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IN THIS ISSUE

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Message from the Chair

The Fall ACS National Meeting held in Philadelphia was a great success, with an excellent set of symposia, useful business meetings, and great networking opportunities. As with most fall meetings it had a tightly packed program – this year's was one of the largest programs in recent times! CINF had a wide range of symposia covering Open Notebook Science, materials informatics, drug repurposing, chemical information in patents, science and legislation, etc.

The Fall Meeting saw the presentation of the 2012 Herman Skolnik award to Dr. Peter Murray-Rust and Prof. Henry Rzepa for their work in opening standards to facilitate first-class science, and promoting new ways to collaborate and exchange chemical data. The awardees organized an excellent symposium that addressed a broad expanse of areas in chemical information influenced by their work. Despite a few technical hitches, the symposium proceeded well. The award presentation was followed by a memorable reception hosted at the Chemical Heritage Foundation.

For the social side we had a variety of events including the Welcoming Reception, Harry's Party and the CINF Luncheon, too. The Welcoming Reception also hosted the CINF Scholarship for Scientific Excellence, which highlighted some excellent work by several graduate students. The CINF Luncheon featured Dr. William Brock, who spoke about his recent book on the history of chemistry.

The business meetings were quite productive this time. The Division has decided on making these meetings more efficient by moving as many in-person committee meetings to virtual forums as possible. It was also decided that the Division would be hosting webinars on topics related to chemical information. The first such webinar is scheduled for October 3 and will feature Dr. Alex Clark speaking on mobile chemistry. Thanks go to Antony Williams and David Martinsen for handling the logistics.

This will be my last message as Division Chair and I will pass the baton on to the next Chair, Antony Williams. I wish Tony all the best and I have no doubt that the Division will have great leadership in the coming year.

I'd like to note that it has been an honor to serve the Division. I had a great opportunity to work with my fellow CINF officials and it was the best part of my tenure. Having played various roles in the Division over the last nine years, I can attest to the fun and benefits of interacting with CINF members. There are lots of areas in which new members can get involved in the Division. I highly recommend that anybody with an interest in chemical information get in touch with a CINF member and learn about the Division's activities. As always, if you're already a CINF member and you would like to see things done differently or have an opinion related to our activities, we'd like to hear from you!

Finally, I'd like to thank all the symposium organizers, presenters, and sponsors for their time, effort and generous contributions, without which the National Meetings would not be so successful!

Rajarshi Guha, Chair, ACS Division of Chemical Information

Letter from the Editor

Welcome to the most comprehensive post-conference issue of *Chemical Information Bulletin* (62 pages!). It reflects on the richness of the Division's technical program, recognition of excellence of its renowned scientists as well as younger researchers, dedication of its members to various committees, and, furthermore, their willingness to write timely reports of the ACS National Meeting in Philadelphia for the readers of this Bulletin.

I have asked Rachelle Bienstock, CINF Program Chair 2011-12, about her experience of the division programming. Readers will find Rachelle's reflections continue a sequence of "behind the stage" interviews of the former CINF Program Chairs, Rajarshi Guha (2009-10) and Leah Solla (2007-08).

Full reports of eight symposia are included in this issue. These are: *Science and the Law: Analytical Data in Support of Regulation in Health, Food and Environment* by Bill Town, *Hunting for Hidden Treasurers: Chemical Information in Patents and Other Documents* by David Deng, *Cheminformatics and Drug Repurposing* by José Medina-Franco and Rachelle Bienstock, *Future of the History of Chemical Information* by Leah McEwen, *Herman Skolnik Award Symposium Honoring Henry Rzepa and Peter Murray-Rust* by Wendy Warr, *Global Opportunities in Chemical Information* by Tom Blackadar, Jignesh Bhate and Rachelle Bienstock, *Legal, Patent, and Digital Rights Management in Publishing* by Charles Huber, plus *Before and After Lab: Instructing Students In 'Non Chemical' Research Skills*, organized for the Biennial Conference on Chemical Education, by Andrea Twiss-Brooks. The reports are listed in the order in which they were presented at the Meeting.

CINF's four symposia and two poster sessions (twenty eight presentations total) were recorded at the Philadelphia meeting. Unfortunately, this fall the recorded content was moved from open access (used to be available about six weeks after the Meeting) to ACS Presentations on Demand**.** The recorded content will be available free only to the ACS Members registered for the Fall 2012 National Meeting (and for members with emeritus or dues waiver status). Even Non-ACS Members, e.g., Division Affiliates, registered for the Meeting are now asked to pay an extra access fee.

For traditional content this issue features award announcements by Andrea Twiss-Brooks and Bonnie Lawlor; updates on the ACS thematic programming by Guetner Grethe; reports from two CINF Committees: Communications and Publications by Bill Town, and Education by Charles Huber; ACS Council by Bonnite Lawlor and Andrea Twiss-Brooks; ACS Council Committee on Nomenclature, Terminology and Symbols by Peter Rusch; highlights from the Joint Board-Council Committee on Publications by Leah McEwen; and sponsor acknowledgments of CINF symposia and social networking events by Graham Douglas.

In conclusion, I would like to thank all authors for their generous contributions to this issue. Many thanks to Mark Luchetti for designing the cover page, to Rhonda Ross for providing the CAS chart, to Bonnie Lawlor and Wendy Warr for proofreading this issue, and to Wendy Warr for taking photographs at the Philadelphia Meeting (http://www.flickr.com/photos/cinf/).

Svetlana Korolev, Editor, Chemical Information Bulletin

AWARDS AND SCHOLARSHIPS

2012 Herman Skolnik Award Presented

The Division of Chemical Information's 2012 Herman Skolnik Award Symposium honoring Dr. Peter Murray-Rust and Prof. Henry Rzepa took place on Tuesday, August 21, 2012 at the 244th American Chemical Society National Meeting in Philadelphia, PA. The symposium, organized by the awardees, featured a morning session titled "Molecular Science and the Semantic Web" and an afternoon session titled "Intelligent Machines and Chemical Data." Speakers covered a broad range of topics such as chemical blogging, Chemical Markup Language, InChI, open chemistry, and semantic tagging for chemical concepts. (More complete coverage of the symposium is provided by an article authored by Wendy A. Warr elsewhere in this issue). The Herman Skolnik Award recognizes outstanding contributions to and achievements in the theory and practice of chemical information science and related disciplines. The award presentation took place at the close of the day-long symposium. A reception honoring Peter and Henry took place in the evening at the Chemical Heritage Foundation. The reception was generously co-sponsored by Imperial College, Microsoft Research, Schrodinger, Unilever, and the *Journal of Cheminformatics*.

Andrea Twiss-Brooks, Chair, CINF Awards Committee

2012 Val Metanomski Meritorious Service Award Presented

The Division of Chemical Information (CINF) presented the Val Metanomski Meritorious Service Award to Dr. Wendy A. Warr at the CINF Luncheon held on Tuesday, August 21, 2012 during the American Chemical Society National Meeting in Philadelphia, PA. The award is made to a member of CINF for outstanding contributions to the Division. Dr. Wendy Warr was recognized for sustained active contribution to major tasks over many years. The award consists of an engraved plaque, which was presented by CINF Chair, Dr. Rajarshi Guha.

Congratulations, Wendy!

Andrea Twiss-Brooks, Chair, CINF Awards Committee

2012 CINF Scholarships for Scientific Excellence Sponsored by FIZ CHEMIE Berlin Presented

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) funded by FIZ CHEMIE Berlin is designed to reward graduate and post-graduate students in chemical information and related sciences for scientific excellence and to foster their involvement in CINF.

Applicants presented their posters at the CINF Welcoming Reception and the Sci-Mix session of the 2012 Fall ACS National Meeting in Philadelphia. Three scholarships valued at $1,000 each were given out at the CINF Luncheon during the same meeting. The winners were presented with cash awards and plaques by Dr. Jost Bohlen, Head of Product Development & Internet, FIZ CHEMIE Berlin. CINF scholarships have been awarded consecutively for the last fourteen ACS National Meetings kindly sponsored by commercial organizations.

The names of the recipients and the titles of their posters were:

Christin Schärfer, Center for Bioinformatics, University of Hamburg, Hamburg, Germany. "*Torsion Fingerprint Deviation: A novel measure to compare small molecule conformations.*"
Co-authors: Tanja Schulz-Gasch, Matthias Rarey, Wolfgang Guba.

Barbara Zdrazil, Department of Medicinal Chemistry, University of Vienna, Vienna, Austria. "*Prioritization of docking poses in human serotonin and dopamine transporters by the use of Common Scaffold Clustering.*"
Co-authors: Amir Seddick, Rene Weissensteiner, Harald H. Sitte, Gerhard F. Ecker.

Rodolpho C. Braga, Federal University of Goiás, Goiânia, Brazil. "*Integrated chemoinformatics approaches to virtual screening in the search of new lead compounds against Leishmania.*"
Co-authors: Luciano M. Liao, José C.B. Bezerra, Marina C.B. Vinaud, Carolina H. Andrade.

Guenter Grethe, CINF Scholarship for Scientific Excellence Coordinator

From left to right: Jost Bohlen, Rodolpho Braga, Christin Schärfer, Barbara Zdrazil

2013 Herman Skolnik Award Recipient Announced

Dr. Richard D. (Dick) Cramer will be the recipient of the 2013 Herman Skolnik Award presented by the ACS Division of Chemical Information. The award recognizes outstanding contributions to and achievements in the theory and practice of chemical information science and related disciplines. The prize consists of a $3,000 honorarium and a plaque. Dr. Cramer will also be invited to present an award symposium at the Fall 2013 ACS National Meeting.

Cramer is best known as the inventor of the technique of Comparative Molecular Field Analysis (CoMFA) and its introduction to the molecular and drug design fields (JACS 1998, 110, 5959-5967). The technique and its implementation was one of the first widely available and usable 3D QSAR software methods and was developed in collaboration with David Patterson and Jeffrey Bunce. The CoMFA process was one of the first patents in the cheminformatics and computational chemistry fields and has been used in the pharmaceutical industry as the standard method for small molecule bioactivity prediction for the last twenty-five years.

