

2:25 CHAS 49. Heavy lifting of compliance: A graduate student perspective. A. Manlove, B. Anderson, N. Nunez

2:50 Intermission.

3:05 CHAS 50. UC-Davis: SOP task force committee. P.N. Serrano

3:30 CHAS 51. Continuing to promote careful chemistry in the post-settlement era. J.G. Palmer, L.S. Wong

3:55 Concluding Remarks.

ience. K. Deards, S. Krane, R. Guha, A. Magid

11:40 Panel Discussion.

### Computer-Aided Peptide Design

#### In-Silico Peptide Modeling

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#### Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

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## CINF

### Division of Chemical Information

E. Alvaro, Program Chair

#### OTHER SYMPOSIA OF INTEREST:

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin (see COMP, Tue)

Applications of Cheminformatics & Computational Chemistry in Environmental Health (see ENVIR, Wed, Thu)

#### SOCIAL EVENTS:

Reception, 6:30 PM: Sun

Luncheon, 12:00 PM: Tue

#### BUSINESS MEETINGS:

Business Meetings, 12:30 PM & 3:00 PM: Sat

## SUNDAY MORNING

### Section A

Park Central San Francisco  
Metropolitan I

#### Materials Informatics & Computational Modeling

Cosponsored by COMP and POLY

R. J. Bienstock, M. A. Pasquinelli, *Organizers, Presiding*

8:30 CINF 1. Computer-aided design of novel materials with desired electronic and physical properties. T. Moot, O. Isayev, J. Cahoon, A. Tropsha

8:55 CINF 2. Leveraging informatics and machine learning to predict physical properties of organic compounds. M. Liosi, T. Spyriouni, X. Krokidis, L. Subramanian

9:20 CINF 3. Rational materials design via machine learning. J. Hachmann

9:45 Intermission.

9:50 CINF 4. Machine learning for large-scale MOF screening. D. Coupry, L. Groot, M.A. Addicoat, T. Heine

10:15 CINF 5. Accelerating materials research through the effective use of data. T. Mueller

10:40 CINF 6. Dark reactions project: Machine learning-assisted materials discovery using failed experiments. J. Schrier

11:05 Intermission.

11:10 CINF 7. Predicting properties of organic materials with models that blend informatics with quantum chemistry. D. Yaron, H. Li, C.R. Collins

11:35 CINF 8. Computer-based design of advanced materials: Chemically specific multiscale modelling of polymer-clay nanocomposites. P.V. Coveney, J. Suter, D. Groen

### Section B

Park Central San Francisco  
Metropolitan II

#### Open Access: Current Landscape, Challenges & Future Directions

E. Kajosallo, Y. Li, *Organizers*

G. Baysinger, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CINF 9. Perspectives on open access. M.G. Hicks

9:05 CINF 10. Current landscape and the future direction of open access publishing. J. Heber

9:35 CINF 11. Setting a fee for publication. J. McLennan

10:05 Intermission.

10:20 CINF 12. Free the science: Innovations and business model for scientific publishing. M. Yess

10:50 CINF 13. Open access and the Royal Society of Chemistry. R. Kidd, R. Anand

11:20 CINF 14. American Chemical Society's view of open access. D.P. Henderson

11:50 Concluding Remarks.

### Section C

Park Central San Francisco  
Metropolitan III

#### Careers in Chemical Information

S. K. Cardinal, K. Deards, *Organizers*  
K. Deards, *Presiding*

8:10 Introductory Remarks.

8:15 CINF 15. Twenty five years in cheminformatics: A career path through a diverse series of roles and responsibilities. A.J. Williams

8:45 CINF 16. Old chemists never die; They just go through transformations. D. Alberts

9:05 CINF 17. Challenges of the corporate librarian vs. academic librarian. V.K. Tucci

9:25 CINF 18. Computational chemistry career at the NIH. R.J. Bienstock

9:45 Intermission.

10:00 CINF 19. Interpreting chemistry: A day in the life of a data curator. S. Ward, M.P. Lightfoot, A. Sarjeant

10:20 CINF 20. Do's and don'ts of the job search: What you need to know to succeed. K. Deards

10:40 CINF 21. Preparing for careers in chemical information: A diversity of experience. K. Deards, S. Krane, R. Guha, A. Magid

11:40 Panel Discussion.

