

4:25 Open Meeting. Committees on Publications and Chemical Abstracts Service.

#### Section B

Salt Palace Convention Center  
251 F

#### Are Chemical Information Professionals Ready for the Future?

E. Kajosalto and M. Lafferty, *Organizers*

1:30 37. Scientific data stewardship: Meeting the challenge in academic libraries.

B. A. Losoff

2:00 38. Data awareness: Should chemistry information professionals care?

L. R. Solla, D. Dietrich

2:30 39. NIH public access policy: Opportunity for a new library service? E. Kajosalto

3:00 Panel Discussion.

**Nanomaterials Modeling and Informatics Nanotubes and Nanocomposites** Sponsored by COMP, Cosponsored by CINF and NANO

#### MONDAY EVENING

#### Section A

Salt Palace Convention Center  
Hall 5

#### Sci-Mix

R. Guha, *Organizer*

8:00–10:00

18–22. See previous listings.

40. Clustering of NF- $\kappa$ B inhibitors by their interaction in the signaling pathway.

Y. Patel, C. Heyward, P. D. B. Kell

#### TUESDAY MORNING

#### Section A

Salt Palace Convention Center  
254 A

**Library Design, Search Methods and Applications of Fragment-based Drug Design** Cosponsored by COMP

R. Bienstock and A. Tropsha, *Organizers*

8:30 Introductory Remarks.

8:35 41. Molecular similarity searching using inference network. A. Abdo, N. Salim

9:05 42. A fragment based de novo application in the context of the active site.

C. Detering, H. Claußen, M. Gastreich

9:35 43. Withdrawn.

10:05 Intermission.

10:10 44. Fragment based docking and linking engine of eHITS. Z. Zsoldos

10:40 45. Druglike pieces for the virtual chemistry jigsaw puzzle: Toward optimized fragment spaces. C. Wegscheid-Gerlach, J. Degen, H. Briem, M. Rarey, A. Zaliani

11:10 Concluding Remarks.

#### Section B

Salt Palace Convention Center  
251 F

**Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen Crystal Form Analysis, Experiment and Prediction** Cosponsored by COMP, CHAL, and MEDI

B. Town and F. H. Allen, *Organizers*

8:30 Introductory Remarks.

8:35 46. Application of computational methods in pharmaceutical solid form selection.

R. Docherty

‡ Cooperative Cosponsorship

9:05 47. Investigating crystal engineering principles using a data set of pharmaceutical cocrystals. P. A. Wood

9:35 48. Cocrystal design and packing analysis based on a family of crystal structures containing a common molecule.

S. L. Childs

10:05 Intermission.

10:15 49. Hydrogen bond propensities: Knowledge-based predictions to aid solid form selection. P. T. A. Galek

10:45 50. Crystal structure prediction: A decade of blind tests. F. J. Leusen

**Nanomaterials Modeling and Informatics Nanoparticles, Nanotoxicity and Molecular Machines** Sponsored by COMP, Cosponsored by CINF and NANO

**Online Resources for Chemical Education Green and Organic Chemistry Applications** Sponsored by CHED, Cosponsored by CINF

**Public Outreach: Better Living through Chemistry** Sponsored by CHED, Cosponsored by CINF

#### TUESDAY AFTERNOON

#### Section A

Salt Palace Convention Center  
254 A

**Adaptive Scoring Functions** Cosponsored by the CSA Trust and COMP

D. K. Agrafiotis and E. J. Martin, *Organizers*

2:00 Introductory Remarks.

2:05 51. Force field based scoring of protein-ligand binding affinities. J. Aqvist

2:40 52. Structure based drug design and LIE models for GPCRs. P. Kolb, D. M. Rosenbaum, A. M. M. Jorgensen, J. J. Irwin, B. K. Shoichet, B. K. Kobilka

3:15 53. Learning scoring function parameters from binary data. M. H. Seifert

3:50 Intermission.