Early in his career in the research group of E.J. Corey, he was involved with the first artificial intelligence methods to predict chemical synthesis, coining the acronym 'LHASA' (Logic and Heuristics Applied to Synthetic Analysis) for the project, which is known today as one of the very first attempts at computer aided design in chemistry. While his entire later career has been in industry, Cramer has taken an academic approach to solving complex problems and this has resulted in a number of break-through developments that are synonymous with innovation in chemical information and QSAR. He has remained active in research and publishing at the forefront of his field. His work on 'topomeric' descriptors, (*J. Med. Chem*. **2003**, *46*, 374-388) which allows CoMFA without tedious alignment of ligands is proving a very successful tool in drug discovery allowing the design of more selective ligands (*J. Med. Chem*. **2011**, *54*, 3982-3986). Admired by his colleagues, Cramer is described as personable and open to discussing science with all and any interested parties, a "gentleman" scientist.

While Cramer is known to the chemical information world as a top rate scientist, he has made major contributions to another field entirely: baseball[1]. He became interested in applying computers to baseball statistics and developed a program to feed detailed baseball statistics into the commentator's box. Cramer consulted with a number of major league teams, and is featured in the book *Moneyball* by Michael Lewis (recently made into a major motion picture).

Cramer received his AB degree in Chemistry and Physics from Harvard University in 1963 and his PhD in Physical Organic Chemistry from the Massachusetts Institute of Technology in 1967. He worked for Polaroid Corporation (1967-1969) and then completed a two-year fellowship under direction of E.J. Corey. After more than a decade working with Smith Kline & French Laboratories, he moved to Tripos in 1983 as Vice President of New Products. Cramer currently serves as Senior Vice President, Science, and Chief Scientific Officer for Tripos, a Certara-Company.

Andrea Twiss-Brooks, Chair, CINF Awards Committee

[1] Murphy, John. "Still hitting home runs/ PROFILE: Richard Cramer", *Scientific Computing World:* September / October 2003 http://www.scientific-computing.com/features/feature.php?feature_id=107

The Howard and Sally Peters Award for Non-Traditional Careers in Chemistry

The ACS Division of Chemistry and the Law (CHAL) has just established an award for Non-traditional Careers in Chemistry in honor of Howard and Sally Peters. This is the first award established by CHAL in more than twenty years. It was presented for the first time to both Howard and Sally for their significant contributions to non-traditional careers in chemistry at a dinner following the CHAL Executive Committee meeting held on Sunday, August 19, 2012 during the 244th American Chemical Society National Meeting in Philadelphia, PA. It was also announced at the CHAL reception held Monday, August 20, 2012 at the Chemical Heritage Foundation.

The award presented to Howard and Sally was the first of many annual presentations to come. Beginning in 2013, CHAL plans to recognize two ACS members each year. Recipients of the award will be those who have significantly contributed to or who have been significantly involved in non-traditional careers in chemistry. There will be an annual honorarium for the award and further details about the award will be featured in the coming months on CHAL's official website which can be found at www.chemistryandthelaw.org.

Howard was instrumental in establishing CHAL as a subdivision of the Division of Chemical Information (CINF) during the 1980's. He and Sally combined have 50+ years of membership in CHAL, about 50 years on the ACS Council, and 80 years of ACS membership. Sally has also been a long-term member of CINF.

On behalf of all members of the Division of Chemical Information and those of us who have followed non-traditional career paths in chemistry, I offer sincere congratulations on a well-deserved honor!

Bonnie Lawlor, CINF Councilor

Sally and Howard Peters provided an entertaining presentation with delightful treats "Chocolate, Food of the Gods" at the CINF Luncheon, 2011 Fall ACS National Meeting, Denver, CO.

TECHNICAL PROGRAM

CINF Technical Program Highlights: An Interview with Rachelle Bienstock, CINF Program Chair 2011-12

Dr. Rachelle J. Bienstock received her undergraduate degree in Chemical Engineering from The Cooper Union in New York City and her Ph.D. in Chemistry from The University of Michigan in Ann Arbor, Michigan. Following postdoctoral studies at the University of Texas Southwestern Medical Center (Dallas), involving NMR and molecular modeling of constrained peptide analogs and peptidomimetics, she joined The National Institute of Environmental Health Sciences, (NIEHS), Research Triangle Park, NC, as a molecular modeler and computational chemist. Her main research interests are protein structure and protein complex prediction methodologies, computational and structure-based ligand design methods and protein-protein and protein-ligand docking studies.

Svetlana Korolev: Rachelle, could you tell us about your professional service interests that brought you to CINF? What were your motivations to volunteer for the CINF Program Chair 2011-12? Are you a member of any other ACS divisions or other professional societies?

Rachelle Bienstock: Rajarshi Guha had posted a message on the Computational Chemistry List (CCL) server indicating that he was looking for people who would like to organize and suggest interesting symposium topics for the CINF Division program for National ACS Meetings. So I suggested a symposium on Computational Methods for Fragment Based Ligand Design for the Salt Lake City Meeting in 2009, which was so popular and well-attended that it was followed by a second part symposium in 2010 at the San Francisco meeting. Rajarshi then suggested that I might like to assume the Program Chair position at the end of his term. It seemed like a good idea as I had participated in some Program Committee meetings and enjoyed contributing topics to the CINF program at National Meetings. I am also a member of the COMP, MEDI and BIOL Divisions of ACS and the American Association for the Advancement of Science (AAAS).

SK: The Fall 2012 ACS National Meeting was the last meeting for you as the CINF Program Chair and, coincidently, the CINF program was organized at its fullest length from Sunday morning to Thursday afternoon inclusively. Would you assess the last meeting as the most successful program during your tenure? What were the CINF technical program highlights in Philadelphia?

RB: The CINF program at the Philadelphia meeting was a bit of a challenge because not only did we have a substantial program, but we were blessed with two renowned Skolnik winners: Dr. Peter Murray-Rust and Prof. Henry Rzepa. Both Peter and Henry wanted to honor many of their collaborators and colleagues with the opportunity to speak so we had a rather extensive and packed Skolnik symposium all in a single day! Additionally, we had some speakers give their addresses via the Internet and had a real time twitter feed about the meeting ongoing simultaneously. While it was a challenge, it was really pioneering for an ACS Meeting.

Some of the other programming highlights from the Philadelphia Meeting were: the one-and-a-half day session on patents held jointly with the Division of Chemistry and the Law, and The Chemistry

Small Business Divisions; the sessions on drug repurposing featuring Chris Lipinski as a speaker; on the history of chemical information; and on the new developments in electronic lab notebooks. Our program was really interesting to members and most of our sessions had standing room only attendance packed into tiny rooms in the Marriott. Even the Thursday morning session traditionally the "General papers" but subtitled "chemical databases, drug discovery and chemical structure representation" had a substantial audience.

SK: In the registration statistics of the ACS National Meetings over the past five years 2008-12, we see spikes in the numbers of attendees at the Spring meetings in San Diego (16,859 in 2012) and San Francisco (18,064 in 2010) and that correlates with the peaks of the CINF abstract submissions for the meetings. Could you comment on a magic formula of "Spring + San city = Success" and on the factors that the CINF Program Committee considers when programming for spring versus fall meetings, and for specific locations?

RB: One of the significant problems due to the current economic downturn is that many companies are no longer sponsoring employees for travel to conferences. Because San Francisco and San Diego have significant numbers of local attendees the travel problem is circumvented. At the recent meetings in Denver, Anaheim and Philadelphia we saw significant numbers of speakers asking for sponsored travel funds and then withdrawing their talks if the funds are not received. CINF is now frequently looking at the local venue and trying to involve individuals in the local area in CINF programming so that travel will be less of an issue. For the upcoming Indianapolis meeting, we are trying to involve David Wild and faculty members at Indiana University and people at Eli Lilly and Company so that travel funds will be less of an obstacle. However, we try not to let location impinge too heavily on the quality and content of our programming.

SK: Rachelle, in your highlights of the CINF Program at the 2012 Spring ACS Meeting in San Diego you observed that "no conference is now going without mobile chemistry." The first InChI Symposium took place in San Diego, too. Could you mention some other emerging themes for CINF programming? How successful has the ACS thematic programming been in influencing the CINF programming during your tenure?

RB: As you mentioned, the development of mobile applications and their usefulness in chemistry has had a significant impact on CINF programming. Additionally, recent ACS thematic programming has focused heavily on medical and health themes like in Philadelphia. We had symposia on "Science and the Law" with emphasis on regulation in health aspects and "cheminoformatics in the hands of the medicinal chemist" as well as "cheminformatics opportunities in personalized medicine and chemogenomics." At the San Diego meeting, one of our CINF symposia was featured in the LIFE thematic flyer included in the registration packets mailed to all attendees. Aside from mobile chemistry, open publishing, and medicinal and biological cheminformatic applications, I expect to see themes focused on new materials/nanomaterials and cheminformatics, semantic web and chemical database linking in the future.

SK: Rachelle, you organized two notable CINF symposia on a topic of fragment-based ligand design at Spring ACS National Meetings in 2009 and 2010, which resulted in publishing of the ACS Symposium Book Series Library Design, Search Methods, and Applications of Fragment-Based Drug Design *in September, 2011. Could you share with us your experience of the symposium book*

publishing? Were there any difficulties? Are you planning to continue programming on this topic at future ACS Meetings?

RB: Certainly publishing a book with ACS was a rewarding experience, especially since it was published and available so expediently as an E-book. However the greatest difficulty, which I had not anticipated, was persuading participants in the symposia to write chapters for the book! Because of the demands for the material in chapters to be novel and peer-reviewed, like a research article, many researchers preferred to publish in a journal rather than in an ACS symposium series volume. As fragment-based design and computer methodologies associated with growing and linking, and developing of novel fragments evolve, CINF will revisit this topic. It certainly was a popular topic and the symposium sessions were well attended.