### Computer-Aided Peptide Design

#### In-Silico Peptide Modeling

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#### Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

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## SUNDAY AFTERNOON

### Section A

Park Central San Francisco  
Metropolitan I

#### Materials Informatics & Computational Modeling

Cosponsored by COMP and POLY

R. J. Bienstock, M. A. Pasquinelli, *Organizers, Presiding*

1:30 CINF 22. Computational studies of interfacial fracture in polymer composite materials. R.M. Elder, M.S. Walter, D. Knorr, T.W. Sirk

1:55 CINF 23. Guiding the synthesis of polyester electrolytes with hydrophobicity calculations. R.T. Mathers

2:20 Intermission.

2:25 CINF 24. Challenges and opportunities in modeling UV-Vis absorption spectra of organic chromophores: Utilization of Max A. Weaver Dye Library for TD-DFT benchmarking. E. Jakubikova

2:50 CINF 25. Design and optimization of polymers with high charability and high Tg using machine learning. R. Chaudret, L. Subramanian, R. Avakian, A. Mukhopadhyay

3:15 Intermission.

3:20 CINF 26. Quasi one-dimensional transport mechanisms in superionic conductors. J. Eapen, A. Annamareddy

3:45 CINF 27. Prediction of salt-responsive morphological phase diagrams for polyelectrolytes in semidilute regime. N.K. Li, T.A. Deaton, Y.G. Yingling

4:10 CINF 28. Thermal conductivity and reduced-order approximation based on covariance of heat current. J. Eapen, A. Raj

### Section B

Park Central San Francisco  
Metropolitan II

#### Open Access: Current Landscape, Challenges & Future Directions

G. Baysinger, Y. Li, *Organizers*

E. Kajosallo, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 CINF 29. Open access activities at Thieme publishers. S. Haak

1:50 CINF 30. Open research at Springer Nature. N. Quaderi

2:20 CINF 31. Seeing the forest for the trees: What's happening around the world with open access? A. Wise, P. Carton

2:50 CINF 32. Open access to chemical information. J. Zhang, P.A. Thiessen, A. Gindulyte, E. Bolton

3:20 Intermission.

3:35 CINF 33. ArXiv and SCOAP3: Evolution of open access and funding models. C. Hoover

4:05 CINF 34. bioRxiv: The development of a preprint service for the life sciences. J.R. Inglis

4:35 CINF 35. ChemRxiv – Building a preprint server for the benefit of the chemistry community. K. Davies, D.P. Henderson

5:05 Concluding Remarks.

### Section C

Park Central San Francisco  
Metropolitan III

#### Textbooks & the Practice of Science: Before, During & After Gutenberg

Cosponsored by CHED and HIST

R. E. Belford, T. Gupta, *Organizers*

G. D. Patterson, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF 36. William Henry and The Elements of Experimental Chemistry. G.D. Patterson

1:55 CINF 37. Cannizzaro's sunto: A legendary text of chemistry. C.J. Giunta

2:15 CINF 38. Alexandre Édouard Baudrimont and his Introduction à l'étude de la chimie par la théorie atomique (Introduction to the Study of Chemistry by the Atomic Theory). V.V. Mainz

2:35 CINF 39. Chemistry for a popular audience: Josiah Parsons Cooke's The New Chemistry. R.A. Egoif

2:55 Intermission.

3:10 CINF 40. Basic organic textbook: From its beginning to its (digital) end. M.C. Caserio

3:30 CINF 41. Mechanistic turn in inorganic textbooks: Basolo and Pearson's Mechanisms of Inorganic Reactions. J.A. Labinger

3:50 CINF 42. Edgar Fahs Smith and elements of chemistry at Penn. G.D. Patterson

4:10 CINF 43. Panel discussion on lessons learned from historical textbooks. G.D. Patterson

4:30 Concluding Remarks.

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**Computer-Aided Peptide Design****Computational Approaches to Peptide ADME**

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**Should I Move My Computational Chemistry or Informatics Tools to the Cloud?**

