CINF

DIVISION OF CHEMICAL INFORMATION

R. Guha, *Program Chair*

OTHER SYMPOSIA OF INTEREST:
Medicinal Chemistry in Rare, Orphan and Neglected Diseases (see *MEDI*, Sun)
Advances in Conformational Sampling (see *COMP*, Sun - Mon)
New Drug Targets (see *BIOL*, Tue)
SOCIAL EVENTS:
Reception, 6:30 PM: Sun
Luncheon, 12:30 PM: Tue
Harry's Party, 5:30 PM: Mon

SUNDAY MORNING

Section A

The Moscone Center
Room 212 East

Sustainable Chemical Information Education through Faculty and Librarian Partnerships

J. Currano and J. Garritano, *Organizers*

8:00 Introductory Remarks.

8:05 1. "Chemical Information Instructor" feature: Telling the story of successful faculty-librarian partnerships in the Journal of Chemical Education. **A. Twiss-Brooks**

8:35 2. Teaching students to use REAXYS in order to find synthetic methods for making benzylic acid from benzaldehyde. **S. K. Cardinal**, W. D. Jones

9:05 3. In depth chemical information instruction in a second year organic chemistry course at Indiana University-Purdue University Indianapolis. **E. Snajdr**

9:35 4. Qualitative analysis in the library. **J. N. Currano**

10:05 Intermission.

10:20 5. Integrating library instruction into SAGES seminars at Case Western Reserve University for undergraduate chemistry students: A strategic plan. **S. Guo**

10:50 6. USC Chemistry OIL program. **N. Xiao**

11:20 7. Beyond Google: Integrating chemical information into the undergraduate chemistry curriculum. **M. C. Peters**

11:50 8. No chemistry librarian: How chemistry faculty can participate in collection development and its

increased use. **A. W. Kozlowski**

Section B

The Moscone Center
Room 206/210

Metabolomics: A Field at the Boundaries between Chemistry and Biology

Applications and Infrastructures

Cosponsored by ANYL and MEDI
C. Steinbeck, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 9. Beyond Metlin: Extending metabolite databases to enhance identifications in metabolomics. **G. Suizdak**

9:45 10. Stable isotope-resolved metabolomics analysis of UDP-GlcNAc & UDP-GalNAc: Computational resolution and modeling of their converging biosynthetic pathways. **H. N. B. Moseley**, A. C. Belshoff, R. M. Higashi, T. W.-M. Fan, A. N. Lane

10:10 11. Functional and structural network modeling of metabolomics datasets. **D. K. Barupal**, G. Wohlgemuth, O. Fiehn

10:35 Intermission.

10:50 12. Computational aspects of metabolomic Quantitative Trait Locus (mQTL) mapping and metabolome-wide genome-wide association studies. **M.-E. Dumas**, J.-B. Cazier, J. K. Nicholson, D. Gauguier

11:15 13. Metabolite identification pipeline based on MS fragmentation. **M. Rojas-Chertó**, **J. E. Peironcely**, P. T. Kasper, A. Bender, J.-L. Faulon, T. Reijmers, L. Coulier, R. Vreeken, T. Hankemeier

11:40 14. Consensus-phenotype integration of metabolomic and transcriptomic data enhances the detection of pathways associated with drug response. R. Cavill, A. Kamburov, M. S. C. Blagrove, T. J. Athersuch, J. K. Ellis, R. Herwig, **T. M. D. Ebbels**, H. C. Keun

12:05 15. Designing a cyberinfrastructure for metabolomics. **M. Arita**

Section C

The Moscone Center
Room 200 East

Cheminformatics Tools and High-throughput Approaches for the Discovery of New Materials

Microporous and Composite Materials

Cosponsored by COMP, INOR and PHYS

M. Haranczyk, *Organizer*
B. Smit, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 16. Computational discovery of new zeolite-like materials. **M. W. Deem**, D. J. Earl

9:35 17. Using multiple levels of computer modeling to accelerate development of metal organic frameworks materials for membrane applications. **D. S. Sholl**, S. Keskin, T. Watanabe, E. Haldoupis, S. Nair

10:05 18. Informatics approaches for analyzing zeolites. **E. Blaisten-Barojas**

10:35 Intermission.