SK: Rachelle, let's review some challenges and support venues for Program Chairs. (There used to be a Planning for Program Chair Conference organized by ACS). How do Program Chairs collaborate with other divisions and with MPPG? How important is the role of the CINF fundraising efforts for financial support of speakers in order to put together high quality programs?

RB: Other than from Rajarshi Guha, the previous CINF Program Chair, I had little assistance. The PACS system is not too user-friendly for organizing the program, although Robin Green and Farai Tsokodayi at ACS provided excellent support. Collaborating with other divisions really involves personally reaching out to the other program chairs. We have been fortunate that other divisions, particularly MEDI, COMP, CHAL, CHED, and SCHB, wanted to build bridges and co-sponsor programming with CINF. Fundraising and financial support has been a challenging issue in the current economic climate. We also had some difficulties with speakers, who are accustomed to having all their expenses paid when they come to present at a conference. Graham Douglas has worked very hard in securing sponsorship for events.

SK: As Program Chair have you been getting any data about CINF programming from ACS? Have you heard any other feedback on the program? Would you like to share your recommendations with CINF members considering their involvement in CINF programming?

RB: I have not received any feedback from ACS regarding CINF programming. However, I have been told informally from our members and other attendees that the program was interesting and of high quality. Many people commented to me on the diversity and the breadth of the program. They liked the fact that we did not repeat the same topical sessions at every meeting. The topics are really influenced by Committee members and Division members in general. Our programming is only as good as the varied input we receive from our members and attendees. We try to cast a broad net and invite all CINF members to participate in suggesting topics or organizing symposia. We welcome all suggestions and participants to the Program Committee either by attending the Committee meetings or emailing your suggestions to the Program Chair.

SK: Rachelle, who is going to be your successor as the CINF Program Chair 2013-14? Could you give us a sneak preview of the CINF technical program planned for the 2013 National Meetings?

RB: Jeremy Garritano, Chemistry and Chemical Engineering Librarian at Purdue University, will be my successor. He is already busily organizing the Spring 2013 New Orleans Meeting. Since he is from the "librarian" side of the CINF membership as opposed to the "computational" side of CINF membership, I'm sure that Jeremy will bring a new flavor to CINF programming. We already have an exciting meeting planned with sessions on scholarly communication, advances in virtual high–throughput screening, public databases, library cafes, challenges for libraries in global universities, multiparameter optimization, linking bioinformatic and cheminformatic data, foodinformatics (in line with the ACS theme), as well as on finding information about food chemistry and safety. I am even organizing a symposium myself on computational *de novo* "rational" design of proteins and peptides.

SK: Are you planning on contributing to the CINF Division in any other role after completing your term as CINF Program Chair?

RB: Well, I am planning on organizing and chairing a symposium in New Orleans, and I hope to continue to be a participant in CINF and a contributor to CINF programming without the responsibilities of being Program Chair.

SK: Rachelle, thank you very much for sharing with us your experiences as the CINF Program Chair 2011-12.

Proposed CINF Program for the Spring 2013 ACS National Meeting

Advances in Virtual High-Throughput Screening	Joel Freundlich, Sean Ekins
Advances in Visualizing and Analyzing Biomolecular Screening Data	Deepak Bandyopadhyay
Balancing Chemistry on the Head of a Pin: Multi-Parameter Optimization	Edmund Champness, Matthew Segall
CINF Scholarship for Scientific Excellence (poster)	Guenter Grethe
Computational de novo ("rational") design of proteins/peptides	Rachelle Bienstock
Food for Thought: Alternative Careers in Chemistry	Donna Wrublewski, Patricia Meindl
FoodInformatics: Applications of Chemical Information to Food Chemistry	Jose Medina-Franco, Karina Martinez Mayorga
General Papers; Sci-Mix (poster)	Jeremy Garritano
Going Global: Challenges for Libraries in Global Universities	Andrea Twiss-Brooks, David Martinsen
Library Cafes, Intellectual Commons and Virtual Services	Leah McEwen, Norah Xiao, Olivia Bautista Sparks, Teri Vogel
Linking Bioinformatic Data and Cheminformatic Data	Ian Bruno, John Overington
Public Databases Serving the Chemistry Community	Antony Williams, Sean Ekins
Scholarly Communication: New Models New Media, New Metrics	David Martinsen, William Town

Science and the Law: Analytical Data in Support of Regulation in Health, Food and the Environment

This one-day symposium examined the interaction between legislation and the underlying science which supports legislation, both in the development and application/compliance phases. In particular, the use of analytical methods and data in the regulation of health, food, and the environment has a major impact on the drafting of new legislation and on the public debate that typically precedes any new legislation. Existing databases used by legislators and those responsible for implementing legislation were considered in each sector. In addition, consideration was given to the impact of science on the regulation of new areas, such as functional foods, and the appropriate fora for the regulator and regulated industry to discuss technical issues.

Consumers face a barrage of product claims each day. These claims create consumer expectation of safety and product performance and, assuming they are accurate, facilitate well informed choice. But increased scrutiny of claims, especially where the claim involves potential health outcomes, means that claim substantiation and the science behind it are more important than ever.

Speakers in the symposium said that greater collaboration is needed to ensure that product claims are based on the best available scientific evidence. "What we need is not science for science's sake, but science for society's sake," said David Richardson. He also said that "regulators must ensure that any claims are based on the best available scientific evidence and using the best tools and methods available in order to ensure the highest standards for consumers, while at the same time fostering and advancing innovation in the products they regulate. This can only be achieved if all interested parties, whether they be NGOs, academics, regulators or industry scientists, are brought together to advance regulatory science and leverage its potential to promote and protect public health."

Other speakers in the symposium discussed claims made in the realm of regulated products, ranging from the very familiar, health and nutritional claims on food, to the newer, less familiar territory of potential future claims around "modified risk" tobacco products, which according to the Family Smoking Prevention and Tobacco Control Act of 2009 (FSPTCA) also comes under the remit of the U.S. Food and Drug Administration (FDA). The FDA is currently the only regulator with a mandate to evaluate submissions to place modified risk tobacco products on the U.S. market.

David Richardson, a food scientist at Reading University in the UK, says that the use of claims in the food and dietary supplement market is widespread. But supermarket shelves may look very different as regulators crack down on false and misleading claims. In the European Union (EU) for example, regulation published in May this year (Regulation EC No 432/2012) concerning the well-established nutrient functions of vitamins and minerals could see hundreds of nutritional and health claims become illegal. The European Commission has published a list of more than 1600 unauthorized claims on the EU Register. All labels and commercial communications must comply with the regulation by 14th December 2012 following a six-month transitional period. The result, he says, is that we must achieve an important balancing act between overcoming challenges in generating and presenting scientific data to justify a claim and achieve conclusive evidence of cause and effect, while not reducing a company's willingness to invest in new research and innovation or impacting international trade.

But whereas health claims on food and nutritional supplements are commonplace, the possibility of making reduced-risk claims is a new prospect for modified risk tobacco products which manufacturers might seek to place on the U.S. market. Under the FSPTCA, companies can apply to the FDA to market lower-risk tobacco products in the U.S. providing they provide scientific proof that marketing of the product will not only reduce harm to individual users, but also benefit the population as a whole. The FDA has started to draft guidance on the kind of scientific and other data needed to forecast and monitor a proposed modified risk tobacco product's potential impact on public health, including: product characterization; the amount of human exposure to harmful constituents; perceptions about the product and effects on human health. "Right now, this is a very new area of science and there is a shortage of established regulatory science to help assess the health risks of modified-risk tobacco products," says Christopher Proctor, Chief Scientific Officer at British American Tobacco. "We need reliable credible evidence to further this area of science and fill the gaps identified by the regulators. The FDA has set out a large number of research questions that they want answered in order to help them create the scientific underpinning to regulations, and it is going to take a considerable multi-disciplinary research effort, involving a range of research contributors, to complete the science they need."

The sentiment was echoed by Rodger Curren, of the Institute for in vitro Sciences in the US, who said that transparency, data sharing, and active communication between scientists, industry and regulators is the best way to ensure the intelligent application of science to regulatory policy. Rodger described how such an approach was key to the successful use and acceptance of new in vitro ocular models for hazard testing of anti-microbial cleaning products. He said that this approach could be modeled for use in the safety assessment of other consumer products, thus supporting the 3Rs (reduce, reuse, and recycle) approach and avoiding new animal experimentation.

Among the other speakers, Istvan Pelczer (Frick Chemistry Laboratory, Princeton) discussed **"**Honey analysis by high-sensitivity cryo-13C-NMR" detection of the fraudulent production of honey possible by this technique.

Judith Currano (Chemistry Library, University of Pennsylvania) shared her thoughts on "Hunting and gathering: locating information on the cusp between science and legislation." Her talk used a case study approach to examine methods of finding information on the science and legislation dealing with food, drugs, and the environment.

K. Scott Phillips (Division of Chemistry and Materials Science, FDA) presented research on contact lenses at FDA in a talk entitled "Contact lens materials and multipurpose solutions: lessons learned from laboratory research." This talk discussed research efforts in the areas of materials chemistry and bioanalytical chemistry, the project's contribution to current regulatory science knowledge, and potential implications that the data have for public health.

Lucinda Buhse (Division of Pharmaceutical Analysis, FDA) enlightened us on **"**Rapid screening methods for pharmaceutical surveillance." An ever-increasing percentage of products and ingredients is now coming from overseas, potentially increasing consumer exposure to poor quality, counterfeit, and adulterated pharmaceutical products. In response to this situation, the FDA has developed rapid and portable screening methods to assess the quality and safety of pharmaceutical products at ports of entry.

George Lunn (Office of New Drug Quality Assessment, FDA) informed us about "Analytical procedures and the regulation of new drug development." The information that should be submitted to the FDA is governed by the Food, Drug, and Cosmetic Act, Title 21 of the Code of Federal Regulations, and various guidances. This talk focused on these requirements and recommendations.

