyer**

9:00 CINF 9. Reaction networks analysis for algorithmic process development. **A. Lapkin**, P. Jacob

9:25 CINF 10. International chemical identifier for reactions (RInChI): The key to managing reaction databases effectively. **J.M. Goodman**, G. Blanke, G. Grethe, H. Kraut

9:50 CINF 11. *De facto* standard or a free-for-all? A benchmark for reading SMILES. **N. O'Boyle**, J. Mayfield, R.A. Sayle

10:15 Intermission.

10:30 CINF 12. Reporting crystal structure data: Recent insights. **C. Tovee**, S. Ward, A. Sarjeant, I. Bruno

10:55 CINF 13. Extending machine learning capabilities for semi-automated annotation of biological assays in BioAssay Express. **P. Gedeck**, H. McGinty, B.A. Bunin, A. Clark

11:20 CINF 14. Blockchain for research. **J. van Rossum**

11:45 Discussion.

Section C

Westin Boston Waterfront
Harbor Ballroom III

Chemical Structure Searching for Patent Information

Cosponsored by CHAL and CPRM
R. J. Bienstock, *Organizer*
E. N. Cheeseman, M. McBride, E. S. Simmons, *Organizers, Presiding*

8:30 Introductory Remarks.

8:45 CINF 15. Chemical structure searching for patents through the years. **E.S. Simmons**

9:15 CINF 16. Same structure, different answers: Examining the impact of chemical indexing policy on retrieval of patent references. **S.R. Adams**

9:45 CINF 17. Beyond the search: Deep analysis of chemical patents and Markush claims. **J. Biagi**, Á. Figyelmesi

10:15 Intermission.

10:30 CINF 18. State of chemical structure searching 30 years on OR The human element – the power behind structure searching in the CAS content collection. **E.N. Cheeseman**

11:00 CINF 19. Chemical indexing and searching with Orbit Chemistry modules. **A. Kandi-Masakidi**

11:30 CINF 20. Chemistry in patents: Unique perspectives within Derwent World Patents Index. **S. Hajkowski**

Moving the Safety Values of the ACS Forward

Sponsored by PRES, Cosponsored by AGFD, ANYL, BIOL, BMGT, CA, CARB, CCS, CHAS‡, CINF, COLL, CPT, ENFL, ENVR, I&EC, ORGN, PROF and SCHB

SUNDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Ballroom II

Chemoinformatic Approaches to Enhance Drug Discovery Based on Natural Products

J. L. Medina-Franco, *Organizer, Presiding*
N. Sánchez-Cruz, *Presiding*

1:30 CINF 21. Natural product databases: Chemical space, diversity and suitability of virtual screening. **F. Saldivar**, J. Medina Franco

1:55 CINF 22. Characterization of the chemical space of purchasable natural products. Y. Chen, C. de Bruyn Kops, M. Garcia de Lomana, N. Friedrich, **J. Kirchmair**

2:20 CINF 23. Exploring natural product analogs in chemical universe databases. **M. Awale**, J. Reymond

2:45 Intermission.

3:00 CINF 24. OpenZika: Discovery of new antiviral candidates against Zika virus. **M. Mottin**, A.S. Carvalho, C.C. Melo-Filho, B.J. Neves, R.C. Braga, C.S. Lima, S. da Silva, J.F. Shimizu, N.C. Mesquita, L.O. Regasini, A.C. Jardim, E. Muratov, G. Oliva, A.L. Perryman, S. Ekins, C.H. Andrade

3:25 CINF 25. Designing synthetically accessible natural-product mimetics by machine learning. **G. Schneider**, L. Friedrich, F. Grisoni, D. Merk

3:50 CINF 26. Similarity search and pharmacophore modeling approaches to aid natural products drug discovery against tropical infectious diseases. **E. Pavadai**, G. Kaur, P. Mutai, K. Chibale

4:15 CINF 27. Identification of bichalcones as natural product sirtuin inhibitors by virtual screening and *in vitro* testing. B. Karaman, Z. Alhalabi, S. Swyter, S. Mihigo, K. Andrae-Marobela, M. Jung, W. Sippl, **F. Ntie-Kang**

4:40 Concluding Remarks.