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**SUNDAY EVENING****Section A**Park Central San Francisco  
Franciscan I & II**CINF Scholarships for Scientific Excellence: Student Poster Competition**S. J. Chalk, *Organizer***6:30 - 8:30****CINF 44.** Application of spectral and diffusion geometry descriptors to shape-based virtual screening. **M. Seddon**, D. Cosgrove, M. Packer, V.J. Gillet**CINF 45.** Evaluating performance of chemical fingerprinting methods and machine learning algorithms for in silico prediction of Ames mutagenicity. **D. Mehta**, P. Volarath, K. Arvidson**CINF 46.** Shape described by numbers – Comparing the shape fingerprint and shape multipole methods. **J. Zarnecka**, A.G. Leach, S.J. Enoch**CINF 47.** Water, water, everywhere...: Modeling water molecules in protein-ligand complexes. **E. Nittinger**, P.A. Gibbons, V. Tsui, D.F. Ortwine, M. Rarey**CINF 48.** Mobilizing EPA's Comptox Chemistry Dashboard data on mobile devices. **K. Blinov**, **A. McEachran**, A.J. Williams**CINF 49.** Free online access to experimental and predicted chemical properties through the EPA's CompTox Chemistry Dashboard. **K. Mansouri**, C. Grulke, R. Judson, A.J. Williams**CINF 50.** Cheminformatics modeling of closantel analogues potentially relevant for creating river blindness. **M.A. Kuenemann**, S. Kuchibhotla, P. Kyaw Zin, D. Fourches**CINF 51.** Generation of structure-based pharmacophores in unbound state (apo) protein binding sites. **T. Seidel**, V. Reiner, G. Ibis, T. Langer

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**CINF 52.** Visualization in CDD vault: A new reactive web platform for multidimensional drug discovery data mining and visualization. **W.W. Smith**, B.A. Bunin, K. Gregory**CINF 53.** Investigating transport properties with multi-scale computable mesh models from heterogeneous structural datasets. **C. Lee**, J. Moody, J. McCammon, M. Holst, R.E. Amaro**CINF 54.** Toward automated verification of curated chemical property data. **A. Loyola**, S.J. Chalk**CINF 55.** Withdrawn.**CINF 56.** Semantically capturing NIST SRD 81 data using the SciData data model. **T. Schumann**, S.J. Chalk**MONDAY MORNING****Section A**Park Central San Francisco  
Metropolitan I**Advances in High-Throughput Screening**

Cosponsored by COMP and MEDI

R. J. Bienstock, S. Sirmulla, *Organizers*, *Presiding***8:15** Introductory Remarks.**8:20 CINF 57.** Maximizing PubChem for drug discovery. **S. Kim**, E. Bolton, S.H. Bryant**8:45 CINF 58.** Web servers and high throughput virtual screening. **R.J. Bienstock****9:10 CINF 59.** Recent advances in Autodock Vina molecular docking software. **S. Sirmulla****9:35** Intermission.**9:45 CINF 60.** Hyperspace, warp speed and time warp: Searching the chemical universe at ludicrous speed. **C. Detering****10:10 CINF 61.** PubChem BioAssay: What it takes to build a public HTS data warehouse. **Y. Wang****10:35 CINF 62.** Confidently targeting high quality hits from high-throughput screening. **M.D. Segall**, T. Mansley, P. Hunt, E. Champness**11:00** Intermission.**11:10 CINF 63.** Discovery of novel inhibitors of the galactokinase from high throughput and *in silico* screening. **M. Shen**, X. Hu, Y. Zhang, L. Liu, M. Boxer, M.D. Hall**11:35 CINF 64.** Structural modeling and identification of small molecule agonists of human relaxin family peptide receptor 1. **X. Hu**, C. Myhr, E. Barinaeva, I. Agoulnik, M. Ferrer, J.J. Marugan, N. Southall, A. Agoulnik**Section B**Park Central San Francisco  
Metropolitan II**Advances in Data Visualization**E. Davis, *Organizer*, *Presiding***8:10** Introductory Remarks.**8:15 CINF 65.** Expanding the target dimension: How to visualize a lot of models. **A. Clark****8:40 CINF 66.** Visualizing molecules in and out of context. **C. Batchelor**, N. Bailey, P. Corbett, J. White, J. Boyle**9:05 CINF 67.** Withdrawn.**9:30 CINF 68.** Scaffold histories: Visualizing temporal trends in scaffold properties. **B. Zdravil**, R. Guha**9:55** Intermission.**10:10 CINF 69.** Shoring up the (data) base: Advances in materials data processing and visualization. **P. Schaal**, R. Padilla, S.J. Chalk, M. Klinge**10:35 CINF 70.** Data visualisation: Saying it all in a bite-sized chunk. **E. Champness**, M.D. Segall, P. Hunt, T. Mansley**11:00 CINF 71.** Scalable web-based molecular graphics and visualization of structure quality metrics. **A.S. Rose**, A.R. Bradley, Y. Valasatava, J. Duarte, A. Pric, P. Rose**11:25 CINF 72.** Semi-interactive creation of 2D protein-ligand pose diagrams with PoseView-2. **T. Otto**, **M. Rarey****11:50** Concluding Remarks.**Section C**Park Central San Francisco  
Metropolitan III**Textbooks & the Practice of Science: Before, During & After Gutenberg**Cosponsored by CHED and HIST<sup>†</sup>R. E. Belford, G. D. Patterson, *Organizers*  
T. Gupta, *Organizer*, *Presiding***8:45** Introductory Remarks.**8:50 CINF 73.** Extensible electronic textbook. **R.E. Belford**, J.L. Holmes**9:10 CINF 74.** Supporting transmission of knowledge for chemical safety education: An information workflow supplement to the laboratory textbook. **L. McEwen**, S.B. Sigmann, R. Stuart**9:30 CINF 75.** Chemistry in context: How do we most effectively engage the non-science majors? **B.D. Fahlman****9:50 CINF 76.** Facts versus foundation -- The evolution of learning needs for contemporary science students. **A.S. Tseng****10:10** Intermission.**10:25 CINF 77.** Indian textbooks: From the beginnings to the modern times. **P. Roy Chowdhury****10:45 CINF 78.** Alchemy to chemical science: The advance of texts for over 5,000 years in China from the oracle bones to e-learning resources and methodologies. **R.J. Rusay**, B. Koo, R. Daugherty, G. Dasgupta, D.S. Larsen**11:05 CINF 79.** Instructor support is key to adoption of open educational systems. **J.B. Halpern**, D.S. Larsen**Should I Move My Computational Chemistry or Informatics Tools to the Cloud?**