10:45 19. Screening tools for identification of porous materials for CO_2 separation. **M. Haranczyk**, J. Kloke, K. Theisen, B. Liu, G. Carlsson, B. Smit

11:15 20. 3D-Characterization and modeling of composite materials. **O. Wirjadi**

SUNDAY AFTERNOON

Section A

The Moscone Center
Room 212 East

Green Chemistry: Multidisciplinary Use of Chemical Information Resources

R. Schenck, *Organizer, Presiding*

2:00 Introductory Remarks.

2:10 21. Growing focus on green chemistry: What the CAS databases reveal. **R. Schenck**

2:40 22. California's green chemistry initiative: Application of life cycle assessment in public policy. **B. Boughton**

3:10 23. ChemSpider: How an online resource of chemical compounds, reaction syntheses, and property data can support green chemistry. **A. J. Williams**, V. Tkachenko

3:40 Intermission.

3:55 24. From biochemical pathways to retrobiosynthesis. **C. H. Schwab**, O. Sacher, B. Bienfait, J. Gasteiger

4:25 25. Green chemistry database and analytical compliance suite (GC-DACS) . **G. R. Thompson**

4:55 26. Importance of benchmarking Green Chemistry. G. Gurau, **R. D. Rogers**

5:25 Concluding Remarks.

Section B

The Moscone Center
Room 206/210

Metabolomics: A Field at the Boundaries between Chemistry and Biology

Analytical Aspects

Cosponsored by ANYL and MEDI
C. Steinbeck, *Organizer, Presider*

2:00 27. Software advancements for performing compound identification QC on large metabolomic datasets. **C. DeHaven**

2:25 28. Fold-change analysis and visualization of multispectral datasets in NMR-based metabolomics. **S. L. Robinette**, A. S. Edison

2:50 29. Data mining tool for automated metabolite identification and quantification using *J*-resolved NMR spectroscopy. S. He, C. Ludwig, J. M. Easton, H. Chen, S. Tiziani, A. Lodi, S. Manzoor, A. D. Southam, T. N. Arvanitis, U. L. Guenther, **M. R. Viant**

3:15 Intermission.

3:30 30. Identification of parent-fragment pairs via rigorous statistical modeling of LC-MS metabolomic data. **A. Ipsen**, E. Want, J. Lindon, T. Ebbels

3:55 31. Generation of in-silico MS/MS mass spectra using combinatorial algorithms and reaction prediction expert systems. **T. Kind**, K.-H. Liu, D. Y. Lee, O. Fiehn

SUNDAY EVENING

Section A

The Moscone Center
Room 110 – 111 North

2010 CINF Scholarship for Scientific Excellence

G. Grethe, *Organizer*

6:30 - 8:30
32. Using aggregative Web Services for drug discovery. **Q. Zhu**, M. S. Lajiness, D. J. Wild

33. Semantifying polymer science using ontologies. **E. O. Cannon**, N. Adams, P. Murray-Rust

34. PDZ domain: A computational insight into protein similarity and ligand specificity. **C. S. D. Sisu**, G. H. Grant

35. Homology modeling and molecular dynamics of the APJ receptor, a co-receptor for cellular entry of HIV. **N. J. M. Macaluso**, R. C. Glen

36. Assigning stereochemistry using GIAO NMR shift calculation. **S. G. Smith**, J. M. Goodman

37. Combination of target-specific pose filters and force field-based scoring functions to improve the structure-based virtual screening. **J.-H. Hsieh**, S. Yin, X. S. Wang, S. Liu, N. V. Dokholyan, A. Tropsha

38. Toxicity reference database (ToxRefDB) to develop predictive toxicity models and prioritize compounds for future toxicity testing. **H. Tang**, H. Zhu, L. Zhang, A. Sedykh, A. Richard, I. Rusyn, A. Tropsha