Section B

Westin Boston Waterfront
Lewis

Reporting & Reproducibility of Chemistry Research Data

Cosponsored by ETHX and ORGN
Financially supported by Chemical Structure Association Trust; IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)
M. G. Hicks, H. A. Lawlor, L. R. McEwen, V. F. Scalfani, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CINF 28. Assessing the quality of scientific data. **J. Rumble**

2:00 CINF 29. Scope of ELNs and repositories to improve scientific documentation and reporting: Examples taken from the Chemotion-ELN and Chemotion-Repository. **N. Jung**, P. Tremouilhac, S. Braese

2:25 CINF 30. Bottom-up training in reproducible research: Undergraduate level approaches. **A.C. Evans**

2:50 Intermission.

3:05 CINF 31. Reproducibility in organic syntheses. **R.L. Danheiser**

3:30 CINF 32. Progress in delivering transparency in research data by the National Center for Computational Toxicology at the US EPA. **A.J. Williams**, J. Edwards, C. Grulke, J. Cowden

3:55 CINF 33. Better reporting for better measurements: Enzyme kinetics as a case study. W. Stroberg, **S. Schnell**

4:20 CINF 34. Networking chemically capable robots using Twitter for RealTimeChem. **L. Cronin**, D. Caramelli, D. Salley

4:45 Discussion.

Section C

Westin Boston Waterfront
Harbor Ballroom III

Chemical Structure Searching for Patent Information

Cosponsored by CHAL and CPRM
R. J. Bienstock, *Organizer*
E. N. Cheeseman, M. McBride, E. S. Simmons, *Organizers, Presiding*

1:30 Introductory Remarks.

1:45 CINF 35. Structure searching for patent information: The need for speed. **J. Mayfield**, N.M. O'Boyle, R.A. Sayle

2:15 CINF 36. Pros and cons of 22 million patent-extracted structures in PubChem. **C. Southan**

2:45 CINF 37. Automating chemical structure and inhibition data extraction from patents: A text mining approach. **A. Hinton**

3:15 Intermission.

3:30 CINF 38. Searching for patent information in PubChem. **S. Kim**, P. Thiessen, A. Gindulyte, E. Bolton

4:00 CINF 39. Navigating around patented routes with the help of computer-driven retrosynthetic analysis. **K. Molga**, P. Dittwald, B. Grzybowski

4:30 CINF 40. Software for presenting results of chemical structure searches. **J.A. Willmore**

Moving the Safety Values of the ACS Forward

Sponsored by PRES, Cosponsored by AGFD, ANYL, BIOL, BMGT, CA, CARB, CCS, CHAS‡, CINF, COLL, CPT, ENFL, ENVR, I&EC, ORGN, PROF and SCHB

SUNDAY EVENING

Section A

Westin Boston Waterfront
Galleria

CINF Poster Session

E. Alvaro, S. J. Chalk, *Organizers*

6:30 - 8:30

CINF 41. Easy exploration of synthetically accessible chemical space via synthesis-aware enumeration. **I. Tubert-Brohman**, K.D. Konze, S. Bhat, S. Watts

CINF 42. Computational approach towards understanding genotoxic and mutagenic biological pathways of azo dyes within organisms. **R.J. Bienstock**, L. Perera, M.A. Pasquinelli

CINF 43. From just in case to just in time – just maybe not. **P. Borrego**, K. Zdepski

CINF 44. Data visualization and analysis of the NIST TRC ThermoML Dataset. **S. Bagdadi**, K. Skinner, S.J. Chalk

CINF 45. Combined computational chemistry and machine learning approach to assess the drug-likeness of fullerene nanostructures. **B. Rasulev**, N. Fjorodova