Sponsored by COMP, Cosponsored by CINF

**MONDAY AFTERNOON****Section A**Park Central San Francisco  
Metropolitan I**Advances in High-Throughput Screening**

Cosponsored by COMP and MEDI

R. J. Bienstock, S. Sirmulla, *Organizers*, *Presiding***1:15** Introductory Remarks.**1:20 CINF 80.** Spectral and diffusion geometry descriptions of molecular shape. **M. Seddon**, D. Cosgrove, M. Packer, V.J. Gillet**1:45 CINF 81.** Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration. **A.P. Bhati**, S. Wan, D.W. Wright, P.V. Coveney**2:10 CINF 82.** Advanced HTS triage methods to identify false negative compounds. **L. Zhang**, M. Boehm, F.E. Lovring**2:35** Intermission.**2:45 CINF 83.** Withdrawn.**3:10 CINF 84.** Combining *de novo* design and macromolecular target prediction for high-throughput virtual screening. **G. Schneider**, L. Friedrich, A. Button, P. Schneider**3:35 CINF 85.** Chemical biology informatic approaches to enable high-throughput screening: Focused compounds sets, target enrichment, and hit expansion. **P. Kutchukian**, A. Wassermann, I. Wallace, C. Chang, W.L. Pettrilli, T. Kremer, M. Kansara, C.L. Waller, J.E. Imbriglio, M. Glick**4:00** Intermission.**4:10 CINF 86.** AbbVie target prediction tool. **A. Seal**, **R. Gupta**, D. Debe, P. Hajduk**4:35 CINF 87.** Open innovation drug discovery: Structure blinded virtual screening. **N.I. Franklin****5:00** Concluding Remarks.**Section B**Park Central San Francisco  
Metropolitan II**The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit**Cosponsored by CHED, CPRM and ETHX<sup>†</sup>J. N. Currano, P. A. Mabrouk, *Organizers*, *Presiding***1:10** Introductory Remarks.**1:15 CINF 88.** Authorship issues in academia of low and lower middle-income countries. **L. Anestidou****1:40 CINF 89.** What constitutes authorship? Guidance from the Committee on Publication Ethics (COPE). **H.L. Tierney****2:05 CINF 90.** Teaching students where credit is due: Attribution 101 for the mash-up generation. **J.N. Currano****2:30 CINF 91.** Influence of graduate students on authorship decision-making in undergraduate research partnerships. **A. Andes**, P.A. Mabrouk, A. Pattani**2:55** Intermission.**3:10 CINF 92.** Authorship issues and conflict in the U.S. academic chemical community. **J. Seeman**<sup>†</sup>Cooperative Cosponsorship

**3:35 CINF 93.** ORCID iDs & Project Credit: Contributor badges and getting credit for your work. C. Craig

**4:00 CINF 94.** Do not lose your invention by improperly naming inventors on the patent. X. Pillai

**4:25 CINF 95.** Hey—You stole my invention! Avoiding ethical pitfalls in determining inventorship, authorship, and honoring Non-Disclosure Agreement (NDA) obligations. J.L. Krieger