Thomas Hartung (School of Public Health, Johns Hopkins University) described some ground breaking work on "Mapping the human toxome for new regulatory tools." The lecture summarized the lessons learned from the development, validation and acceptance of alternative methods for the creation of a new approach for regulatory toxicology. Beside the technical development of new approaches, a case was made that we need conceptual steering, an objective assessment of current practices by evidence-based toxicology (modeled on evidence-based medicine), and implementation into legislation.

The session closed with a presentation from Frederick Stoss (Silverman Library, University at Buffalo - The State University of New York) entitled "Environmental databases: a trip down memory lane and new journeys in the 21st century." This presentation compared the "environmental" content of several STEM bibliographic databases.

Bill Town, Symposium Organizer

Hunting for Hidden Treasures: Chemical Information in Patents and Other Documents

There is a huge chemical space in scientific and legal documents, such as chemical patents, journal articles, internal documents, and other publications, that is an important resource of intellectual property, but due to historical reasons and technical limitations, much of this space is not indexed or digitized. How to extract this information and to make use of it has long been a challenging task. This symposium included a series of discussions of current developments to analyze chemical space in documents, which can benefit not only scientists in the pharmaceutical industry and academia, but also individuals in cheminformatics, publishing, patent laws and government agencies.

Since there has not been a similar symposium before, the participation at this one was overwhelming, with twenty two abstract submissions. All talks were grouped into three half-day sessions. The Sunday morning session was focused on Markush structure analysis in chemical patents, Sunday afternoon was focused on exemplified structure analysis in patents, and Monday afternoon was focused on chemical information in non-patent documents. All sessions were organized and chaired by David Deng (ChemAxon). The agenda and abstracts of all sessions are available here. (With the permission from the authors, some presentation slides are available online. The links are inserted under the author names.)

Although this time all CINF meeting rooms were far away from the convention center and the COMP sessions, it did not deter attendees. All three sessions were well attended with 40-50 participants.

Sunday Morning: Markush Structures in Patents

Markush structures are widely used in chemical patents to define large chemical spaces, and they contain essential chemical information for patent analysis. However, the flexibility and complexity of Markush structures preclude easy transformations from patent document to digital format. Currently, two organizations have systematically indexed most chemical patents: Thomson Reuters and Chemical Abstracts Service. After the opening remarks, the symposium started with talks of representatives from both organizations.

Donald Walter (Thomson Reuters) talked about how Thomson Reuters indexes Markush structures, and the coverage of their Markush database. Also, he demonstrated how one can enumerate, filter and search this database using ChemAxon's Markush technology. Roger Schenck (Chemical Abstracts Service) described how CAS builds its contents from patents and literature, and gave illustrative examples on how CAS treats inconsistencies in the documents and translated literature.

In addition to the two giants in patent Markush indexing there are also smaller and independent organizations who index Markush structures on their own. Without mishap, Jayaraman Packirisamy (Sristi Biosciences) would have reported how his company indexed Markush database of natural products, e.g. a cancer database of over 1500 Markush scaffolds of almost all cancer targets from patents. The curation is also done with ChemAxon's Markush technology. Unfortunately, Packirisamy could not come to the conference to deliver the presentation in person.

After the first three presentations had introduced the complex nature of Markush structures and its tedious process of indexing, someone wondered if the indexing can be done automatically. In this context, Josef Eiblmaier (InfoChem) talked about ChemProspector, a five-year project to automatically extract Markush structures from patent documents. ChemProspector uses image recognition technology to extract the Markush scaffold, then scans the text to extract chemical name entities as R-group definitions and retrieve Markush structure variations. For nested R-group recognition, ChemProspector obtains satisfactory results for level-1R-groups and reasonable results for level-2R-groups. However, deeply nested R-groups (level-3 and beyond) are still very challenging to retrieve accurately.

After fours talks on Markush curation, the next three presentations dealt with patent analysis.

Daniel Lowe (NextMove Software) described a system for automatically downloading patent applications from various sources, correcting and extracting relevant chemical information, indexing and storing the results in a searchable database. These structures can be used to identify novel scaffold or as keys to cluster patents.

David Cosgrove (AstraZeneca) gave an overview of a new system for encoding and searching Markush structures and a structure activity relationship analysis of chemical patents. The Periscope system uses a new language (MIL) to describe a Markush structure and has a graphic interface to display Markush structures. After exemplified structures and activity values are extracted, structures go through R-group decomposition. The R-group fragments and the activities are then used for Free-Wilson analysis yielding an improved result.

Christopher Kibbey (Pfizer) discussed his research on patent structure analysis at Pfizer. His team uses reduced graphs and generates fragment fingerprints to present a structure. These reduced graphs are compatible with Markush structure variations. They can be used to overlay structures, provide "similarity-like" score and do "substructure-like" matches. To generate a representative subset of a Markush library, his group chooses "level enumeration" which uses only the first instance of each R-group definition during enumeration. Combined with reduced graph, a Markush library can be easily compared to a query structure, which provides valuable IP assessment.

Sunday Afternoon: Exemplified Structures in Patents

Besides Markush structures, a patent also contains many exemplified structures and prophetic structures. They are often scattered in the documents as images or texts. The Sunday afternoon session discussed developments in technologies, such as OSR (image to structure), OCR (text to structure), text mining, and others, to extract and analyze these structures from patents. An interesting observation was made that seven out of the eight speakers were representing European companies in this half-day session. Does this mean Europe is leading in patent analysis?

The first two talks discussed OSR technology. Rostislav Chutkov (GGA) presented Imago, the open-source OSR toolkit. Advanced structure features, such as crossing bonds, abbreviated groups, and R-groups, are supported. Also, results from Imago can be improved by tuning the method with a training set of images and structures. Aniko Valko (Keymodule) introduced the latest development in CLiDE. From version 3.2.0 to 5.5.4 major improvements have been achieved with less run time. Now CLiDE is better at retrieving atom labels, functional groups as formula, stereochemistry, and structures in tables, and at removing noise.

The next three talks were about OCR technology and name-to-structure conversion.

Roger Sayle (NextMove software) talked about automatic spelling correction after OCR. Due to the limitation of the OCR technology, texts converted from non-text documents often contain errors. Effective automatic “spelling” correction can significantly improve chemical entity extraction. The same technology can also be applied to protein target names or even non-alphabetic entities such as CAS Registry Numbers.

Lutz Weber (OntoChem) spoke about automated SAR extraction from patents. First, chemical information, including structures, compound classes, and biological effects, is extracted from patent texts. Second, relationships about the compounds and effects are analyzed for their syntax with an automated tool. Last, the normalized relationship n-tuples are generated, and a structure activity relationship can be derived for search engines.

Daniel Bonniot (ChemAxon) provided an update on ChemAxon’s patent mining technology. Based on ChemAxon's Naming technology, Daniel and his colleagues have developed “Document to Structure,” a tool to extract all chemical information from images and text in documents. As a powerful tool for patent mining it works with non-searchable PDF, and all converted structures are returned with their locations in the document. Another tool “Document to Database” can pull documents from file systems and extract all chemical and biographical information. A free website

Chemicalize.org has been setup to demonstrate extracting information from web pages and documents.

Alex Klenner (Fraunhofer SCAI) presented his research on the exploration and visualization of chemical information in patents. After pre-processing documents with ChemoCR and Tesseract, images and text are converted into structures. All structures are "stamped" into the original PDF as "pop-up" displays along with hyperlinks to public web services. Additionally, all retrieved structures are stored in a ChemAxon JChem database, enabling structure search and filtering options. This workflow can access grid resources for parallel processing.

Nicko Goncharoff (SureChem) presented the SureChem database of 12 million unique structures from US, EP, WO and JP patents. These structures are automatically extracted from patent images using CLiDE, and from text using OPSIN and ChemAxon's Naming. The system also uses ChemAxon's Structure Checker and Standardizer for structure validation, and is hosted on Amazon Cloud with ChemAxon's JChem Cartridge for searching. All structures have been made publicly available in PubChem.

Amy Kallmerten (PerkinElmer) presented Structure Genius, a system that extracts structures from images in documents. All structures are indexed and stored in the centralized database for search and analysis.

Monday Afternoon: Chemical Information in Non-Patent Documents

Patent mining can be quite challenging, but extracting chemical information from other scientific documents, e.g. internal document database at a global corporation, is not any easier. The last half-day session was dedicated to analyzing chemical information in all documents.

The session started with an overview of the challenges in chemical literature mining by Vidyendra Sadanandan (Molecular Connections). Different chemical entity recognition applications were summarized, and challenges in chemical text mining were outlined. Typical challenges include typographical errors, image format, terminology inconsistency, legal uncertainty, access costs, etc.

As the two major players in literature indexing, Thomson Reuters and Chemical Abstracts Service, both offer comprehensive literature searching. Robert Stembridge (Thomson Reuters) talked about the challenges of collaborations between the information scientist and the chemists, and Thomson Reuters database search result visualization. Jim Brown (FIZ Karlsruhe) spoke about numeric property searching in STN databases.

David Sharpe (Royal Society of Chemistry) spoke about extracting information from literature and correcting the errors therein. Two user cases were presented: the first, Project Prospect that processes literature documents and generates enhanced HTML, and the second, fixing chair form of sugars/cyclohexanes.

Abraham Heifets (University of Toronto) presented SCRIPDB, a publicly-accessible database of chemical structures and reactions. It contains over 10 million compounds found in over 100,000

patents granted since 2001. A case study of using this database for synthetic accessibility analysis was discussed.

Guenter Grethe (for Akos GmbH) introduced CWM Global Search, which is a single user interface allowing for federated search over more than 60 scientific databases and drug discovery data sources publicly available on the internet. The search query can be chemical structures or names, CAS Registry Numbers, or free text.

SharePoint has been widely adopted as a repository for unstructured data within the enterprise. However, it lacks chemistry storage and search features. The last two talks in this symposium were about enabling chemical information extraction and searching in SharePoint.