CINF 46. Outlook on the development of antidiabetic compounds: Databases, scaffolds and current trends. **A. Madariaga**, K. Martinez Mayorga

CINF 47. Leveraging IUPAC recommendations for the ontological description of PubChem Data. **K. Skinner**, J. Rotne, S. Bagdadi, S.J. Chalk

CINF 48. Text mining the IUPAC recommendations: Opportunities for knowledge discovery. **J. Rotne**, S.J. Chalk

CINF 49. Symmetry and chirality analysis of substituted ferrocenes. **A.W. Kaspi-Kaneti**, I. Tuvi-Arad

CINF 50. Cheminformatics-based differential modeling of dynamic ERK1/2-inhibitor interactions. **J. Ash**, J. Hughes-Oliver, D. Fourches

CINF 51. Data integration and fragment analysis reveal important structural motifs for ligand selectivity among hepatic organic anion transporting polypeptides. A. Türkova, **B. Zdrazil**

CINF 52. Development of a taxonomy and indexing policy for InChI open education resources and publications. **V.F. Scalfani**, **R.E. Belford**

CINF 53. Supporting the assessment of the purging of potential mutagenic impurities via analysis of known reactions. **S.J. Webb**, M. Burns, E. Rosser

CINF 54. SynJet: A novel chemical dispensing platform for high throughput reaction screening and optimization. **J.D. White**, J.P. Malerich, S. Mallya, D. Stout, B. McCoy, D. Krieger, N. Collins

MONDAY MORNING

Section A

Westin Boston Waterfront
Harbor Ballroom II

Ethics of Data Sharing

Cosponsored by ETHX‡
J. N. Currano, P. A. Mabrouk, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 55. Research integrity: Perspectives from the NSF Office of Inspector General. **J. Kroll**

9:00 CINF 56. Connecting the dots between data management and research integrity. **S. Moore**

9:25 CINF 57. Long term viability of computational chemistry/biology research. **K.M. Merz**

9:50 CINF 58. Social aspects of chemical safety information. **L.R. McEwen**, **R. Stuart**

10:15 Intermission.

10:25 CINF 59. Computational analysis of publications' texts for bioassay protocol classification. **O. Tarasova**, I.S. Mayorov, D. Filimonov, V. Poroikov, I. Mayzus, A. Rzhetsky

10:50 CINF 60. Data sharing: Ethics in research. **K.M. Elkins**

11:15 CINF 61. Crystallographic crime: Detection and prevention of fake data. **A. Sarjeant**, I. Bruno

11:40 CINF 62. Chemistry data: Distortion and dissemination in the internet era. **A.J. Williams**

12:05 Discussion.

12:25 Concluding Remarks.

Section B

Westin Boston Waterfront
Lewis

Publishing Chemical Data

Cosponsored by ETHX and ORGN
Financially supported by Chemical Structure Association Trust, IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)
M. G. Hicks, H. A. Lawlor, L. R. McEwen, V. F. Scalfani, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 63. Publication of raw and curated NMR spectroscopic data for organic molecules. **C. Steinbeck**

9:00 CINF 64. Publishing spectral data in the cloud. **G.M. Banik**, K. Kunitsky, M. D'Souza, T. Abshear

9:25 CINF 65. Flow of experimental thermophysical and thermochemical data through the NIST Thermodynamics Research Center. **D. Riccardi**, A. Kazakov, S. Townsend, V. Diky, C. Muzny, K. Kroenlein

9:50 CINF 66. Web Force-Field (WebFF) Project: Molecular dynamics force-field repository for soft materials at multiple levels of granularity. **F.R. Phelan**, H. Sun

10:15 Intermission.