**4:50** Discussion.

**5:05** Concluding Remarks.

## Section C

Park Central San Francisco  
Metropolitan III

### Textbooks & the Practice of Science: Before, During & After Gutenberg

*Cosponsored by CHED and HIST*

T. Gupta, G. D. Patterson, *Organizers*

R. E. Belford, *Organizer, Presiding*

**1:50** Introductory Remarks.

**1:55 CINF 96.** Developing and assessing effective cyberlearning within the Libretex libraries. D.S. Larsen

**2:15 CINF 97.** Textbooks in transition: A new low-cost model for distributing chemistry textbooks and tools. M.A. Bishop

**2:35 CINF 98.** Democratization of learning and re-embedding the textbook. B. McCollum

**2:55 CINF 99.** MindTap general chemistry: Integrating scientific exploration and problem-solving within a textbook. W.J. Vining, S.M. Young, R. Day

**3:15** Intermission.

**3:30 CINF 100.** What should a textbook for 21st-century students look like? J. Moore, C.L. Stanitski

**3:50 CINF 101.** High school students and critical reading of science misinformation and inaccurate claims. A.S. Tseng

**4:10 CINF 102.** Textbooks and the SI base units. A challenge for authors and editors. P.F. Rusch

**4:30 CINF 103.** Panel discussion on textbooks of the future. R.E. Belford

**4:50** Concluding Remarks.

### Data Science Challenges in Computational Chemistry

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### Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

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## MONDAY EVENING

### Section A

Moscone Center  
Hall D

#### Sci-Mix

E. Alvaro, *Organizer*

**8:00 - 10:00**

**28, 44-45, 48-51, 53-54, 56, 86-87, 91, 101.** See previous listings.

**108, 121, 139, 160.** See subsequent listings.

## TUESDAY MORNING

### Section A

Park Central San Francisco  
Metropolitan I

### Text-Mining & Natural Language Processing for Chemical Information: From Documents to Knowledge

R. J. Bienstock, J. L. Nauss, *Organizers, Presiding*

**9:00 CINF 104.** From documents to knowledge. J.L. Nauss

**9:25 CINF 105.** Improving chemical names matching for verification, rating, and validation of PubChem compound records. L. Zaslavsky, D.M. Lowe, C. Wei, Z. Lu, E. Bolton

**9:50 CINF 106.** Advanced grammars for state-of-the-art Named Entity Recognition (NER). R.A. Sayle, D.M. Lowe

**10:15** Intermission.

**10:30 CINF 107.** Mining protein interactions from biomedical literature using semantic similarity. C. Schmitt, S. Cox, L. Christopherson, E. Scott, S. Firrincieli, N. Baker, E. Tutubalina, A. Tropsha

**10:55 CINF 108.** Automatic extraction of bioactivity data from patents. D.M. Lowe, S. Senger, R.A. Sayle

**11:20 CINF 109.** Text-mining strategies to support computational research in chemical toxicity. N. Baker, T. Knudsen, A.J. Williams, K. Crofton

### Section B

Park Central San Francisco  
Metropolitan II

### Open Access: Current Landscape, Challenges & Future Directions

G. Baysinger, E. Kajosal, *Organizers*  
Y. Li, *Organizer, Presiding*

**8:30** Introductory Remarks.

**8:35 CINF 110.** Increasing public access to federally-funded R&D results – The Department of Energy's Access Model and DOE PAGES. B. Hitson, J. Gilmore, C. Robinson, S. Studwell

**9:05 CINF 111.** Building communities and infrastructure to support openness. S. Bowman

**9:35 CINF 112.** Open access reporting: Improving the accuracy of data collection during the publishing process. M. Qiu, S. Akay, M. Blickem, S. Monasky

**10:05** Intermission.

**10:20 CINF 113.** Getting more than what you're paid for: Technologies driving revenue in an OA landscape. J. Wilcock

**10:50 CINF 114.** CHORUS – Driving the uptake and monitoring of public access by leveraging established standards and infrastructure for cost efficiency. S. King

**11:20 CINF 115.** Tales from the front lines: Supporting open access journals & repositories with research metrics. A. Michalek

**11:50** Concluding Remarks.

### Section C

Park Central San Francisco  
Metropolitan III

### Advanced Materials: Issues in Nanoinformatics & Nanosafety Data

Y. Cohen, M. G. Hicks, R. Liu, L. McEwen, *Organizers, Presiding*

**8:10** Introductory Remarks.

**8:15 CINF 116.** Meeting the challenges of nanoinformatics. J. Rumble

**8:40 CINF 117.** Conceptual analysis and chemical information: A case study in nanoscience. J.R. Bursten

**9:05 CINF 118.** Nanoinformatics platform for environmental impact assessment of engineered nanomaterials. M. Bilal, P. Church, H. Liu, R. Liu, Y. Cohen