39. Chem2bio2RDF: Semantic systems chemical biology. **B. Chen**, X. Dong, D. Jiao, H. Wang, Y. Ding, D. J. Wild

40. Application of novel data mining techniques to improve chemical array design decisions during lead optimisation. **G. Papadatos**, M. Alkarouri, V. Gillet, P. Willett, V. Kadirkamanathan, C. Luscombe, G. Bravi, N. Richmond, S. Pickett, J. Pritchard, A. Cooper, S. Macdonald

41. Biological and chemical network construction from linked open data. **D. Jiao**

42. Novel approach to drug discovery integrating chemogenomics and QSAR modeling: Applications to anti-Alzheimer's agents . **R. Hajjo**, S. Wang, B. L. Roth, A. Tropsha

43. Use of QSAR models to validate the HTS assay data in PubChem: Application to the serotonin receptor 5-HT1A ligands. **M. Luo**, S. X. Wang, A. Golbraikh, A. Tropsha

44. Speeding up chemical database searches. **R. J. Nasr**, P. Baldi

45. OrbDB: A database of molecular orbital interactions. **M. A. Kayala**, C. A. Azencott, J. H. Chen, P. F. Baldi

46. PropOrb: A frontier molecular orbital interaction proposer. **C.-A. Azencott**, M. A. Kayala, P. Baldi

MONDAY MORNING

Section A

The Moscone Center
Room 212 East

Visual Analysis of Chemical Data

Data Integration

Cosponsored by COMP
J.-C. Bradley, A. Lang, and N. O Boyle, *Organizers*

8:45 Introductory Remarks.

8:50 47. Dataviz explosion: Considering effectiveness in classrooms and across disciplines. **E. Dorland**

9:30 48. ASAP: Emphasizing multidimensional drug discovery . **W. P. Walters**, Y. Bennani, T. Kramer

9:55 49. Visual analyses for guiding compound selection and design. **E. Champness**

10:20 50. Contextual visualization of biological and chemical networks using linked open life science data. **D. Jiao**, Y. Ding, D. J. Wild

10:45 Intermission.

11:00 51. iTunes™ for chemistry and biology: Addressing usability in cheminformatics. D.-T. Nguyen, Y. Wang, R. Guha, **N. Southall**, R. Huang, **A. Jadhav**

11:25 52. Interaction Maps: Understanding compound pathway space. **Y. Tanrikulu**, M. Weisel, R. Kondru, H. M. Bitter

11:50 53. PubChem: A public cheminformatics system for bioactivity analysis. **Y. Wang**

Section B

The Moscone Center
Room 206/210

Cheminformatics Tools and High-throughput Approaches for the Discovery of New Materials

Electronic and Optical Materials

Cosponsored by COMP, INOR and PHYS
B. Smit, *Organizer*
M. Haranczyk, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 54. High throughput synthesis and screening system for discovery of improved materials for rechargeable batteries. B. Li, F. Matsumoto, B. Howard, R. Olugbile, D. Greenburg, C. Riley, C. O'Neill, M. S. Bailey, **S. S. Kaye**

9:35 55. The Clean Energy Project: Finding new renewable energy materials, one screensaver at a time. **A. Aspuru-Guzik**

10:05 56. Compound discovery and design via materials informatics: An "omics" approach to materials science. **K. Rajan**

10:35 Intermission.

10:45 57. Organic electronic materials by design: Finding a needle through the haystack. **G. R. Hutchison**, N. O'Boyle

11:05 58. Searching chemical space by inverse design. **B. C. Rinderspacher**, J. Andzelm, A. Rawlett, J. Dougherty, R. Lambeth

11:25 59. High-throughout quantum chemistry and virtual screening for materials solutions. **M. D. Halls**

Beyond the Bench: Non-Traditional Careers in Chemistry

CHAL's 25th Anniversary Series

Sponsored by CHAL, Cosponsored by CINF

MONDAY AFTERNOON

Section A

The Moscone Center
Room 212 East 

What Happened to My Library?: Managing Organizational and Space-related Challenges

A. Twiss-Brooks, *Organizer*
E. Kajosalo, *Organizer, Presiding*

1:45 Introductory Remarks.