4:05 54. 2-D and 3-D adaptive scoring functions for iterative kinase medium-throughput screening (iKMTS) with Profile-QSAR and AutoShim. E. J. Martin, D. C. Sullivan, P. Mukherjee

4:40 55. Combining quantitative data and qualitative knowledge to score reaction energies. C-A. Azencott, M. A. Kayala, P. Baldi

#### Section B

Salt Palace Convention Center  
251 F

**Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen Scientific and Regulatory Issues of Crystal Forms** Cosponsored by COMP, CHAL, and MEDI

B. Town and F. H. Allen, *Organizers*

2:00 56. Drug development and solid form selection: Multicomponent crystals.

W. Jones

2:30 57. Supramolecular heterosynthons and their role in cocrystal design.

M. Zaworotko, M. L. Cheney, D. Weyna

3:00 58. Cambridge Structural Database analysis of complementary molecular properties in cocrystals. L. Fábian

3:30 Intermission.

3:40 59. Applications of the CSD to structure determination from powder data.

A. J. Florence, R. Taylor, N. Shankland, K. Shankland

4:10 60. Pharmaceutical crystal forms at the dynamic intersection of science and intellectual property law. A. V. Trask

4:40 Concluding Remarks.

**Nanomaterials Modeling and Informatics Nanostructure Modeling with Simulation and DFT** Sponsored by COMP, Cosponsored by CINF and NANO

#### WEDNESDAY MORNING

#### Section A

Salt Palace Convention Center  
254 A

**Adaptive Scoring Functions** Cosponsored by the CSA Trust and COMP

D. K. Agrafiotis and E. J. Martin, *Organizers*

8:30 Introductory Remarks.

8:35 61. Developing scoring functions for a class of proteins. C. M. Venkatachalam, S. Varma-O'Brien, T. J. Ehlers, J. Koska

9:10 62. Development of novel iterative knowledge-based scoring functions for protein-ligand and protein-protein interactions. X. Zou

9:45 Intermission.

10:00 63. eHITS scoring function.

Z. Zsoldos, D. Harris

10:35 64. Development of scoring functions for computing protein-ligand binding affinities. R. A. Friesner

11:10 65. At what point does docking morph into 3-D QSAR? R. D. Clark

#### Section B

Salt Palace Convention Center  
251 F

**Science in the Service of Genealogy**

C. Huber, *Organizer*

9:00 66. Navigating the Family History Archive: Digitizing the Family History Library collection. D. L. Meldrum, J. Jump

9:30 67. Understanding genetic genealogy and the importance of DNA databases.

B. Greenspan, M. Blankfeld

10:00 68. Identification of the remains found at the crash site of Northwest Flight 4422 using forensic genealogy and DNA analysis. C. Fitzpatrick, O. Loreille

10:30 69. How the Pilgrims brought colon cancer to the New World and how Utah Population Database outed them.

D. W. Neklason, J. Stevens, K. Boucher, R. Kerber, G. Mineau, R. Burt

**Online Resources for Chemical Education General Chemistry Applications** Sponsored by CHED, Cosponsored by CINF

#### WEDNESDAY AFTERNOON

#### Section A

Salt Palace Convention Center  
254 A

**Adaptive Scoring Functions** Cosponsored by the CSA Trust and COMP

D. K. Agrafiotis and E. J. Martin, *Organizers*

2:00 Introductory Remarks.

2:05 70. Adaptive scoring for comparing ligand binding sites and predicting binding modes and affinities. L. A. Kuhn, M. E. Toner, J. R. Van Voorst, M. I. Závodszy

2:40 71. Avoiding pitfalls in molecular docking. S. A. Hindle, C. Detering, M. Gastreich, H. Claußen

3:15 Intermission.

3:30 72. Designing drugs against multiple parameters: Scoring functions for multiparameter ligand based de novo design.

B. B. Masek, K. M. Smith, S. C. Nagy, J. R. Damewood, C. L. Lerman

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4:05 73. Scoring synthetic feasibility: A very different problem. A. P. Johnson, K. Boda, G. J. Myatt, J. C. Baber

#### Section B

Salt Palace Convention Center  
251 F

#### General Papers

R. Guha, *Organizer*

2:00 Introductory Remarks.

2:05 74. Text mining for chemistry and building a public platform for document markup. A. J. Williams

2:30 75. Extending the scope of journal articles: Certifying and publishing experimental data. I. Sens, J. Brase, S. Haak, G. F. Herrmann

2:55 76. Ontologies for nanotechnology.