10:30 CINF 67. Reciprocal journal-to-chemistry connectivity in PubChem from the IUPHAR/BPS Guide to Pharmacology and other sources. **C. Southan**, J.L. Sharman, E. Faccenda, A.J. Pawson, S.D. Harding, J.A. Davies

10:55 CINF 68. Open data in chemistry: The fast track to scientific content. **J. Eiblmaier**, D. Geppert, H. Saller

11:20 CINF 69. Research data management using FAIR data repository with integrated machine learning. **V. Tkachenko**, B. Sattarov, A. Korotcov, R. Zakharov

11:45 CINF 70. SynOne - The use of an expert-defined chemical-compound class taxonomy to map organic synthesis articles from the chemistry literature. **F. Shortt de Hernandez**, T. Menke, J. Rochlitz

Growing with Project SEED: 50 years and 10,000+ Students

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MONDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Ballroom II

Where are the Standards: Biologics Registration & HELM

Representation of Biologics: Informatics Standards & Challenges

C. Bellamy, E. Bolton, D. Deng, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CINF 71. HELM: Continuing to set the standard for biomolecular representation. **S. Rotstein**

2:00 CINF 72. Current development and new challenges of HELM representation. **D. Deng**, T. Yuan, J. Lee, R. Hotchandani

2:25 CINF 73. Registering chemically modified oligonucleotides: Implementations and challenges. **Y. Potier**

2:50 Intermission.

3:00 CINF 74. Similarity analysis of oligonucleotides based on HELM notation. **M. Weisser**

3:25 CINF 75. monomer.org: The global hub for (bio)polymer informatics. **D.J. Milton**

3:50 CINF 76. Trials and tribulations of curating peptide and antibody ligands for the IUPHAR/BPS Guide to Pharmacology. **C. Southan**, J.L. Sharman, E. Faccenda, A.J. Pawson, S.D. Harding, J.A. Davies

4:15 Intermission.

4:25 CINF 77. Building a bridge between human-readable and machine-readable representations of biopolymers. **N. O'Boyle**, R.A. Sayle

4:50 CINF 78. Bridging the gap between small molecule and biologics editing: Drawing, viewing and sharing complex biomolecules with BioEddie and BiomoleculeToolkit. **A.D. Costache**, R. Knispel

5:15 Concluding Remarks.

Section B

Westin Boston Waterfront
Lewis

Publishing Chemical Data

Cosponsored by ETHX and ORGN
Financially supported by Chemical Structure Association Trust, IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)
M. G. Hicks, H. A. Lawlor, L. R. McEwen, V. F. Scalfani, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CINF 79. Publishing chemical data in public data repository. **J. Zhang**, P. Thiessen, A. Gindulyte, E. Bolton

2:00 CINF 80. ChEMBL – encouraging deposition of drug discovery data. **A. Gaulton**, P. Bento, J. Chambers, E. Felix, A. Hersey, D. Mendez, J.F. Mosquera, P. Mutowo, M. Nowotka, A. Leach

2:25 CINF 81. Data sharing and publication at NIST. **R.J. Hanisch**

2:25 CINF 82. Publishing chemical data sustainably: A crystallographic case study. **I. Bruno**, A. Sarjeant

2:50 CINF 83. Documenting chemical data. **P. Linstrom**

3:15 Intermission.

3:30 CINF 84. Profiling common types of data in chemistry research articles: What has changed in five years? **Y. Li**

3:55 CINF 85. Publication data standards and Supporting Information review at *Organic Letters*. **A.M. Hunter**

4:20 CINF 86. Sustainable processes for chemical data publishing – our experiences as a society publisher. R. Kidd, **G. Jones**

4:45 CINF 87. Enabling FAIR data in the Earth and space sciences. **S. Stall**, K. Lehnert, L. Wyborn, E. Robinson, H. Glaves, M. Parsons, B. Hanson, J. Cutcher-Gershenfeld, B. Nosek, L. Yarmey

MONDAY EVENING

Section A

Boston Convention & Exhibition Center
Exhibit Hall B2/C

Sci-Mix

R. J. Bienstock, *Organizer*

8:00 - 10:00

41-**48**, **50-54**. See previous listings.