1:50 60. Impacts of closing academic branch libraries. **S. J. Redalje**

2:15 61. e-Books and e-references collection in academic libraries: A case study. **N. Xiao**

2:40 62. Future of the liaison in academic libraries. **M. Lafferty**

3:05 63. New workspaces: From library facility to online service. **L. Solla**

3:30 Panel Discussion.

Section B

The Moscone Center
Room 206/210

The Future of Scholarly Communication

Evolving Business Models

Cosponsored by CHED
D. Martinsen, W. G. Town, and W. Warr, *Organizers*

1:00 Introductory Remarks.

1:05 64. PLoS ONE: A new model for online journal publishing. **P. Binfield**

1:35 65. Impact of emerging economies on publishing. **J. Bhate**

2:05 66. Ensuring sustainability of scientific data resources: Technologies and business models for the future. **C. R. Groom**

2:35 Intermission.

2:45 67. Vision and strategy for the future of RSC Publishing. **R. J. Parker**, J. Milne

3:15 68. Challenges facing the STM industry. **M. O'Malley**

3:45 69. Vision and strategy for scholarly communication at the ACS. **S. King**

4:15 Intermission.

4:20 Open Meeting. CINF Division.

4:30 Intermission.

4:35 Open Meeting. Committees on Publications and Chemical Abstracts Service.

MONDAY EVENING

Section A

The Moscone Center
Hall D

Sci-Mix

R. Guha, *Organizer*

8:00 - 10:00

7. See previous listings

72, 102, 122. See subsequent listings.

TUESDAY MORNING

Section A

The Moscone Center
Room 212 East 

Visual Analysis of Chemical Data

QSAR

Cosponsored by COMP
J.-C. Bradley, A. Lang, and N. O'Boyle, *Organizers*

8:15 70. Network visualization of structure activity landscapes. **R. Guha**

8:40 71. Visualization and analysis of bioisosteric analogs generated with BROOD. **J. J. Corkery**, A. G. Skillman, K. E. Schmidt, B. Kelley

9:05 72. Visualizing polypharmacology in chemical libraries. **D. Marcus**, D. Barasch, A. Rayan, A. Goldblum

9:30 73. Linear scaling mapping of chemical space. **J. S. Delaney**

9:55 Intermission.

10:10 74. Integrated visualization for the interpretation of QSPR and QSAR models. **G. D. Purvis**, W. D. Laidig, D. T. Stanton

10:35 75. VTK: The visualization toolkit and its applications to the analysis of chemical data. **M. D. Hanwell**

11:00 76. Molecular similarity characterization of ADME landscapes. **R. R. Gupta**, **B. Chen**, E. M. Gifford

11:25 77. Chemical information usage patterns under the microscope: The prospects of GIS-based visualization for libraries. **M. P. Brändle**

Section B

The Moscone Center
Room 206/210

The Future of Scholarly Communication

Towards Web 2.0

Cosponsored by CHED
D. Martinsen, W. Town, and W Warr, *Organizers*

8:15 Introductory Remarks.

8:20 78. Scholarly communication in the 21st Century: Changing paradigms of communication and access. **R. Schwarzwalder**

8:50 79. oreChem project: Semantic infrastructure and applications for chemistry scholarship. **C. Lagoze**

9:20 80. Chemistry: Computation, synthesis and communication. **J. M. Goodman**

9:50 81. Primary data for chemistry. I. Sens, S. Haak, J. Brase, **G. F. Herrmann**

10:20 Intermission.

10:35 82. Papers to papers: The future of reading, storing, and producing chemical literature in an academic environment. **J. N. Currano**

11:05 83. Socialized medicine: Medical publishing in the era of the read-write web. **K. R. Anderson**

11:35 84. Scholarly communication between chemists and their uptake and use of Web 2.0 and other new technologies. **W. G. Town**

TUESDAY AFTERNOON

Section A

The Moscone Center
Room 212 East

Visual Analysis of Chemical Data

Molecular Visualization

Cosponsored by COMP
J.-C. Bradley, A. Lang, and N. O'Boyle, *Organizers*

2:00 85. ChemSci3D: An integrated 2D and 3D desktop chemistry interface. **T. J. O'Donnell**

2:25 86. Real-time ray-tracing in molecular graphics. **M. Keil**

2:50 87. Avogadro: Framework for chemical structure analysis and visualization. **M. D. Hanwell**

3:15 88. 2D graphical depiction of zeolite voidspace topology. **K. J. Theisen**, B. Smit, M. Haranczyk

3:40 Intermission.