C. R. Batchelor

3:20 Intermission.

3:30 77. Pistoia alliance: Emerging cross pharma collaboration. A. George, D. Igo, K. Hebbel, N. Lynch, T. Mueller, M. Nolte, C. L. Waller

3:55 78. Cleaning up chemistry for the pharma industry: Delivering a flexible platform for interrogating the FDA DailyMed website. A. Williams, R. Potenzione

4:20 79. The use of EPA software and Scranton University green chemistry web page in the green engineering course in Universidad de los Andes. G. Camargo, F. Segura, A. Altamar, J. E. Tirano

#### THURSDAY MORNING

#### Section A

Salt Palace Convention Center  
254 A

#### General Papers

R. Guha, *Organizer*

8:30 Introductory Remarks.

8:35 80. Building blocks for automated elucidation of metabolites: Machine learning methods for NMR prediction.

C. Steinbeck, S. Kuhn, S. Neumann, B. Eger, G. Torrance

9:00 81. Development of test systems for pharmacophore elucidation. J. C. Cole, E. J. Gardiner, V. J. Gillet, R. Taylor

9:25 82. Integrating LSQ, PLS and robust regression visualization to find best QSPR models. G. D. Purvis III, D. T. Stanton

9:50 Intermission.

10:05 83. Automated compound submission and active learning using HT-ADME in silico models. R. R. Gupta, E. M. Gifford, M. Troutman

10:30 84. Reaction simulation expert system for synthetic organic chemistry.

J. H. Chen, P. Baldi

10:55 85. A BLAST-like tool for cheminformatics and drug discovery. P. Baldi

11:20 86. Binding of alkali metal cations (Li<sup>+</sup>, Na<sup>+</sup> and K<sup>+</sup>) with mono- and bi-cyclic ring fused benzenes: A theoretical study.

T. C. Dinadayalane, J. Leszczynski

## TECH

### Division of Chemical Technicians

K. Hayslip, *Program Chair*

**SOCIAL EVENTS:**  
Luncheon: Tue  
National Chemical Technician Award Dinner: Sun

**BUSINESS MEETING:**  
TECH Open Meeting: Tue

## MONDAY EVENING

## Section A

Salt Palace Convention Center  
Hall 5

## General Papers

K. Hayslip, *Organizer*

## 8:00–10:00

1. TECH: Developing professional bonds. **D. Bailey**
2. The history of the National Chemical Technician Award. **D. Bailey**
3. The many faces of CTA. **V. M. Mautino**
4. The applied chemical technology summit. **M. K. Moore**, **V. M. Mautino**
5. What is a Technician Affiliate Group? **J. Engelman**, **M. K. Moore**, **C. Dunn**
6. Bridging the gap between industry and academia for the improvement of chemical technology programs. **T. Pagano**, **L. K. Quinsland**, **A. Ross**
7. Collaboration between industry and education. **J. K. Galotos**, **E. T. Gradney**

## CHAL

## Division of Chemistry &amp; the Law

**A. I. Ahmed and J. M. Brown**,  
*Program Chairs*

## SUNDAY MORNING

## Section A

Salt Palace Convention Center  
355 C

## Strengthening your Patent Rights in Light of Recent Federal Circuit Court Decisions

**J. M. Brown and X. Pillai**, *Organizers*,  
*Presiding*

- 9:00 1. Strengthening your future patent rights in light of recent federal circuit court decisions. **J. M. Brown**, **X. Pillai**

**Plagiarism: What is it? What Can We Do About It?** Sponsored by CHED, Cosponsored by CHAL, ETHC, and CINF

## SUNDAY AFTERNOON

## Section A

Salt Palace Convention Center  
355 C

**The Chemistry of Chocolate** Cosponsored by PRES

**H. M. Peters**, *Organizer, Presiding*

- 1:30 2. Chocolate is the food of the gods. **H. M. Peters**, **S. Peters**  
2:00 3. The chemistry of cocoa. **W. Hurst**, **M. Payne**, **K. Miller**, **D. Staurt**, **J. Apgar**  
2:30 4. Chocolate: Is it really good for you? **J. A. Vinson**  
3:00 5. Making the food of gods. **S. Beckett**  
3:30 Panel Discussion.