**9:30 CINF 119.** Materials informatics: Computational and cheminformatics approaches towards properties assessment and rational design of advanced materials. B. Rasulev

**9:50** Intermission.

**10:05 CINF 120.** QNAR models for the rational design of nanomaterials. D. Fourches

**10:30 CINF 121.** Data visualization tool for exploring how nanomaterial properties correlate with toxicity in zebrafish assays. G. Lowry, S. Karcher, C. Hendren, M. Wiesner, B. Harper, S. Harper

**10:55 CINF 122.** Investigation of the interactions of macrophage and silver nanowires. E. Ogorodnik, G. Liu

**11:20 CINF 123.** Flexible database management system for nanoinformatics research and data integration. P. Church, M. Bilal, R. Liu, Y. Cohen

**11:45 CINF 124.** Tools and approaches for data deposition into nanomaterial databases. V. Tkachenko, R. Zakharov, A. Kabanov, K. Mills, T. Hickey, A. Tropsha

### Information Flow in Environmental Health & Safety

*Sponsored by CHAS, Cosponsored by CCS and CINF*

## TUESDAY AFTERNOON

### Section A

Park Central San Francisco  
Metropolitan I

### Text-Mining & Natural Language Processing for Chemical Information: From Documents to Knowledge

R. J. Bienstock, J. L. Nauss, *Organizers, Presiding*

**2:00 CINF 125.** Making the old new again: Modern technology provides access to historical chemical information. S.P. Kuhn, J. Tinsley, K.C. Schwall

**2:25 CINF 126.** Evolution of SciFinder to meet the changing needs for scientific information. P.Y. Ayala, Y. Wu, G. Gao, J.W. Taylor

**2:50 CINF 127.** Trends and relations. P. Corbett, N. Bailey, C. Batchelor, J. White, J. Boyle

**3:15** Intermission.

**3:30 CINF 128.** ChemAnalyzer: A text analytics platform for chemical surveillance. S. Gaurav, T. Roy, J. Zeng, L. E. Charles, M. Henry, K. Han, C. Corley

**3:55 CINF 129.** Addition of chemical search capabilities to PATENTSCOPE: Turning a full-text search system into a chemistry database. J. Eiblmaier, C. Mazenc, D. Geppert, L. Isenko, H. Saller

**4:20 CINF 130.** ChemExtractor: Enhanced rule-based capture and identification of PDF based property data. S.J. Chalk, T. Schumann, A. Loyola, M. Bastien, J. Turner

### Section B

Park Central San Francisco  
Metropolitan II

### Open Access: Current Landscape, Challenges & Future Directions

G. Baysinger, Y. Li, *Organizers*

E. Kajosal, *Organizer, Presiding*

**1:15** Introductory Remarks.

**1:20 CINF 131.** Open up the open access conversation at a STEM-focused university. Y. Li

**1:50 CINF 132.** Work in progress: Status of open access at a major research university. G. Baysinger

**2:20 CINF 133.** Qualitative analysis of the Berkeley Research Impact Initiative (BRII) open access fund at UC Berkeley. S. Teplitzky

**2:50 CINF 134.** Open software in chemistry: Challenges and opportunities. L. Soito

**3:20** Intermission.

**3:35 CINF 135.** Using Caltech's institutional repository to track OA publishing in chemistry. D. Wrublewski, G.S. Porter

**4:05 CINF 136.** Impact of recent changes at MIT Libraries on MIT open access policy. E. Kajosal

**4:35 CINF 137.** What price open access: Findings from the Pay It Forward Project. I. Anderson

**5:05** Concluding Remarks.

### Information Flow in Environmental Health & Safety

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## WEDNESDAY MORNING

### Section A

Park Central San Francisco  
Metropolitan I

### Public-Private Partnerships: Fostering Drug Discovery & Data Sharing

*Cosponsored by COMP*

R. J. Bienstock, B. A. Bunin, *Organizers, Presiding*

**8:30** Introductory Remarks.

**8:40 CINF 138.** CCDC: A public-private research partnership. P. Davie, I. Bruno

Technical program information known at press time.