3:55 89. Computational methods for 2D-visualization of molecular interaction patterns. K. Stierand, **M. Rarey**, C. Lemmen

4:20 90. Visualizing combinatorial molecular materials research using Avogadro. **G. R. Hutchison**, M. D. Hanwell

4:45 91. Visualizing chemistry in Second Life. **A. S. I. D. Lang**, **J.-C. Bradley**

5:10 92. Next-generation visualization technologies: How close are we to the Science 2.0?. **O. Isayev**

Section B

The Moscone Center
Room 206/210

The Future of Scholarly Communication

Application of Emerging Technologies

Cosponsored by CHED
D. Martinsen, W. Town and W. Warr, *Organizers*

2:00 Introductory Remarks.

2:05 93. CAS and ACS publications: Together, providing new pathways to chemical research. **J. Morgan**, **M. Dennis**

2:35 94. Adding structure to publishing chemistry. **J. N. Wilde**

3:05 95. Under the hood: A technical view on publishing chemistry in the future. **R. Kidd**

3:35 Intermission.

3:50 96. Interactive publishing of crystal structure data. **B. McMahon**, P. R. Strickland

4:20 97. Science video journal to increase efficiency and standardization in experimental research. **M. Pritsker**

4:50 98. Nano-Publication. **J. J. J. M. Velterop**

TUESDAY EVENING

Section D

The Moscone Center
Hall D

General Posters

R. Guha, *Organizer*

6:00 - 8:00
99. Speeding up chemical database searches. **R. J. Nasr**, P. Baldi

100. Comparison of backfiles offered by major publishers of chemical journals. **A. D. Bolek**

101. Marketing chemical research with custom web databases. **B. Brandys**

102. Advanced materials/processes for information technology: Microfluidic synthesis, nanofabrication, and soft lithography. **K. Choi**

103. New Knovel interface. **S. Gurke**

104. Expanding and understanding metabolite space. **J. E. Peironcely**, A. Bender, M. Rojas-Chertó, T. Reijmers, L. Coulier, T. Hankemeier

105. Metabolite identification based on MS fragmentation. **M. Rojas-Chertó**, P. T. Kasper, J. E. Peironcely, T. Reijmers, R. J. Vreeken, T. Hankemeier

WEDNESDAY MORNING

Section A

The Moscone Center
Room 212 East

Fragment Based Drug Design: Success Stories due to Novel Computational Methods Applications

Cosponsored by COMP and MEDI
R. Bienstock, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 106. Fragment database analysis using molecular shape fingerprints. **J. D. MacCuish**, N. E. MacCuish, M. Hawrylycz, M. Chapman

9:10 107. Qsearch: Pharmacophore-based search in fragment spaces. **T. Lippert**, M. Rarey

9:40 108. Fragment-based lead discovery through chemotype evolution. **D. Erlanson**

10:10 Intermission.

10:25 109. Leading fragments to lead structures: Fragment evolution, merging and core replacement, and…docking. **C. Detering**, M. Gastreich, C. Lemmen

10:55 110. Fragment-based drug design using PASS approach. O. A. Filz, A. A. Lagunin, D. A. Filimonov, **V. V. Poroikov**

11:25 111. Use of virtual fragment screening for lead modification. **Y. Xu**, H. Jansen, E. Martin

Section B

The Moscone Center
Room 206/210

The Future of Scholarly Communication

Authoring and Discovery Tools

Cosponsored by CHED
D. Martinsen, W. Town, and W. Warr, *Organizers*

8:15 Introductory Remarks.