Tamas Pelcz (ChemAxon) presented JChem for SharePoint (JC4SP), which allows many ChemAxon applications to be used in SharePoint. The user may import/view structures, and calculate properties in SharePoint list and blogs. Powered by ChemAxon's Document to Structure, JC4SP can also extract chemical information (names, SMILES, InChIs, CAS Registry Numbers, structure images, embedded structure objects, and even corporate IDs) from various document types. The extracted structures are indexed and searchable.

Rudy Potenzone (PerkinElmer Informatics) presented Search Genius, which can be used with SharePoint for chemical searching. It uses Microsoft FAST Search to identify and index embedded structures in documents. Search Genius can also be inserted into a SharePoint or E-Notebook front end for federated searching.

Summary

Various approaches to automate chemical information extraction and analysis were reported, and the challenges were well discussed at this symposium. It is of no doubt that chemical information in documents is well hidden, and a treasure hunt faces many challenges. Sometimes satisfactory or even acceptable results cannot be obtained particularly when dealing with chemical patents and/or Markush structures. However, a great number of minds have been working real hard to build comprehensive databases and to develop powerful tools in this field, and more will certainly become available.

The symposium will probably be reconvened in a couple of years. Hopefully, with the improvement of computing power and algorithms, we will hear more successful user stories.

David Deng, Symposium Organizer

Recorded content from six CINF symposia and poster sessions held at the Fall 2012 ACS National Meeting is at:
http://presentations.acs.org/common/sessions.aspx/Fall2012/CINF
Free access for the ACS Members registered for the 2012 Fall National Meeting,
Paid access for ACS Members not registered for the Meeting and non-ACS Members.

Cheminformatics and Drug Repurposing

The symposium took place on Sunday, August 19, 2012 from 1:30 PM until approximately 5:30 PM in the Philadelphia Marriott Downtown hotel. Seven speakers from industry, academia and other research labs shared their leading expertise in the area with over 50 attendees. The speakers presented opinions, case studies, and perspectives of this increasingly attractive topic to the Chemical Information community and other research areas.

Chris Lipinski (Consultant for Melior Discovery, USA) opened the symposium providing a broad perspective of the current status of the success of drug discovery efforts. Chris raised the question: "What is wrong with drug discovery?" He then reflected that one of the failures of drug discovery efforts is the current single-target approach. In this context, drug repurposing or drug repositioning is based on an alternative multi-targeted approach. Chris pointed out that a vast number of resources that are available in the public domain are promising for drug repurposing efforts in industry and other research organizations.

Thomas Freeman (Boehringer-Ingelheim, USA) spoke about the current areas of improvement of drug discovery from an industry point of view. He emphasized that the biology involved in the drug development efforts is highly complex and then discussed three major approaches to mine the vast amount of accumulated data for drug repurposing: biological, chemical, and textual data mining. Freeman presented case studies that exemplify the success of these approaches.

Iwona Weidlich (University of Maryland, USA) discussed a comprehensive study conducted in an academic setting to identify approved drugs with HCV RNA polymerase activity. She described a general computational approach to develop predictive QSAR models for molecules in a training set and then apply such models to mine databases of approved drugs. Iwona also covered key aspects of the database preparation, generation of predictive models, and shared personal experiences that face academia conducting drug repurposing projects.

Joshua Swamidass (Washington University in St. Louis, USA), also from an academic point of view, talked about opportunities and challenges that drug repurposing faces. He presented a rigorous statistical-based approach to predict potential biological activities starting from sparse and incomplete data matrices of chemical databases annotated with biological activity across different targets.

Antony Williams of the Royal Society of Chemistry and one of the lead developers of ChemSpider, discussed in detail the Open PHACTS project, a large initiative to mine publicly available databases such as PubChem, ChemSpider, BindingDB, for drug repurposing using cheminformatics tools. He also discussed issues of standards and data validation in available databases which is one significant issue with which OpenPHACTS will deal. The slides from his presentation are available at his slideshare.

Dongsup Kim (Department of Bio and Brain Engineering, KAIST, Republic of Korea), presented the development and applications of the drug-drug relationship score (DRS) for use to predict drug pairs that share common targets. This drug relationship score can then successfully be applied as a

predictive method for new target identification and has successfully predicted pharmacological effects.

Mohamed Abdul Hameed (Biotechnology High Performance Computing Software Applications Institute, USA) closed the symposium presenting the results of a general target fishing strategy based on 3D similarity searching. He described both the validation of the approach using a well-known data set of decoy compounds and then the application of the validated approach for drug repurposing.

Two papers could not be presented due to unavoidable travel conflicts for the presenters, Richard Cramer (Tripos, USA) and Chenglong Li (The Ohio State University, USA).

José Medina-Franco and Rachelle Bienstock, Symposium Organizers

The Future of the History of Chemical Information

Yes, you read it correctly; we are wondering where the venerable story of chemical information is bound. Consider the impact on chemical research of machine-readable documentation over the past 50+ years, and systematic chemical nomenclature the 100+ years before that. Consider the generations of chemists who built this discipline through their scholarly exchange and navigating the politics of their time. Bend those lenses around to look forward and consider what of the current day will most influence the progress of the chemical enterprise and its information in 50 years. What can we learn from our history to help us focus our endeavors to make future history? As we chart our way forward, what are the important principles for chemistry and chemical information, in particular, that we all in the information profession need to keep clear, front and center? These questions were the drivers of a CINF symposium at the recent ACS Meeting in Philadelphia.

We heard from a diverse panel of knowledgeable information professionals what the landscape of today could lead and distill to, based on what we have learned from various perspectives over 100+ years, about chemistry, information, and most importantly, the people involved in it all. Twelve speakers gave reflective analyses based on their respective areas of expertise, tying it to essential issues for CINF with implications for the fellow Divisions of Chemical Education (CHED) and History of Chemistry (HIST) as well. Links to the presentation slides for most talks are included in this report and also available at: http://bulletin.acscinf.org/node/347 (abstract numbers 47-51 & 59-65). My impressions and reflections on the impact of the future of the history of our chemical information are represented below.

Peter Rusch, currently the Chair of and the CINF Liaison to, the ACS Committee on Nomenclature, Symbols and Terminology, set the tone of the day by "cantilevering history." He aptly illustrated how cantilevering, much like in bridge building, is a critical aspect of the work of information professionals, and never is really done. His on-point, prescriptive "prospective retrospection" suggested that those practicing the unrecognized "central science" with its "unobvious" information will need to keep vigilant to the integrity of the science. Important principles to consider are seemingly self-evident, but not to be overlooked in any scenario: price/performance, chemical integrity, personal contact and conversation, and of course, good information habits.

Delving into the long history of chemical nomenclature and structure representation were two talks based on a symposium held at the Royal Society of Chemistry in London in November of 2010 (http://www.rsc.org/Membership/Networking/InterestGroups/CICAG/meetings.asp, scroll down to *"Celebrating the History of Chemical Information"*).

Bill Town gave a thoughtful walk through the histories of confusing nomenclature and eventually more specified compound classification. Early alchemical history was fraught with persecution, resulting in layers of confusion between warring desires of useful classification and secrecy. It took several hundred years to work through multiple systems until the atomic theory and more accurate analysis pulled together understanding. As the need for granularity increased, different nomenclatures and classifications appeared appropriate for organic compounds, inorganic compounds and the elements. Scientists finally started grappling with standardization in the 19th century.

Phil McHale delivered an entertaining evolution of structure representations, from early recognition of atoms and aromatics, through complexities of stereochemistry and delocalized bonds, to implications of Markush generics. Computerized systems depend on clear notation to support robust compound RSVP (register, search, view, print/publish) and have served up a variety of coding schemas based on fragments for substructure searching or linear notation for unambiguous identification. Current structure representation techniques focus on informatics applications, including calculation, prediction, analysis, and leveraging the networked environment through enhancing traditional information formats, linking diverse information streams, and pushing molecular manipulation potential into a variety of social communication venues.

Steve Heller picked up the story of structure representation with a primer on the emerging InChI standard, IUPAC's algorithm-based, open source International Chemical Identifier system. The idea of the InChI is to enable linking across the very diverse landscape of chemical notation, and definitely gives a twist on future thinking, pushing information publishers and vendors into thinking beyond their current systems and focus on transferrable deliverables. This approach is compatible with any registry or indexing system, but the challenge for InChI will be encouraging support and cooperation across the information industry to implement and develop further specifications as the chemical and computational landscapes continue to evolve.

Guenter Grethe traced the evolution of chemical reaction information from early alchemy focusing heavily on methodology. Desire for control brought on more scientific-like approaches to experimentation and the need for more systematic explanation. Printed sources were characterized by complex indexes and vetted methodology. The diversity of information related to reactions lends itself to endless creativity in computational approaches, including synthesis design, which predated reaction information retrieval. Early synthesis design programs used a variety of algebraic, knowledge-based or numeric approaches; later algorithms relied on reaction information. The real challenge with any reaction tool is interacting with the chemists using the systems and classification remains an important mental indexing tool for chemists. RInChI is currently under development and may help navigate some of the many wrinkles that still persist across systems. Guenter's call to honor "the intelligence and creativity of…chemists" is good aspiration as we hurtle into the future.

The afternoon session started off with two information services having long histories of innovation in chemical searching, Web of Science and Chemical Abstracts. Vijay Bhatia and Roger Schenck both focused on the future of evaluation and analysis in information systems at the chemical level. Current trends indicate increasing abundance of chemical information of diverse types and sources and chemically robust systems will need to enable scientists across disciplines to sift through the cornucopia more actively and intellectually, and reach decisions. Search and delivery have vastly improved in quality and efficiency over decades and scientists now need sophisticated tools supporting various informatics techniques. Not all information is created equivalent in content or quality and not in all contexts, especially in such intertwining, cross-disciplinary areas as chemical biology.

