OTHER SYMPOSIAS 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, Sun - Mon)

SOCIAL EVENTS:
Reception, 6:30 PM: Sun
Luncheon, 12:30 PM: Tue
Harry's Party, 5:30 PM: Mon

SUNDAY MORNING

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

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


10:35 Intermission.


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.


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

10:35 Intermission.


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


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.


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

S. L. Robinette, A. S. Edison


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


SUNDAY EVENING

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


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


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


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


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


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

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


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.


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-throughput quantum chemistry and virtual screening for materials solutions. M. D. Halls

Beyond the Bench: Non-Traditional Careers in Chemistry

CHAL's 25th Anniversary Series
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.

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.


**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

9:30 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

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


9:50 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**
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


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. M. Velterop**

**TUESDAY EVENING**

**Section D**

The Moscone Center
Hall D

**General Posters**

R. Guha, *Organizer*

**6:00 - 8:00**


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


**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.


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

10:10 Intermission.


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


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


3:00 Intermission.


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


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, Co-sponsored by CINF*

**THURSDAY MORNING**

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**


10:10 Intermission.

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


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


9:55 Intermission.


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

The Moscone Center
Room 212 East

General Papers

Platforms and Databases

R. Guha, Organizer


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

3:10 Intermission.


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


3:15 Intermission.

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


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