

- 1:40 CHAS 15. Moving from a danger culture to a safety culture. R. Stuart
- 2:00 CHAS 16. Teaching basic technique: A view into preparing for a safer educational and work environment. F.K. Wood-Black, K. Black
- 2:20 CHAS 17. Using traditional safety rules to teach more advanced concepts in chemical hygiene. S.B. Sigmund
- 2:40 CHAS 18. Talk dirty to me: Teaching undergraduate students the importance of good hygiene in the teaching laboratory. L. Gallion, A.M. Wilson, M.J. Samide
- 3:00 CHAS 19. Risk hazard assessment in the general chemistry laboratory. S.D. Wiediger, A. Hyett
- 3:20 Intermission.
- 3:35 CHAS 20. Developing a safety synergy in the chemistry department at Stanford University. C.T. Cox, S. Chan
- 3:55 CHAS 21. Safety Friday: Do in-class safety presentations impact student behavior and perceptions of laboratory safety? A.M. Wilson, P.M. Morgan
- 4:15 CHAS 22. Student view of safety in the undergraduate laboratory. T. Black, F.K. Wood-Black
- 4:35 CHAS 23. Case study: Impact of chemical safety training in undergraduate teaching. O. Oluwaniyi, O.O. Fadare
- 4:55 CHAS 24. Nitric acid acts upon trousers: Learning about hazardous chemicals. K.P. Fivizzani
- 5:15 Concluding Remarks.

## CINF

## Division of Chemical Information

E. Davis, Program Chair

## OTHER SYMPOSIA OF INTEREST:

**Drug Discovery** (see COMP, Sun, Mon, Tue, Wed)

**Applications of Positron Emission Tomography in Drug Discovery** (see MEDI, Sun)

**New Models for Drug Discovery: Public, Private, and Non-Profit** (see MEDI, Mon)

**Putting Chemical Biology in Context** (see BIOL, Tue)

**Citizens First: Communicating Climate Science to the Public** (see CHED, Tue)

**ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of David A. Case** (see COMP, Mon, Tue)

## SOCIAL EVENTS:

**Reception**, 6:30 PM: Sun  
**Harry's Party**, 5:30 PM: Mon  
**Luncheon**, 12:00 PM: Tue

## BUSINESS MEETINGS:

**Business Meeting**, 1:00 PM: Sat

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## SUNDAY MORNING

## Section A

Colorado Convention Center  
Room 110

## Getting to the Best Reaction: Tools for Finding a Needle in a Haystack

R. Schenck, Organizer, Presiding

10:00 Introductory Remarks.

10:05 CINF 1. Automated design of realistic organometallic complexes and catalysts. M. Foscatto, G. Occhipinti, V. Venkatraman, B.K. Alsborg, V.R. Jensen

10:30 CINF 2. Different needles for different tailors: How specialized reaction search algorithms support scientists working in various research areas. V. Eigner Pitto, J. Eiblmaier, H. Kraut, H. Saller, P. Loew

10:55 CINF 3. Classification of scientific journal articles for the NIST Thermodynamic Research Center. A. Dima, Y. Feng, S. Yousef, K. Kroenlein

11:20 CINF 4. Mining electronic lab notebooks for synthetic needles (or gems). P.J. McHale

11:45 Concluding Remarks.

## SUNDAY AFTERNOON

## Section A

Colorado Convention Center  
Room 110

## Defining "Value" in Scholarly Communications: Evolving Ways of Evaluating Impact on Science

S. Rouhi, T. M. Vogel, Organizers, Presiding

1:00 CINF 5. Withdrawn.

1:25 CINF 6. Dynamic evaluation of impact for scholarly communications in the field of thermophysical properties. R. Chirico, V. Diky, J. Magee, A. Bazyleva, C. Muzny, K. Kroenlein

1:50 CINF 7. Impact of crystal structures over the last, and next, 50 years. S. Ward, I. Bruno, C. Groom

2:15 CINF 8. Give me kudos for taking responsibility for self-marketing my scientific publications and increase impact. A.J. Williams, W. Russell, M. Kenneway, L. Peck

2:40 Intermission.

2:55 CINF 9. How do you define the value of something if it's free? Observations on Caltech's Institutional Repository. D.T. Wrublewski, G.S. Porter

3:20 CINF 10. Redefining value: Alternative metrics and research outputs. K. Deards, R.M. Burks, S. Rouhi, W. Gunn

## MONDAY MORNING

## Section A

Colorado Convention Center  
Room 110

## Research Results: Reproducibility, Reporting, Sharing &amp; Plagiarism

M. G. Hicks, Organizer, Presiding

8:30 Introductory Remarks.

8:35 CINF 11. Addressing researcher incentives for publishability over accuracy. S. Davis Bowman, B. Nosek

9:05 CINF 12. Ethics in publishing: Editorial and related experiences. P.S. Weiss

9:35 CINF 13. Data management and the research record in research misconduct investigations. K. Busch

10:05 Intermission.

10:20 CINF 14. Irreproducibility in the scientific literature or: How often do scientists tell the truth, the whole truth and nothing but the truth? R.G. Bergman

10:50 CINF 15. Interplay of prior information and new data in high-throughput small-molecule studies. P.A. Clemons

11:20 CINF 16. STRENDA – proposing minimum information for reporting functional enzymology data. C. Kettner, M.G. Hicks

## MONDAY AFTERNOON

## Section A

Colorado Convention Center  
Room 110

## Research Results: Reproducibility, Reporting, Sharing &amp; Plagiarism

M. G. Hicks, Organizer

C. Kettner, Presiding

1:30 CINF 17. Reproducibility in organic synthesis. R.L. Danheiser

2:00 CINF 18. Data and models, models and data. T.R. Clark, C. Kramer

2:30 CINF 19. Reproducibility and the quality of chemical probes. A. Edwards

3:00 Intermission.