The next two talks considered the role of chemical information incorporating basic knowledge into learning. Through a historical tour of chemical information education, Adrienne Kozlowski delivered a strong sentiment to revive the focus on information skills in education, reminding us that CINF originated in CHED. Bruce Lewenstein focused on the central role of textbooks in chemical education. With this form in particular there are warring factors under the hood that influence what is presented to students, including considerations of economy, education as industry, adoption-rejection, and different takes on basic subjects by different types of scientists. A lively audience discussion considered Internet-based tools and data flows for chemical education, trending towards increased availability of materials, a divergence of large one-stop tools and many specialized approaches, and the mobile environment that lends itself to smaller discrete steps, or "apps." A general concern emerged throughout the day that with less tedious activities required to search, find and work with chemical information, there is in effect less practice and less re-enforcement with students about this important aspect of chemistry research.

Engelbert Zass delivered a rigorous retrospective of the interaction of chemists and their information in tandem with the technical developments of access and use over time. We are at a unique point in this history where career information specialists have directly experienced many approaches to stitching together the pieces necessary for robust chemical searching. Some interesting patterns emerge when considering the long view: there are many core fundamental steps that the tools of any day need to address and the data sources need to be well-structured to support this retrieval; chemists themselves need to weigh in scientifically at many of these steps, the searching process is as unique and critical to chemical research as the individual scientists; and this intellectual engagement has ironically been most often accomplished through usually tedious "work-arounds." Engelbert gave a passionate call that the vigilance of information professionals today needs to be no less; there are as many dangers in today's searching systems demanding multi-step complicated "work-arounds" and the primary responsibility for searching has again shifted back to chemists themselves as in the previous era of printed sources.

A unique and thought-provoking contribution to the consideration of the future of the history of chemical information was provided by Jeff Seeman's focus on chemists' information. As a chemist-historian interested in the unfolding of chemistry through the people who practice and produce it, Jeff seeks information from archival sources as well as the published literature and searching tools. A series of powerful stories around some of the classic discoveries in chemistry gleaned from "primary data" sources illustrated the ongoing importance of considering the past in light of the present and future, for practicing chemists and historians alike. The past is a moving target

depending on the vagaries of technology, economics, politics and how researchers choose to build on it; continued access to this past is a concern for all involved. Chemists themselves should be aware of and engage in thoughtful record keeping of their correspondence, data and other aspects of their research process, especially as the daily interactions around research become increasingly ephemeral in the digital environment.

Robert Buntrock brought the symposium together completing the bridge analogy connecting seekers and information. Through a whirlwind tour of the diverse variety of information sources and a dizzying array of print and early machine "interfaces," the core principles of good information seeking remain the same, from keeping current to experimental design to comprehensive literature reviews and competitive analysis. With the advent of greater access and options for searching online, it is more critical than ever before for information professionals to support chemists. While the construction techniques need updating to meet the technologies, information professionals continue to bridge the same abyss between practicing chemists and the information they need.

Overall it was a great team perspective on how we've arrived to the present day; and how even less well prepared I feel than ever before...but inspired. I don't have any answers. I am still deep in the middle of it all, not quite long enough to fully appreciate where we have been with the intersection of computers, and not quite naive enough to jump into every idea that washes through. I am especially interested in the players: amid international and government players how much of a role will the industry continue to have in shaping information? Is there really a future for the academic side and is this best focused through computer science and information theory approaches, or do we need to bring in an ethnographic approach, or just more chemists? With enhanced data access, linking, parsing and re-mixing just on the horizon, what new complexities and abilities will chemists and their science encounter? The impression is a perfect storm of centripetal forces; and I am looking forward to pushing this momentum into the murky landscape rich in potential for high-value information.

Leah McEwen, Symposium Co-Organizer

Image credit: http://www.foundationnews.org/CME/article.cfm?ID=1003

Herman Skolnik Award Symposium
Honoring Henry Rzepa and Peter Murray-Rust

Introduction

This one-day symposium was remarkable for its record number of speakers (23 in all, plus one withdrawn and one replaced by a demonstration). Despite the number of performers, and some unfortunate technical faults, the whole event proceeded on schedule and without serious mishap. Henry Rzepa's own talk was an opening scene-setter. He told a 1992 tale of some molecular orbitals explaining the course of a chemical reaction in 1992. The color diagram of these lacked semantics, and when it had been sent by fax to Bangor, it even lost its color. Months later the work was published,[1] but the supporting information (SI) is not available for this article, and even if it were available electronically, would it be usable? So, how can it be mined for useful data or used as the starting point for further investigation?

By 1994 Henry and his colleagues had recognized the opportunities presented by the World Wide Web.[2,3] The data for a later article[4] do survive in the form of Quicktime and MPEG animations on the Imperial College Gopher+ server, but they are semantically poor, i.e., they are interpretable by humans, but not by computer. The X-ray crystallography data are locatable using the proprietary identifier HEHXIB allocated by the Cambridge Crystallographic Data Center. Open identifiers such as the IUPAC International Chemical Identifier, InChI, are preferable. It would be better if we had access to semantically-rich data that allows reanalysis of the key intermolecular interactions (described in Henry's blog entry of July 5, 2012, http://www.ch.imperial.ac.uk/rzepa/blog/?p=7027). The answer is a hand-crafted XML document with the SI as a "datument:" a superset of the main article.[5] Molecules and spectra are expressed in Chemical Markup Language (**CML**)[6] and presented using a Java applet and scalable vector graphics (SVG). The underlying data for the article are still semantically alive today.

More recently, Henry has used electronic SI as a data repository for the main article.[7] The molecules are expressed in **CML** and a Jmol applet is used as the presentation layer in the style of an explorable story-board. Quick-response (QR) access to the data in 2011 allowed a re-investigation, with revised conclusions. Datasets should be deposited in digital repositories,[8] using CML where possible, and assigned a handle (equivalent to a digital object identifier, DOI). Metadata can be generated from automated scripts and can be harvested for re-injection into other repositories. In Peter Murray-Rust's Chempound (https://journals.tdl.org/jodi/article/view/5873/5879), the Resource Description Framework (RDF) allows SPARQL (http://www.w3.org/TR/rdf-sparql-query/) semantic queries of data. The repository figshare (http://www.figshare.com) allows users to upload any file format so that figures, datasets and media can be disseminated in a way that the current scholarly publishing model does not allow. Most journals treat such data-rich objects as "gold" Open Access, but there are not yet many articles with such data and you may not have permission to mine them, or even know how to find them. Perhaps gold data need their own DOIs in figshare, SPECTRa[8] etc.

Steve Bachrach's Computational Organic Chemistry blog (http://comporgchem.com/blog/) is data-rich, discussion-rich, and archivable. In other work, device-agnostic HTML5 components have been rendered natively in a browser or the epub3 Reader (the new shrink-wrapper), enabling a mobile ecosystem. Talks later in the symposium enlarged on the topics introduced by Henry.

Visualization

The first invited talk was by Bob Hanson of St. Olaf College who described two open source Java applets, Jmol and JSpecView, that are used for interactive access to molecules and spectra. Jmol is a viewer for chemical structures in 3D. JSpecView, a viewer for spectral data in the JCAMP-DX format, reads a variety of spectral data types, and has recently been integrated into Jmol. Bob also discussed a proposal for a JCAMP file extension, JCAMP-MOL (http://chemapps.stolaf.edu/jmol/docs/misc/Jmol-JSpecView-specs.pdf), that allows Jmol and JSpecView to read molecular structures, spectra and associated correlation data all from the same file. Two new user-defined data labels add 3D Jmol-readable models to the file and also associate spectral bands with specific IR and Raman vibrations, MS fragments, and NMR signals. The purpose of JCAMP-MOL is to allow for a single file that can be read either by the standalone Jmol application or by twin Jmol and JSpecView applets on a Web page. Clicking on an atom or selecting an IR/Raman vibration in Jmol highlights a band or peak or fragment on the spectrum. Clicking on the spectrum highlights one or more atoms, starts an IR vibration, or displays an MS fragment in Jmol. The specification was implemented successfully in Jmol 12.2.18 early in 2012.

The next speaker was Josef Polak of iChemLabs, the company that produces the ChemDoodle chemical structure environment (http://www.ichemlabs.com/products) focusing on 2D graphics and publishing (a product which, incidentally, was used to create all of the posters, pamphlets and conference books at this ACS National Meeting). Josef described how HTML5 adds new functionality in the browser. Java applets and third-party plug-ins such as Flash are being replaced by HTML5 and WebGL, not least in the open source ChemDoodle Web Components, a Javascript chemical graphics and cheminformatics library allowing users to present publication quality 2D and 3D graphics and animations for chemical structures, reactions and spectra. Beyond graphics, this tool provides a framework for user interaction to create dynamic applications through Web browsers, desktop platforms and mobile devices such as the iPhone, iPad and Android devices. The power of mobile technologies was well demonstrated in Josef's presentation when both projectors failed simultaneously: Josef continued, unfazed, while Kevin Theisen of iChemLabs walked around the room showing the slides on his iPad. The ChemDoodle Web Components library is being used by Henry Rzepa in datuments,[5] in the user interface to Jmol, Open Babel (http://openbabel.org/wiki/Main_Page) and ChemSpotlight (http://chemspotlight.openmolecules.net/), and in various educational applications.

Authoring and ELNs

Alex Wade of Microsoft Research talked about the Chemistry Add-in for Word, "Chem4Word" (http://research.microsoft.com/en-us/projects/chem4word/), a joint initiative of Microsoft Research and the University of Cambridge, the goals of which are to simplify the task of authoring a chemical document and to do so in such a way that the document is semantically meaningful, facilitating downstream tasks such as publisher's workflow, entity extraction and semantic applications. Chem4Word is an open source tool that chemically enables Word, allowing direct search of structural repositories and insertion of structures directly into documents. Structures can be locally manipulated within Word and are stored in CML format. Alex explained the nature of Office Open XML files, and demonstrated the chemical editing and re-use cycle: loading structures into Word, from a gallery in Chem4Word itself or from PubChem (http://pubchem.ncbi.nlm.nih.gov/), editing

structures, getting CML data back out of a document, and using and sharing the data in Chemistry for SharePoint.