TUESDAY MORNING

Section A

Westin Boston Waterfront
Harbor Ballroom II

Skolnik Symposium: De Novo Design

G. Schneider, *Organizer, Presiding*

9:00 CINF 88. Molecular recognition studies to advance structure-based drug design. **F.N. Diederich**

9:25 CINF 89. Computer-aided discovery of enzyme inhibitors. **W.L. Jorgensen**

9:50 CINF 90. Massive computational docking experiments to identify noble gases target for new 'atomic drugs'. **D.A. Winkler**, A. Thornton, G. Farjot, I. Katz

10:15 Intermission.

10:30 CINF 91. Progression saturation analysis of analog series using virtual candidate compounds. **J. Bajorath**

10:55 CINF 92. Novel method proposing chemical structures with desirable profile of activities based on chemical and protein spaces. **K. Funatsu**

11:20 CINF 93. Chemography: Toward "universal" maps of drug-like space. **A. Varnek**

Section B

Westin Boston Waterfront
Lewis

Chemistry Librarians of the Future

Cosponsored by CHED
J. R. Garritano, L. R. McEwen, V. F. Scalfani, *Organizers, Presiding*

8:20 Introductory Remarks.

8:25 CINF 94. History and perspective of chemical information services: Time for a return to the library chemist. **V.F. Scalfani**

8:50 CINF 95. Reimagining chemistry librarianship: From the bench to the stacks. **N. Ruhs**

9:15 CINF 96. Changing the landscape of the chemistry librarianship. **N. Bharti**

9:40 Intermission.

9:55 CINF 97. Ten plus years as a chemistry librarian, where have they gone? **J. Carver**

10:20 CINF 98. Pre- and post-research group selection: Evolving roles for chemistry librarians. **K. Deards**, **S. Jeong**

10:45 CINF 99. Nobody else is doing it: Teaching opportunities for the chemistry librarian of the future. **J.N. Currano**

11:10 CINF 100. New models for chemistry library impacts through an international symposium. **M.C. Schlembach**, B.J. McCall

11:35 Discussion.

TUESDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Ballroom II

Skolnik Symposium: *De Novo* Design

G. Schneider, *Organizer, Presiding*

1:30 CINF 101. Artificial Intelligence in drug design. **K. Baringhaus**

1:55 CINF 102. Robot scientists: Automating drug design. **R.D. King**

2:20 CINF 103. Accelerating drug discovery through a fully automated Design-Make-Test-Analyze workflow. **M. Kossenjans**

2:45 Intermission.

3:00 CINF 104. Data-driven drug discovery and repositioning by machine learning methods. **Y. Yamanishi**

3:25 CINF 105. Pattern recognition on neuromorphic hardware inspired by the chemical sense. **M. Schmuker**

3:50 CINF 106. Rethinking molecular design. **G. Schneider**

Section B

Westin Boston Waterfront
Lewis

Chemistry Librarians of the Future

Cosponsored by CHED
J. R. Garritano, L. R. McEwen, V. F. Scalfani, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CINF 107. Workflows for scholarly communication and knowledge creation: Building partnership between researchers and librarians of the future. **Y. Li**

2:00 CINF 108. Chemistry librarians and disciplinary data repositories working in partnership. **I. Bruno**, A. Sarjeant, L. Palumbo, C. Castle

2:25 CINF 109. Science librarians and the future of open science. **D. Wrublewski**, G.P. Clement, T.E. Morrell

2:50 Intermission.

3:05 CINF 110. Hiring a post-doc in chemistry data curation within a research library: The strategies and complexities. **J. Laherty**

3:30 CINF 111. Chemistry librarians as future managers and leaders. **J.R. Garritano**, **A.B. Twiss-Brooks**

3:55 CINF 112. Building chemistry research collections in the 21st century is a cooperative, collaborative effort. **G. Baysinger**

4:20 CINF 113. Stewarding chemical research through standards development: A chemistry librarian's feast. **L.R. McEwen**, **E. Hepler-Smith**

4:45 CINF 114. Reaxys education. **R.E. Belford**

5:10 Discussion.