8:20 112. IUPAC InChI project: A status report. **S. R. Heller**, A. McNaught

8:50 113. Tools for the scholarly communication lifecycle. **A. D. Wade**, L. Dirks

9:20 114. Integrated language for chemical publication. **P. Murray-Rust**, J. A. Townsend, L. Hawizy

9:50 115. Chem4Word. **J. A. Townsend**, P. Muray-Rust, J. Downing, T. Haughton, A. Wade, L. Dirks

10:20 Intermission.

10:35 116. Capturing and publishing chemistry from the bench to paper: Does Google Wave offer a solution?. **C. Neylon**

11:05 117. CAS REGISTRY: Maintaining quality standards as scientific discovery accelerates. **M. J. Toussant**

11:35 118. Chempedia: A social medium for chemical information. **R. L. Apodaca**

12:05 119. Enhancing discoverability across Royal Society of Chemistry content by integrating to ChemSpider, an online database of chemical structures. **A. J. Williams**, V. Tkachenko, S. Shevelev, R. Kidd

WEDNESDAY AFTERNOON

Section A

The Moscone Center
Room 212 East

Fragment Based Drug Design: Success Stories due to Novel Computational Methods Applications

Cosponsored by COMP and MEDI
R. Bienstock, *Organizer, Presiding*

2:00 120. Fragment-based screening of stabilized G protein-coupled receptors. **M. Congreve**

2:30 121. Novel histamine GPCR family antagonists by fragment screening and molecular modeling. **R. J. Law**, T. Hesterkamp, A. Kahrs, M. Whittaker, S. Pal, A. Heifetz

3:00 Intermission.

3:15 122. Mitotic kinesin Eg5 inhibitors generation by computational MED-portion based drug design at PDB scale. K. Oguievetskaia, L. Martin-Chanas, A. Vorotyntsev, O. Doppelt-Azeroual, X. Brotel, S. Adcock, A. de Brevern, **F. Delfaud**, **F. Moriaud**

3:45 123. Starting small and staying small: Fragment-based lead discovery in CNS disease. **V. L. Nienaber**

4:15 124. Finding druggable sites in protein-protein interfaces by computational fragment mapping. **D. Kozakov**, S. Vajda

4:45 Concluding Remarks.

Section B

The Moscone Center
Room 206/210

The Future of Scholarly Communication

Peer Review and Impact Metrics

Cosponsored by CHED
D. Martinsen, W. Town, and W. Warr, *Organizers, Presiding*

2:00 125. Peer review is not perfect but are the alternatives worse?. **W. A. Warr**

2:30 126. Interactive open access publishing and public peer review: Perspectives and effectiveness of transparency and self-regulation in scientific communication and quality assurance. **U. Pöschl**

3:00 127. Impact factors, post-publication peer review and other metrics. **R. P. Grant**

3:30 Intermission.

3:45 128. Eigenfactor: Ranking and mapping the scholarly literature. **J. D. West**

4:15 129. Applying domain expertise assessment to compound annotation for enhanced collaborations between chemists and biologists. **Y. Pouliot**

4:45 Concluding Remarks.

Competition Law and E-publishing in Scientific Fields

Sponsored by CHAL, Cosponsored by CINF

THURSDAY MORNING

Section A

The Moscone Center
Room 212 East

General Papers

Chemical Data Mining

R. Guha, *Organizer*

8:30 130. Exploring molecular networks for polypharmacology analysis. **S. Zhang**

8:55 131. Picking novel actives from large databases using a combined ranking method. **D. Marcus**, D. Barasch, A. Rayan, A. Goldblum

9:20 132. Human proteome in the context of pathways, diseases, drugs, and tool compounds. **F. Nigsch**, J. Jenkins

9:45 133. Atom type preferences, constitutional diversity, and property profiles of known drugs: A knowledge-intensive, comparative assessment of drugability. **V. N. Viswanadhan**, H. Rajesh, V. N. Balaji

10:10 Intermission.