A talk by Jeremy Frey of the University of Southampton also concerned the sharing of data. His team's first approach to the semantic electronic laboratory notebook (ELN) was the Smart Tea project,[9] so-called because, in order to gain a better understanding of the chemist's experimental design and execution process, the team made tea as a chemistry experiment. This early work, at the start of the e-science revolution, pushed the boundaries of the use of RDF, schemas and ontologies. "More Tea" used a tablet interface and RDF World, but these hardware and software technologies still did not have the necessary power. LabTrove (http://www.labtrove.org/) is a more flexible ELN and data management system facilitating the capture of information and the use of this information in a collaborative environment. Jeremy's team has implemented a system ("Blogjects") to "blog" information from instruments: the Smart Research Framework (SRF) LabBroker middleware gets the data into the trove before the users even look. "Tweetjects" is another option. The ELN pages can now be read by both humans and computers, using XHTML (http://www.w3.org/TR/xhtml1/) and (RDFa http://www.w3.org/TR/xhtml-rdfa-primer/). Barcodes can be incorporated, too, and LabTrove can be linked to SharePoint, using RSS, Atom, and the Open Data protocol (OData http://www.odata.org/).

The difference between Jeremy's system and other approaches is that the data are associated with the proposed scientific endeavor prior to or at the point of creation rather than by annotating the data with commentary after the experiment has taken place. This means that scientists and their peers can recreate and adapt the experiment repeatedly having already automated the processes and instrument settings. Prospective provenance describes a scientific experiment that *will be enacted*; retrospective provenance describes the scientific experiment that *was enacted*. Recording provenance allows the experiment itself to be embedded within the literature.

One weakness of the current system is the lack of support for existing external vocabularies and data models. Blog^3 (and TeaTrove^3) will have even greater user focus and semantic rigor. Blog^3 provides an extensible plug-in architecture that enables authentication and authorization; in-line preview and search-engine indexing for all data; an integrated vocabulary and schema-editing environment; and export of all data in a variety of formats.

Simon Coles, also of Southampton University, continued the theme, talking about the ELN in academia. The Dial-a-Molecule Grand Challenge (https://connect.innovateuk.org/web/dial-a-molecule1/) addresses the problem of efficiently making molecules in days, not years. ELNs could be a response to this challenge. Other drivers are information overload, and government and funding agency initiatives to encourage researchers to share data openly. Repositories such as Dryad (http://datadryad.org/) and figshare (http://www.figshare.com) allow data to be published in their own right. Citation of data through DataCite (http://www.datacite.org), for example, promises attribution and recognition for data publication.

An academic ELN should support a range of data acquisition techniques at different scales; promote access to data, sharing and reuse; enable discovery of results in related disciplines; facilitate access to data underpinning publications; enhance communication across the community; and support long-term preservation. ELNs currently on the market are primarily concerned with the protection of

intellectual property and are very poor at supporting academic practice. The solution is to turn the ELN into a publishing platform in its own right with a protocol by which a range of existing platforms and resources can make the content available, based on simple, structured metadata. A number of repositories and alliances already exist and a number of people involved in them got together to produce a "lowest common denominator" solution, easy to implement on any platform, that can nevertheless be made more sophisticated at a later stage.

The multi-layered approach included a knowledge layer, with "core" metadata, an information layer, with "contextual" metadata, and a computation layer with "detail" metadata. Through the knowledge layer, users can discover what is being made available, whether it is of interest, and whether it can be accessed. The information layer determines the granularity at which data should be made available, and the computation layer determines whether the information can be processed automatically. Two case studies illustrate the entry point for layers two and three. One is LabTrove (described by Jeremy Frey earlier). The other is an extension to the IDBS e-Workbook plug-in that enables deposition of 2D structures directly into the Royal Society of Chemistry (RSC) database ChemSpider (http://www.chemspider.com). This could be extended to more content, such as spectra, reactions and properties. Simon's team is developing examples of automatic accessing and processing of data in ELNs layers two and three, and is encouraging wider academic use of ELNs. They will also mine theses and patents and investigate getting data out of old notebooks. The semantic ELN, Blog[3], described by Jeremy Frey, and "iPad in the Lab" are other works in progress.

Blogs

Continuing the blog theme, Steven Bachrach of Trinity University listed a number of examples. Peter Murray-Rust's blog (http://blogs.ch.cam.ac.uk/pmr/), Derek Lowe's *In The Pipeline* (http://pipeline.corante.com/), Paul Bracher's *ChemBark* (http://blog.chembark.com/) and *The Chemistry Blog* (http://www.chemistry-blog.com) provide opinion and news. Some blogs such as James Ashenhurst's *Master Organic Chemistry* http://masterorganicchemistry.com are for teaching. Paul Docherty's *Totally Synthetic* (http://totallysynthetic.com/blog/) and Steve Bachrach's own *Computational Organic Chemistry* http://comporgchem.com/blog/ publish article reviews. Henry Rzepa's blog (http://www.ch.ic.ac.uk/rzepa/blog/) features original research. Blog aggregators include Egon Willighagen and Peter Maas' *Chemical Blogspace* (http://cb.openmolecules.net/) and Jan Jensen's *Computational Chemistry Highlights* (http://www.compchemhighlights.org/).

Two recent examples illustrate post-publication peer review by blog. As a result, initially, of blogging in *Totally Synthetic*, a paper on reduction by sodium hydride[10] was withdrawn for scientific reasons; and a paper with claims about dinosaurs in space[11] was criticized for self-plagiarism and exaggerated claims in several blogs before being withdrawn by the author on the grounds of similarity to his earlier publications. Steve himself has good reasons other than altruism for blogging. He surveys the literature to provide currency to his book and assist in writing the second edition. His blog also forms the basis of a series of review articles for the RSC and demonstrates the use of blogging in chemical communication. Blogging faces pressure from other social media, but it is hard to envisage Twitter as an effective chemical communication medium. Altmetrics (an alternative to journal Impact Factors) and journal review overlay may establish a professional benefit to blogging in future.

Statistics and Property Prediction

Egon Willighagen at Maastricht University gave his presentation remotely. His take-home message was that you can improve your property prediction, training, and validation by adopting semantic pipelines.[12] This means using open look-up lists, dictionaries, and ontologies; removing format limitations; linking to data from other domains; and using calculation provenance. CML is semantic, flexible, and embeddable in HTML and RSS, but it is limited to XML. JavaScript Object Notation (JSON, http://www.json.org/) and Terse RDF Triple Language (Turtle, http://www.w3.org/TeamSubmission/turtle/) are alternative formats to XML for transmitting data between a server and a Web application. They enable linked data. RDF is an open standard, independent of format and database technology, and embeddable in HTML. It can be queried using SPARQL (http://www.w3.org/TR/rdf-sparql-query/). A federated query extension allows execution of queries distributed over different SPARQL endpoints.

One application is a computational toxicity assessment platform[13] generated from integration of two open science platforms related to toxicology: Bioclipse, which combines a scriptable, graphical workbench environment for integration of diverse sets of information sources, and OpenTox, a platform for interoperable toxicology data and computational services. A second application (unpublished) is Egon's work on nanotoxicity carried out in Stockholm last year, using SPARQL to link a wiki to the R statistics environment. Another project in progress is the Open Pharmacological Concepts Triple Store (Open PHACTS, http://www.openphacts.org),[14] a knowledge management project of the Innovative Medicines Initiative (IMI, http://www.imi.europa.eu/).

Rajarshi Guha of NIH discussed the benefits of integrating cheminformatics with statistical software, specifically the Chemistry Development Kit (CDK, (http://sourceforge.net/apps/mediawiki/cdk/index.php?title=Main_Page) and R. R is an environment for modeling that contains many prepackaged statistical and mathematical functions. It is also a matrix programming language that is good for statistical computing. Cheminformatics capabilities include statistics and machine learning and R is well suited to these. There is thus a case for "cheminformatics in R."

CDK provides chemical and more complex objects, input and output of various molecular file formats, fingerprint and fragment generation, rigid alignments, pharmacophore searching, substructure searching, SMARTS support, and molecular descriptors. Rajarshi has implemented CDK (http://github.com/rajarshi/cdk; http://sourceforge.net/projects/cdk/) in R using the rJava package, providing access to variety of CDK classes and methods, and idiomatic R. Currently in rcdk you can access atoms and bonds and get certain properties and 2D and 3D coordinates, but since rcdk does not cover the whole CDK API you might need to drop down to rJava level, and make calls to the Java code, in some cases.

Rajarshi outlined some applications. The fingerprint package implements 28 similarity and dissimilarity metrics, allowing enrichment studies and comparison of datasets.[15] 2D structure images can be visualized. A typical QSAR workflow can be followed.

The PubChem (http://pubchem.ncbi.nlm.nih.gov/) and ChEMBL (https://www.ebi.ac.uk/chembl/) databases can also be accessed directly within R using their public APIs. Published QSAR models

may even become reusable: reproducible data mining is encouraged because DB and HTTP access ensures that an analysis can always be up to date if required.

Open Chemistry

In the final talk of the morning session, Marcus Hanwell of Kitware criticized the proliferation of black box, proprietary codes in chemistry. There is a need for open tools and open standards and more papers should be including data. The Open Chemistry project (http://www.openchemistry.org/) is a collection of open source, cross platform libraries and applications for the exploration, analysis and generation of chemical data. Kitware is developing three independent applications: the Avogadro[2] structure editor, Molequeue, for running local and remote jobs, and ChemData for storing, annotating and searching data. Avogadro (http://avogadro.openmolecules.net/)[16] is an open source molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. The Avogadro library is a framework providing a code library and application programming interface (API) with 3D visualization capabilities. The Avogadro application provides a rich graphical interface using dynamically loaded plug-ins through the library itself. The application and library can each be extended by implementing a plug-in module in C++ or Python. By using the CML file format as its native document type, Avogadro seeks to enhance the semantic accessibility of chemical data types. HDF5 (http://www.hdfgroup.org/HDF5/) will be used to store "heavy data" (e.g., for quantum mechanics). Kitware distributes its products using the very open Berkeley Software Distribution (BSD) license.