WEDNESDAY MORNING

Section A

Westin Boston Waterfront
Harbor Ballroom II

Move Away from the Lamppost & Find Druggable Targets

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

8:30 Introductory Remarks.

8:35 CINF 115. AI-driven target selection in drug discovery - exploring the undiscovered country. **T.I. Oprea**, O. Ursu, C.G. Bologa

9:00 CINF 116. Beyond journal articles – extracting bioactivity data from patents. **A. Gaulton**, E. Cibrián Uhalte, P. Magarinos, G. Papadatos, A. Leach, T.I. Oprea

9:25 CINF 117. Putting hard numbers on druggability: Comparing the IUPHAR/BPS Guide to Pharmacology with other chemistry-mapped sources in Swiss-Prot. **C. Southan**, J.L. Sharman, A.J. Pawson, S.D. Harding, E. Faccenda, J.A. Davies

9:50 Intermission.

10:00 CINF 118. Open targets: An innovative public-private partnership to deliver more sustainable target selection for drug discovery. A. Leach, I. Dunham, **D. Hulcoop**, A. Hersey, A. Gaulton, P. Magarinos

10:25 CINF 119. Computational methods help find chemical matter to uncover novel biology. **Y. Wang**, J.L. Jenkins

10:50 CINF 120. Integrative informatics approaches for unraveling the mysteries of rare diseases: Shedding the light on Potocki-Shaffer syndrome. **R. Hajjo**

11:15 CINF 121. How to present knowledge about dark targets from 60 data sources and 10 data types. T. Sheils, D. Nguyen, **R. Guha**, N. Southall

11:40 Concluding Remarks.

Section B

Westin Boston Waterfront
Lewis

Machine Learning Scoring Functions

S. Sirimulla, *Organizer, Presiding*

8:30 CINF 122. Protein–ligand absolute binding affinity prediction via 3D-convolutional neural networks. **G. De Fabritiis**

8:55 CINF 123. Two faces of machine learning scoring functions - model complexity vs feature engineering. **M. Wojcikowski**, M. Kukielka, M. Stepniewska-Dziubinska, P. Siedlecki

9:20 CINF 124. Hydrogen bonding: *Ab initio* accuracy from fast interatomic Gaussian approximation potentials. **M. Öeren**, G. Csanyi, D.J. Ponting, P. Hunt, M.D. Segall

9:45 CINF 125. Artificial intelligence for predicting molecular electrostatic potentials (ESPs): A step towards developing ESP-guided knowledge-based scoring functions. **M. Verdonk**, R. Lewis, A. Bender, P.C. Rathi

10:10 Intermission.

10:20 CINF 126. Deep learning based scoring function for predicting protein-ligand binding affinities. M. Hassan, d. castaneda, **S. Sirimulla**

10:45 CINF 127. Evaluating lead optimization performance of a structure-based convolutional neural network. **A. Heifets**, M. Mysinger, I. Wallach, K.T. Nguyen

11:10 CINF 128. Mechanism-of-action elucidation using deep convolutional neural networks. **A. Rossi**, I. Wallach, M. Mysinger, K.T. Nguyen, A. Heifets

11:35 CINF 129. Simulated playground for evaluating machine-learning algorithms for bioactivity prediction. **J. Thompson**, S. schrodl, M. Mysinger, I. Wallach

Section C

Westin Boston Waterfront
Harbor Ballroom III

Semantics in Chemistry Vocabulary & Terminology

S. J. Chalk, L. R. McEwen, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CINF 130. Semantic properties and units for chemistry. **S.J. Chalk**

9:00 CINF 131. Data standards, formal ontologies and software tools to facilitate integration, classification and modeling of drug discovery data. **S.C. Schürer**, J. zheng, J. Turner, A. Koleti

9:25 CINF 132. Towards an IUPAC ontology for chemistry. **S.J. Chalk**

9:25 CINF 133. ChemOnt: A semantic-based ontology for chemical and biological data integration. **Y. Djoumbou Feunang**, D. Wishart, N. Karu, A. Marcu, E. Lo, A. Guo

9:50 CINF 134. From text mining to knowledge: PubChem knowledge panels provide synopsis of chemical, gene, protein and disease term co-occurrences in biomedical literature. **L. Zaslavsky**, A. Gindulyte, P. Thiessen, E. Bolton

10:15 Intermission.