## Nontraditional Careers in Chemistry

Sponsored by YCC, Cosponsored by Chemical Information Careers Committee, CINF, CHAL, SOCED, CEPA, SCHB<sup>†</sup>, and POLY

The official technical program for the 237th National Meeting is available online at [oasys2.confex.com/acs/237nm/techprogram/](http://oasys2.confex.com/acs/237nm/techprogram/).

## MONDAY MORNING

## Section A

Salt Palace Convention Center  
355 C

## The 25th Anniversary of the Hatch-Waxman Act: Trends in Pharmaceutical Patent Law Over the Past Twenty Five Years: CHAL's 25th Anniversary Series

**J. J. Hasford**, *Organizer, Presiding*

- 9:00 6. Paragraph IV patent challenges: Undisclosed risks for a blockbuster drug. **J. J. Hasford**  
9:30 7. The first step to ANDA litigation: Orange Book listability with the FDA. **T. L. Irving**  
10:00 8. Why Hatch-Waxman is not a model for biosimilars legislation. **S. Watt**  
10:30 9. Citizen's petitions and their effect on FDA's review of ANDAs. **S. Lee**  
11:00 Panel Discussion.

## MONDAY AFTERNOON

## Section A

Salt Palace Convention Center  
355 C

## The 25th Anniversary of the Hatch-Waxman Act: Trends in Pharmaceutical Patent Law Over the Past Twenty Five Years: CHAL's 25th Anniversary Series

**A. I. Ahmed**, *Organizer, Presiding*

- 1:30 10. Pharmaceutical patent litigation. **A. I. Ahmed**  
2:00 11. Patents, competition, antitrust and generic drugs: Resolving Hatch-Waxman Act issues. **K. Drake**  
2:30 12. FTC scrutiny of patent settlements in Hatch-Waxman cases. **M. McKitthen**  
3:00 13. Application of eBay injunction standard to pharmaceutical patent litigation. **E. Kunz**

## MONDAY EVENING

## Section A

Salt Palace Convention Center  
Hall 5

## Sci-Mix

**H. M. Peters**, *Organizer, Presiding*

- 8:00–10:00  
14. Chocolate is the food of the gods — especially on the Queen Mary 2. **H. M. Peters**  
15. National Inventors Hall of Fame Inductees 2009. **H. M. Peters**

## TUESDAY MORNING

## Section A

Salt Palace Convention Center  
355 C

## Legal Perspectives on a Shrinking World: Intellectual Property, Business and Regulatory Issues in Nanotechnology

Cosponsored by SCHB and NANO  
**J. Bunker**, *Organizer, Presiding*

- 9:00 Introductory Remarks.  
9:10 16. When are nanoparticles new chemicals? A size-based criterion for molecular identity. **V. L. Colvin**  
9:45 17. Biomedical nanotechnology: Patent trends and strategies for protecting your intellectual property. **R. Thiessen**  
10:20 18. Addressing business and legal issues in nanotechnology start-up companies. **L. Astle**  
10:55 19. Patenting nanotechnology: A review of recent U.S. Patent Office decisions on nanotech inventions. **J. J. Mallon**

## Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen Crystal Form Analysis, Experiment and Prediction Sponsored by CINF, Cosponsored by COMP, CHAL, and MEDI

## TUESDAY AFTERNOON

## Section A

Salt Palace Convention Center  
355 C

## New Policies Under the Obama Administration Related to Chemistry and the Law

**J. Bogart**, *Organizer, Presiding*

- 1:00 20. A new light for antitrust developments. **J. Bogart**  
1:30 21. Emerging issues in clean technology law. **L. Saber**  
2:00 22. Recent developments for ERISA and health care plans. **S. Labowsky**  
2:30 Panel Discussion.