3:15 CINF 20. MIRAGE – the minimum information required for a glycomics experiment: Rationale and progress. W. York, C. Kettner, R. Planzinger

3:45 CINF 21. Reporting and reuse of crystal structure data and knowledge. I. Bruno, S. Ward, C. Groom

4:15 CINF 22. Reproducibility and variance of literature compound structure and bioassay data. J.P. Overington

## MONDAY EVENING

## Section A

Colorado Convention Center  
Halls C/D

## Sci-Mix

E. Davis, Organizer

8:00 - 10:00

1, 3-6, 11, 20. See previous listings.

CINF 23. Chemical literature: A comparison of most important databases for searching the chemical literature from an undergraduate perspective. N. Bharti

CINF 24. From lab to the libraries: A new route for chemistry librarianship. N. Bharti

CINF 25. 3Dmol.js: Simple visualization and sharing of 3D molecular data. D. Koes, N. Rego

26, 34-37, 44. See subsequent listings.

## TUESDAY MORNING

## Section A

Colorado Convention Center  
Room 110

## Research Results: Reproducibility, Reporting, Sharing &amp; Plagiarism

M. G. Hicks, Organizer, Presiding

8:30 Introductory Remarks.

8:35 CINF 26. Sharing and reproducibility/replication: An NIH view. P. Bourne

9:05 CINF 27. Globalization of Big Data: Access, integration, and quality control issues. S. Boyer, E. Bolton, R. Martin, E. Louie, T.D. Griffin, G. Fu, B. Yu

9:35 CINF 28. Flagging and curating erroneous chemical and biological records using cheminformatics to ensure data reproducibility. D. Fourches

10:05 Intermission.

10:20 CINF 29. Increasing open communication to facilitate reproducibility. C. Soderberg

## TUESDAY AFTERNOON

## Section A

Colorado Convention Center  
Room 110

## Molecular &amp; Structural 2D &amp; 3D Chemical Fingerprinting: Computational Storing, Searching, &amp; Comparing Molecular &amp; Chemical Structures

R. J. Bienstock, Organizer, Presiding

1:30 Introductory Remarks.

1:35 CINF 30. Insights into molecular similarity from crystal structures. C. Groom, S. Ward, I. Bruno, S. Vyas, N. Feeder

2:00 CINF 31. Do chiral fingerprints and descriptors work? S. Swamidass, G.P. Miller, T. Hughes, J. Hartman, S. Cothren

2:25 Intermission.

2:40 CINF 32. Similarity to SAR – interactive navigation of similarity relationships to guide optimization. M.D. Segall, E. Champness, J. Chisholm, C. Leeding, P. Hunt, A. Elliott, S. Dowling, H. Garcia

3:05 CINF 33. Database fingerprint clustering methods using KNIME. R.J. Bienstock

3:30 CINF 34. Highly visual representation methods for comparison of chemical structures and related properties. J.W. Sager, P. Mounteney, C.P. Snyder, T.E. Mansley

3:55 Concluding Remarks.

## WEDNESDAY MORNING

## Section A

Colorado Convention Center  
Room 110

## Development &amp; Use of Data Format Standards for Cheminformatics

D. Martinsen, Organizer, Presiding

9:00 Introductory Remarks.

9:05 CINF 35. Overview of the analytical information markup language. S.J. Chalk

9:35 CINF 36. Thermophysical property dissemination utilizing an XML-based standard. K. Kroenlein, R. Chirico, V. Diky, A. Bazyleva, J. Magee, C. Muzny

10:05 CINF 37. Standard data format for computational chemistry: CSX. S.J. Chalk, N.S. Ostlund, M. Sopek, B. Wang

10:35 Intermission.

10:50 CINF 38. Development of an ontology specific to computational chemistry. M. Sopek, S.J. Chalk, B. Wang, L. Nardozi, N.S. Ostlund

11:20 CINF 39. Importance of data standards for large scale data integration in chemistry. A.J. Williams, V. Tkachenko, A. Pshenichnov, K. Karapetyan, C. Coba

11:50 Concluding Remarks.

## WEDNESDAY AFTERNOON

## Section A

Colorado Convention Center  
Room 110

## Development &amp; Use of Data Format Standards for Cheminformatics

D. Martinsen, Organizer, Presiding

1:30 Introductory Remarks.

1:35 CINF 40. InChI as the chemical data format standard for cheminformatics. S.R. Heller

2:05 CINF 41. Using HL7 SPL standard for modeling substance information. Y. Borodina, F.L. Switzer, G. Schadow

2:35 Intermission.

2:50 CINF 42. JCAMP-MOL: A JCAMP-DX extension to allow integrated delivery of structural models and correlated spectral data. R.M. Hanson, R.J. Lancashire

3:20 CINF 43. Communicating crystal structures: Successes, challenges, and opportunities. I. Bruno, C. Groom, S. Ward

3:50 CINF 44. Building a standard for standards: The ChAMP project. S.J. Chalk, A. Williams

4:20 Concluding Remarks.

\* Cooperative Cosponsorship