The official technical program for the 253rd ACS National Meeting is available at:

[www.acs.org/SanFran2017](http://www.acs.org/SanFran2017)

**9:05 CINF 139.** PubChem BioAssay: Grow with the support of the community. **Y. Wang**

**9:30 CINF 140.** Selection of cross-docking candidates and comparison of evaluation metrics in Continuous Evaluation of Ligand Pose Prediction (CELPP). **S. Liu, J. Wagner, C. Churas, S.M. Gathiaka, J. Grethe, M. Chiu, H. Yang, S. Burley, R.E. Amaro, M.K. Gilson**

**9:55 Intermission.**

**10:05 CINF 141.** Synthetically accessible virtual inventory (SAVI). **Y. Pevzner, V. Ihlenfeldt, M.C. Nicklaus**

**10:30 CINF 142.** Cross-platform HELM editor empowers HELM adoption. **J. Lee, R. Hotchandani**

**10:55 CINF 143.** HELM: A line-notation and software infrastructure for managing biopolymers. **J. Milton**

**11:20 CINF 144.** Tangled up in data: Enabling strong collaborations with transparent information sharing. **J. Neitz**

## Section B

Park Central San Francisco  
Metropolitan II

### General Papers

**E. Alvaro, Organizer, Presiding**

**8:15** Introductory Remarks.

**8:20 CINF 145.** Withdrawn.

**8:40 CINF 146.** PubChem's literature and patent information for drug discovery. **S. Kim, P.A. Thiessen, T. Cheng, B. Yu, B.A. Shoemaker, J. Wang, E. Bolton, Y. Wang, S.H. Bryant**

**9:00 CINF 147.** QUDT toolkit: Development of framework to allow management of digital scientific units. **S.J. Chalk, R. Hodgson, S. Ray**

**9:20 CINF 148.** Mapping the 3D structures of small molecule binding sites. **J. Meyers, N. Brown, J. Blagg**

**9:40 CINF 149.** Predictions are tough, especially about the future: Assessing model quality, need for rapid automated model updates, and distributed computing. **V.R. Polyakov, E.J. Martin**

**10:00** Intermission.

**10:15 CINF 150.** HLA-triggered adverse drug reactions: Challenges and opportunities for molecular modeling. **G. Van Den Driessche, D. Fourches**

**10:35 CINF 151.** Can machine learning methods usefully rank small molecules for their selective growth inhibition of cancer cell lines with the BRAF V600E gene mutation? **J. Langham**

**10:55 CINF 152.** Using the Structured Product Labeling format to index versatile chemical data. **V. Tkachenko, Y. Borodina, A.J. Williams**

**11:15 CINF 153.** Reinventing the IUPAC Gold Book. **S.J. Chalk, M. Kinnan, L. McEwen, H.A. Lawlor, D. Martinsen**

**11:35 CINF 154.** Computational screening of hydrogen storage in experimental metal-organic frameworks. **Y. Chung**

## Section C

Park Central San Francisco  
Metropolitan III

### Assessment of Chemistry Collections & Services

**V. F. Scaffani, A. B. Twiss-Brooks, Organizers, Presiding**

**8:30** Introductory Remarks.

**8:35 CINF 155.** What about the books? Usage trends of chemistry monographs among graduate students in an era of transition. **D.W. Flaxbart**

**9:00 CINF 156.** Matching chemistry collections and user needs: A data-driven approach. **E. Alvaro**

**9:25 CINF 157.** Assessment of chemistry thesis and dissertation titles for collection development. **V.F. Scaffani**

**9:50** Intermission.

**10:05 CINF 158.** Chemistry library as rallying point: Assessing how to save a branch library. **J.R. Garritano**

**10:30 CINF 159.** Withdrawn.

**10:55 CINF 160.** Assessing data management practices and needs through data management plans. **B. Westra**

**11:20** Concluding Remarks.

## WEDNESDAY AFTERNOON

### Section A

Park Central San Francisco  
Metropolitan I

### Public-Private Partnerships: Fostering Drug Discovery & Data Sharing

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**R. J. Bienstock, B. A. Bunin, Organizers, Presiding**

**1:30** Introductory Remarks.

**1:35 CINF 161.** Extracting medicinal chemistry knowledge by a secure matched molecular pair analysis platform: Standardization enables merging with public data. **A. Dossetter, E.J. Griffen, A.G. Leach, S. Montague**

**2:00 CINF 162.** Enabling precision drug repurposing through innovative public-private partnerships. **D.J. Wild, J.J. Yang**

**2:25 CINF 163.** Innovative medicines initiative: From semantic data integration to risk assessment. **D. Digles, D. Goldmann, B. Zdravil, G.F. Ecker**

**2:50** Intermission.

**3:00 CINF 164.** Present and futuristic collaborative drug discovery informatics innovations (CDD vault + bioassay express). **B.A. Bunin**