## Applications of Crystal Structure Information in Pharmaceutical Materials Development: Honoring Frank Allen Scientific and Regulatory Issues of Crystal Forms Sponsored by CINF, Cosponsored by COMP, CHAL, and MEDI

## WEDNESDAY MORNING

## Section A

Salt Palace Convention Center  
355 C

## The Law and Chemistry of Dietary Supplement Regulations

**S. Turujman**, *Organizer, Presiding*

- 9:00 Introductory Remarks.  
9:10 23. Overview of the Dietary Supplement Health and Education Act: Definition of a new dietary ingredient. **M. McGuffin**  
9:40 24. Chemistry review of a new dietary ingredient notification at FDA. **S. Turujman**  
10:10 25. Dietary supplement cGMPs. **B. Williams**  
10:40 26. Interaction of dietary supplements with drugs: Adverse events. **M. Hardy**  
11:10 27. USP monographs for dietary supplements: The USP Dietary Supplement Verification Program. **J. Atwater**  
11:40 28. Label health claims. **L. Israelsen**

## WEDNESDAY AFTERNOON

## Section A

Salt Palace Convention Center  
355 C

## The Many Faces of CHAL: Where Chemistry Meets the Law Cosponsored by Kirton &amp; McConkie

**J. M. Brown**, *Organizer, Presiding*

- 1:30 29. Intellectual property enforcement and defense. **T. E. Zenger**  
2:05 30. Patentability of chemical inventions: Obviousness of chemical compounds in view of recent court decisions. **J. R. Marrott**  
2:40 31. Comprehensive, systematic intellectual property capture and management. **K. E. Horton**  
3:15 Intermission.  
3:25 32. Prosecution of chemical patent applications in the United States. **C. Metcalf**  
4:00 33. Global protection of intellectual property. **E. R. Witt**

## THURSDAY MORNING

## Section A

Salt Palace Convention Center  
355 C

## The Many Faces of CHAL: Where Chemistry Meets the Law

**A. I. Ahmed**, *Organizer, Presiding*

- 9:00 34. Biomonitoring: Its expanding role in public health evaluations and litigation. **L. S. Kurfirst**  
9:30 35. Design patents as part of a chemical IP portfolio. **S. R. Adams**  
10:00 36. Nanotechnology in consumer products: An update on regulatory responses and litigation. **L. S. Kurfirst**

## THURSDAY AFTERNOON

## Section A

Salt Palace Convention Center  
355 C

Ethics of Access to Copyrighted Scientific Print Publications Cosponsored by ETHC<sup>‡</sup>

**E. S. Slater**, *Organizer*

**J. M. Brown**, *Organizer, Presiding*

- 1:30 37. Ethics of access to copyrighted scientific print publications. **E. S. Slater**, **B. D. Crawford**, **C. P. Lake**, **S. King**

## COLL

## Division of Colloid &amp; Surface Chemistry

**J. Texter**, *Program Chair*

## SUNDAY MORNING

## Section A

Salt Palace Convention Center  
Combo Rooms 150 A-C

## Frontiers in Nanoparticle and Nanoporous Materials

## Surface Enhanced Raman Spectroscopy

Cosponsored by NANO

**J. Shumaker-Parry and M. D. Porter**,  
*Organizers*

**C.-J. Zhong**, *Organizer, Presiding*

- 8:30 1. Exploring single molecule SERS, the plasmonic periodic table, and plasmon microscopy. **R. P. Van Duyne**  
9:00 2. Structural control for tuning IR plasmons and local fields of gold and silver nanoscintors. **R. Bukasov**, **J. Shumaker-Parry**  
9:20 3. Binding kinetics of antibody-functionalized nanoparticles to a rotating capture surface. **R. J. Lipert**, **G. Wang**, **M. D. Porter**  
9:50 4. Rapid and sensitive detection of herpes simplex virus using a surface-enhanced Raman scattering based immunoassay platform. **H. P. Wampler**, **E. W. Taggart**, **M. C. Granger**, **M. D. Porter**  
10:10 Intermission.  
10:20 5. Molecularly-mediated engineering and assembly of nanoparticles. **C.-J. Zhong**  
10:50 6. Optical properties and applications of rationally designed metal nanostructures: Hollow gold nanospheres. **J. Z. Zhang**, **A. Schwartzberg**, **T. Y. Olson**, **C. Li**  
11:20 7. Development of surface enhanced Raman scattering immunoassay labels using gold nanoparticles. **M. M. Bradley**, **R. Narayanan**, **R. J. Lipert**, **J. D. Driskell**, **M. D. Porter**