10:30 CINF 135. OntoloBridge: A semi-automated ontology update request system. **J. Turner**, A. Clark, H. McGinty, B.A. Bunin, S.C. Schürer

10:55 CINF 136. Semantic representation of crystallography experiments. **I. Bruno**, A. Sarjeant

11:20 CINF 137. Ontology design patterns for laboratory chemical process hazards. **L.R. McEwen**, C. Shimizu, M. Sarkar

11:45 Discussion.

WEDNESDAY AFTERNOON

Section A

Westin Boston Waterfront
Harbor Ballroom II

The More the Merrier: Combine Drugs Together

R. Guha, A. Zakharov, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CINF 138. Understanding drug and compound combinations and modelling synergy – Methods and applications. **A. Bender**

2:05 CINF 139. Computational approach to HIV-1 drug resistance prediction based on relationships between viral genotype and combination of antiretroviral medicines. **O. Tarasova**, D.E. Kireev, D. Filimonov, V. Poroikov

2:35 CINF 140. Chemical mixture evaluation using molecular-weight corrected fingerprints. O. Ursu, C.G. Bologa, **T.I. Oprea**

3:05 Intermission.

3:20 CINF 141. SynergySeq – Integration of disease and perturbation gene expression data to prioritize synergistic drug combinations in cancer. **S. Schürer**, V. Stathias, A. Jermakowicz, N. Ayad

3:20 CINF 142. SSR: Structure-synergy relationships. **L. Chen**, K. Wilson, M.D. Hall, R. Guha

3:50 CINF 143. Novel computational approach for predicting drug-carrier formulations of poorly soluble drugs. **V.M. Alves**, D. Hwang, **E. Muratov**, M. Sokolsky-Papkov, E. Varlamova, N. Vinod, C.C. Melo-Filho, R. Marreto, S. Taveira, C.H. Andrade, **A. Tropsha**, A. Kabanov

4:20 Concluding Remarks.

Section B

Westin Boston Waterfront
Lewis

Reaction Analytics

F. van den Broek, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 144. Brief history of reaction analytics. **F. van den Broek**

2:00 CINF 145. Automatic discovery and enumeration of new tactical combinations. **S. Szymkuc**, E. Gajewska, M. Startek, P. Dittwald, B. Grzybowski

2:25 Intermission.

2:40 CINF 146. Retrosynthetic software for practicing chemists: Novel and efficient *in silico* pathway design validated at the bench. **L. Rickershauser**

3:05 CINF 147. Learning to plan chemical syntheses. M. Segler, **M. Waller**

3:30 Intermission.

3:45 CINF 148. Powerful algorithms in CASD systems: How important is the quality of the underlying data? Overview of results obtained with a transform library approach. **V. Eigner Pitto**, M.G. Hutchings, H. Saller

4:10 CINF 149. Exploring the use of conditional generative adversarial networks (cGAN) to analyze chemical reactions via electron density fields. **M. Clark**

Section C

Westin Boston Waterfront
Harbor Ballroom III

Drug Discovery: Cheminformatic Approaches

E. Davis, *Organizer, Presiding*

1:30 CINF 150. Bringing assay protocols into the age of informatics. **A. Clark**

1:55 CINF 151. Library enhancement through performance analysis of different components of high-throughput screening library against a variety of targets. **A. Saha**, M.D. Hack, T. Mirzadegan

2:20 CINF 152. Chemical intelligence that makes hidden knowledge effortlessly reachable. **J. David**, A. Tarcsay, G. Imre

2:45 CINF 153. Statistical-based database fingerprint: Application in ligand-based virtual screening. **N. Sánchez-Cruz**, J. Medina Franco

3:10 Intermission.