**3:25 CINF 165.** Supporting compound optimisation in not-for-profit and academic research. **M.D. Segall, T. Mansley, P. Hunt, K. Chibale, T. Paquet, J. Duffy**

**3:50 CINF 166.** tranSMART platform for translational medicine: An open source, open data and open science platform. **R. Potenzzone, K. Ellison**

**4:15** Discussion.

**4:30** Concluding Remarks.

## Section B

Park Central San Francisco  
Metropolitan II

### General Papers

**E. Alvaro, Organizer, Presiding**

**1:00 CINF 167.** VIMAL: A cheminformatics toolkit for design of novel antiviral agents through textmining of scientific literature. **M. Karthikeyan, R. Pahujani, R. Vyas**

**1:20 CINF 168.** Know the breadth of your sources: The CAS content collection is your comprehensive resource. **E.N. Cheeseman**

**1:40 CINF 169.** Streamlining pharmaceutical supply chain processes: The emerging application of solid-state structural informatics. **M.J. Bryant, A.G. Maloney, N. Feeder**

**2:00 CINF 170.** Open Science Data Repository - the platform for materials research. **V. Tkachenko, R. Zakharov, I. Presniakov, S. Kalmykov**

**2:20 CINF 171.** Software tool that provides the critical information needed to enable toxicity-focused research. **N. Vaidya**

**2:40** Intermission.

**2:55 CINF 172.** Chemistry Validation and Standardization Platform Version 2.0. **V. Tkachenko, R. Zakharov, C. Grulke, A.J. Williams**

**3:15 CINF 173.** Withdrawn.

**3:35 CINF 174.** ZINC: A free database of commercially available compounds for virtual screening. **J.J. Irwin**

**3:55 CINF 175.** Biomedical literature mining for protein-protein interactions analysis using electronic mailing system. **M. Karthikeyan, R. Vyas**

## MONDAY MORNING

### Section A

Park Central San Francisco  
Stanford

### Non-Traditional Careers in Chemistry

**K. E. Bianco, Organizer**

**R. Franz, Presiding**

**9:00 CHAL 2.** Alternative careers in chemistry, an international perspective. **R. Franz**

**9:30 CHAL 3.** A PhD is not enough—Working at the intersection of science and business. **J. Chen**

### Section B

Park Central San Francisco  
Stanford

### Patent Challenges & Chocolate: A Sweet & Sour Symposium

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

**10:30 CHAL 4.** Interplay between patent office IPR challenges and district court patent infringement cases. **J.J. Hasford**

**11:00 CHAL 5.** Chocolate: Food of the Gods - 2016 Helen Free Award Lecture. **H.M. Peters, S.B. Peters**

### Chemical Forensics

### Investigations of Alleged Use & Source Attribution of Chemical Weapons

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## MONDAY AFTERNOON

### Section A

Park Central San Francisco  
Stanford

### The Use of Scientific Information in IP-Related Matters

**E. N. Cheeseman, Organizer, Presiding**

**1:30 CHAL 6.** What exactly are you looking for? Searching for chemical information. **E.N. Cheeseman**

**2:00 CHAL 7.** Patent claims reciting scientific information: The now heightened definiteness requirement. **T.A. Ostomel**

**2:30 CHAL 8.** Your next breakthrough starts here – CAS content and solutions foster discovery and innovation. **K. Zielenbach**

**3:00 CHAL 9.** Survey of biosequence in patent claims and the impact on biosequence search methods. **K.L. Hoppe**

**3:30 CHAL 10.** Patents and basic scientific research: Discovery versus invention. **P. Campbell**

**4:00 CHAL 11.** Importance of Markush searching for FTO purposes. **P.F. Blasi**

### Chemical Forensics

### Chemical Attribution Signatures of Illicit Drugs & Toxic Chemicals

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## CHAL

### Division of Chemistry and the Law

**K. Bianco and J. Kennedy, Program Chairs**

#### SOCIAL EVENTS:

**Luncheon, 12:00 PM:** Mon

**Reception, 6:00 PM:** Mon

#### BUSINESS MEETINGS:

**Business Meeting, 5:00 PM:** Sun

## SUNDAY AFTERNOON

### Section A

Park Central San Francisco  
Stanford

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

**A. H. Berks, Organizer**

**X. Pillai, Organizer, Presiding**

**A. Berks, Presiding**

**1:00 CHAL 1.** Review of recent Federal Circuit decisions relevant to what scientists need to know about patent filing and prosecution. **X. Pillai, A. Berks**