10:25 134. Improving the consistency of data fusion in virtual screening. I. Mott, P. Gedeck, **V. J. Gillet**

10:50 135. Extending interaction fingerprints: A novel approach to characterizing protein binding sites. **C. Higgs**, W. Sherman, J. Blaney

11:15 136. Molecular signatures of promiscuous enzyme-substrate interactions. **J.-L. Faulon**, P. Carbonell

11:40 137. Metabolic regioselectivity models for nine CYP P450 isozymes. **J. M. Zaretzki**, T.-W. Huang, C. M. Breneman, C. Bergeron, K. P. Bennett

Section B

The Moscone Center
Room 206/210

General Papers

Algorithms and Toolkits

R. Guha, *Organizer*

8:15 138. Novel topological molecular key for cheminformatics. **P. Liu**, D. Agrafiotis

8:40 139. Classification of enzyme function based on similarities in reaction mechanisms and common substrate substructures. **D. E. Almonacid**, P. C. Babbitt

9:05 140. Chem_BLAST: A rule-based method to develop advanced structural ontologies for chemical bioinformatics and the PDB, the PubChem. **T. N. Bhat**

9:30 141. Chemical entity extraction and interpretation. **D. M. Lowe**, P. T. Corbett, P. Murray-Rust, R. C. Glen

9:55 Intermission.

10:10 142. PolyGWT: A Google Web Toolkit application to assist polymer research. **E. O. Cannon**, P. Murray-Rust

10:35 143. OpenTox: An open source predictive toxicology software framework. **B. Hardy**, **D. A. Gallagher**, S. Chawla

11:00 144. Combining disparate cheminformatics resources into a single toolkit: The Cinfony library. **N. M. O'Boyle**, G. R. Hutchison

THURSDAY AFTERNOON

Section A

The Moscone Center
Room 212 East

General Papers

Platforms and Databases

R. Guha, *Organizer*

1:30 145. Role of Rh(III) as negative catalyst in N-chlorosuccinimide oxidation of glycine in alkaline medium: A kinetic and mechanistic study. **A. K. Singh**, M. Singh, R. Srivastava, J. Srivastava, S. Rahmani

1:55 146. Psychological barriers to good decision-making: How addressing cognitive biases could improve drug discovery. **M. D. Segall**, A. Chadwick

2:20 147. NCI/CADD: Open-access chemical structure web platform. **M. Sitzmann**, W.-D. Ihlenfeldt, M. C. Nicklaus

2:45 148. OrbDB: A database of molecular orbital interactions. **M. A. Kayala**, C. A. Azencott, J. H. Chen, P. F. Baldi

3:10 Intermission.

3:25 149. Application of crowdsourcing for metadata curation of digitized texts. **A. J. Williams**, R. Kidd, V. Tkachenko, S. Shevelev

3:50 150. Five years of collaborative drug discovery in the cloud. **B. A. Bunin**, S. Ekins, M. Hohman, S. Ernst, K. Gregory

4:15 151. CWM Global Search: An Internet search engine for the chemist. **A. J. Kos**, H.-J. Himmler

4:40 152. www.emolecules.com: The comprehensive source of commercially available, in stock chemicals. **K. Gubernator**

Section B

The Moscone Center
Room 206/210

General Papers

Small Systems and Large Calculations

R. Guha, *Organizer*

2:00 153. Petascale lattice-Boltzmann simulations of dynamical processes in ternary amphiphilic liquid crystalline systems. R. S. Saksena, **P. V. Coveney**

2:25 154. Novel, accurate high-throughput 3D pharmacophore screening algorithm. **G. Wolber**, T. Seidel, F. Bendix, P. Markt

2:50 155. Structure – toxicity relationship study for organophosphorus compounds: QSAR analysis. **Y. Paukku**, D. Magers, G. Hill

3:15 Intermission.

3:30 156. EEM-Hückel model for partial atomic charges. **M. Waldman**, R. Fraczkiewicz, W. S. Woltosz

3:55 157. PropOrb: A frontier molecular orbital interaction proposer. **C.-A. Azencott**, M. A. Kayala, P. Baldi

4:20 158. Fast and accurate prediction of the 3D structure of small molecules. **A. Andronico**, A. Randall, P. Baldi