3:20 CINF 154. Rational solvent selection in asymmetric hydrogenation using molecular descriptors and machine learning. **Y. Amar**, A.M. Schweidtmann, P.P. Deutsch, A. Lapkin

3:45 CINF 155. Phenotypic screening aided by multitask prediction methods. **A. de la Vega de León**, V.J. Gillet

4:10 CINF 156. CCCTK: High performance molecular informatics toolkit for the design of anti-cancer molecule. **M. Karthikeyan**

THURSDAY MORNING

Section A

Westin Boston Waterfront
Grand Ballroom A

Drug Discovery: Cheminformatic Approaches

Cosponsored by AGRO
E. Davis, *Organizer, Presiding*

8:30 CINF 157. Implementing genetic algorithms and evolutionary strategies in conformer analysis. **N. Harms**, R.H. West

8:50 CINF 158. Predicting accumulation in Gram-negative bacteria to design better antibiotics. **B. Drown**, M. Richter, P.J. Hergenrother

9:10 CINF 159. Gearing transcriptomics towards high-throughput screening: Compound shortlisting from gene expression using *in silico* information. N. Aniceto, **A. Bender**, F. Nigsch

9:30 CINF 160. How to achieve better results using ligand-based virtual screening of big chemical databases. P. Pogodin, A. Lagunin, A. Rudik, D. Filimonov, D. Druzhilovskiy, M.C. Nicklaus, **V. Poroikov**

9:50 Intermission.

10:05 CINF 161. Making virtual REAL: Expansion of the synthetically feasible chemical space. **Y. Moroz**

10:25 CINF 162. NextMove for Chemspace: Millisecond search in a database of 100 million structures. **O. Gavrylenko**, Y. Moroz, R.A. Sayle, J. Mayfield

10:45 CINF 163. Automated workflow for reproducible analysis of protein-ligand scoring functions. **D. Castaneda Mogollon**, S. Sirimulla, M. Hassan

11:05 CINF 164. Driving efficiency and innovation in life sciences R&D. **J.F. Donahue**

11:25 CINF 165. Analysis of anti-flavivirus and anti-enterovirus activity based on ViralChEMBL data. **A. Orlov**, A. Nikitina, V. Palyulin, D.I. Osolodkin

Section B

Westin Boston Waterfront
Lewis

Reaction Analytics

F. van den Broek, *Organizer, Presiding*

8:30 CINF 166. Machine learning and continuous flow: Detection and correction of flow-incompatible reaction conditions. **P.P. Plehiers**, C.W. Coley, W.H. Green, G.B. Marin, C.V. Stevens, K. Van Geem

8:55 CINF 167. Predicting reaction conditions for computer-generated SAVI reactions by machine learning from reaction databases. **V. Delannée**, M.C. Nicklaus

9:20 Intermission.

9:35 CINF 168. Using machine learning to recommend suitable conditions for organic reactions. **H. Gao**, T. Struble, C.W. Coley, W.H. Green, K.F. Jensen

10:00 CINF 169. Analysing matched molecular pair transformations in drug discovery projects as a function of time and molecular environment. S. Ashenden, T. Kogej, O. Engkvist, E. Rivers, A. Madin, K. Goldberg, I. Storer, **A. Bender**

10:25 Intermission.

10:40 CINF 170. Regioselectivity: An application of expert systems and ontologies to chemical (named) reaction analysis. **R.A. Sayle**, J. Mayfield, T. Blaschke, N.M. O'Boyle

11:05 CINF 171. Representing organic reactions through InChI differences. **M.A. Walker**, **J. Paliakkara**

11:30 CINF 172. Automatically finding and fixing mistakes in detailed kinetic models of combustion. **N. Harms**, R.H. West