Artificially Intelligent Chemists

Peter Murray-Rust opened the afternoon session with some thoughts on building artificially intelligent chemists. He was helping to build a knowledge base for the Dial-a-Molecule Grand Challenge (https://connect.innovateuk.org/web/dial-a-molecule1/), but found that many publishers were unwilling to allow him to mine their content. There was interest in artificial intelligence (AI) in the 1970s, but over the next 35 years little progress was made. Some early examples are Ralph Christoffersen's work on quantum pharmacology[17] and Malcolm Bersohn's work on retrosynthesis.[18] In those days knowledge bases depended on look-up, heuristics, rules, logic, brute force, tree pruning and computing chemical reality. Nowadays most of the tools we need are available but the will to use them is not there. Peter presented a diagram of the 2012 knowledge base, and perception and communication of the transformed knowledge. Knowledge is represented in CML, ontologies and other domains. AI means putting all the components together.

Peter discussed a chemical application of John Searle's Chinese room thought experiment (http://en.wikipedia.org/wiki/Chinese_room). The experiment supposes that there is a program that gives a computer the ability to carry on an intelligent conversation in written Chinese. If the program is given to someone who speaks only English to execute the instructions of the program by hand, then in theory, the English speaker would also be able to carry on a conversation in written Chinese. However, the English speaker would not be able to understand the conversation. Here are Frog and Zog asking Magic Chemical Panda a chemical question and getting an answer:

There is no "Magic Chemical Panda" in Peter's box (http://vimeo.com/48280639). Chemical names are found by look-up and if the precise name is not found, the rule book is used to manipulate symbols and relate ethanoic to ethanoate, say. The Open Parser for Systematic IUPAC Nomenclature (OPSIN) name to structure software,[19] is a symbol manipulation system with a rule base.

Peter's team has also worked on CML and Chem4Word in the intelligent laboratory: Ami,[20] uses image recognition, voice recognition, sensors and RFID tags. Peter continues to capture semantics "by stealth" and he uses patents because publishers have prevented him from mining the journal literature. "Open" means *really* open and not pretending that your API is open. It is possible to make revenues from open source software: Kitware, ChemDoodle and GGA Software have proved this.

Computational Chemistry and NMR

Peter has been working with the Environmental Molecular Sciences Laboratory (EMSL) at Pacific Northwest National Laboratory (PNNL) on enriching the NWChem open source computational chemistry software (http://www.nwchem-sw.org/) with CML. Wibe ("Bert") de Jong was unable to present a talk about this in person, but Marcus Hanwell deputized. NWChem now generates semantic data, enabling Avogadro to extract and visualize NWChem semantic output. The team has completed a CML generator for Gaussian basis function based quantum methods based on the FOX library (http://fox-toolkit.org/), using an infrastructure based on PNNL's Extensible Computational Chemistry Environment data generator (http://blogs.ch.cam.ac.uk/pmr/2011/11/02/searchable-semantic-compchem-data-quixote-chempound-fox-and-jumbo/). Work currently in progress aims to get all NWChem data stored into CML output file, to reduce the CML data by avoiding replication, and to integrate CML with the appropriate format for bigger data blocks. Then plane wave capability will be made semantically rich. Another goal is to use Peter's JumboConverter to convert old NWChem output files into CML, and store them in MyEMSL. The CML CompChem dictionary and conventions are being extended to enable integration of NWChem and NMR data which can be accessed and visualized in MyEMSL through EMSLHub.

In another EMSL talk, Karl Mueller addressed the subject of NMR data. EMSL is collaborating with the Australian Commonwealth Scientific and Industrial Research Organization (CSIRO) in an NMR project. PNNL has about 12 very large NMR instruments, but the data have not been captured well in the past. Karl gave one example of an experiment in which he was involved.[21] He showed diagrams of the workflows for translating and processing raw data from an experiment and for simulating and processing raw data from calculations in Gaussian, NWChem, etc. He also showed some screenshots from a potential MyEMSL Workbook for NMR. The team initially planned to continue updating the JCAMP NMR dictionary with relevant terms and definitions, to update the JCAMP parser, to test the output and to begin working on code to extract binary data for Agilent and Varian.

To make further progress the development of a repository for NMR data must address three important issues: the large number of different NMR experiments in existence, many with multiple versions and variations; the intricate processing steps often required to convert raw time domain data into usable spectra (and the need for a detailed record); and the large number of divergent NMR data formats. A proper record of an NMR experiment must contain original digitized numerical values, information about the source instrument, and saved instrument parameters, all in a standardized file format. The processed spectrum (as saved by the experimentalist) should include software version and processing parameters, in a standardized file format. The standardized file for a high-level experiment description should include sample, pulse sequence, magnetic field, detected isotope, decoupled and undetected isotopes, pulse times, delays, phase cycles, and temperature, etc., and interpretation, and instrument-parameter to experiment-parameter translation.

New approaches such as blogging are also of interest so Karl has been collaborating with Jeremy Frey in the use of LabTrove. To put all these approaches together, community buy-in, and partnerships are being developed with other national facilities in multiple countries, other NMR data model efforts, and NMR spectrometer companies.

Natural Language Processing and the Semantic Web

Lezan Hawizy was indisposed on the day of the symposium and a video was shown of her presentation about natural language parsing for semantic science. ChemicalTagger is an open source package for "understanding" organic chemistry experiments, developed by Peter Murray-Rust's group, using natural language processing (NLP) approaches. Tools available include Open Source Chemistry Analysis Routines (OSCAR)[22] and OPSIN.[19] ChemicalTagger converts flowing text into structured text. Processes such as dissolve phase, purify phase and yield phase are marked up in the chemical procedure. Components of ChemicalTagger include tokenizers, which split a sequence of text into individual tokens; taggers, which assign parts of speech to each token; a parser which groups tagged tokens into phrases; and a role identifier which assigns roles to the parsed phrases. Taggers include OSCAR for chemical entities, RegEx for chemistry-related entities, and OpenNLP (http://opennlp.apache.org/) for English entities. The parser has a rule-based grammar for molecules, amounts etc. The role identifier assigns action roles (e.g., "dissolving") to phrases, and roles such as "solvent" to molecules. The role identifier was evaluated using 50 experimental paragraphs by comparing the effort of four annotators with each other and with ChemicalTagger, using the Dice coefficient to measure similarity. There was about 90% agreement between human and machine tagging.

Daniel Lowe has expanded the work to chemical reactions. The software identifies experimental sections, uses ChemicalTagger with an additional OPSIN tagger to produce structured data, associates chemical entities with quantities, assigns chemical roles, and carries out atom-atom mapping. Daniel extracted 424,621 reactions from 65,034 patent documents. Hannah Barjat has developed an additional tagger, ACPTagger, for use with the open access journal *Atmospheric Chemistry and Physics*. Lezan showed some visualization features of the resulting system, including geolocations mapped onto a map of the world.

Materials informatics requirements are substantially different from small molecule informatics: while structural representations of small molecules often contain enough information for the development of structure-property relationships, this is frequently not the case for complex materials. Often an account of the provenance of a material must be added to the chemical representation of a material. Additionally, materials data are usually generated in "native vernaculars:" non-portable formats, which do not easily allow for data exchange. To make these data widely accessible, they must be converted to formats with both human as well as machine comprehensible standard syntax and semantics.

Nico Adams of CSIRO has used a complete Semantic Web toolstack, from XML dialects to axiomatically rich ontological models in Web Ontology Language OWL (http://www.w3.org/standards/techs/owl#w3c_all), in the development of modern materials information systems. Nico showed an example of Polymer Markup Language (PML) and the ChemAxiom ontology for polymerization and he produced graphical representations that describe a chemical procedure. Synthetic robots produce a log file that can be decoded by the manufacturer, but Nico had to put in some effort to convert the information into an ontology and graph. Unfortunately the robot does not know what chemistry went into the robot. This has to be caught elsewhere. Nico uses ChemicalTagger.

Janna Hastings of EBI started her talk with her conclusions: classification conveys the type for data; the Semantic Web makes data of all types available, open and interlinked; and classification using OWL ontologies dramatically enhances the potential of the chemical Semantic Web. The subject and object in an RDF triple are types. Molecules are small and three-dimensional. Their structures can vary according to their environment. We say they have the same type when they share important properties. All caffeine molecules have type caffeine. There are many different ways to represent a molecule: by InChI, by a reference number, by a ball and stick model, and so on. None of these is, in itself, a molecule; all these describe and approximate. All data are representations. Science aims to make discoveries of general rules about the things that the data are about. Classification puts the scientific knowledge into the data. RDF is a technology for data representation and OWL is a technology for classification.

Ontologies encode expert domain knowledge in a hierarchically-organized format that a machine can process. One such ontology for the chemical domain is ChEBI.[23] ChEBI provides a classification of chemicals based on their structural features and a role- or activity-based classification. An example of a structure-based class is "pentacyclic compound" (compounds containing five-ring structures), while an example of a role-based class is "analgesic", since many different chemicals can act as analgesics without sharing structural features.

ChEBI has been applied to annotation of chemicals in biological contexts and for diverse tasks of chemical discovery including metabolic network gap prediction, but its growth has been limited to the throughput of manual annotation. A recent publication[23] describes the requirements for structure-based, automated classification; the analysis of structure-based features of chemical classes in ChEBI; and mapping to existing OWL-based technology and cheminformatics-based approaches. Another publication[24] describes feature and maximum common substructure detection for a group of chemicals, asserts class definitions logically using OWL and SMARTS, and demonstrates automated classification using OWL reasoning.

Exploration and Analysis

In the pre-Google era, Henry's team wrote an indexing and search engine called ChemDig;[25] in the post-Google era, Geoffrey Hutchison at the University of Pittsburgh has built ChemSpotlight (http://chemspotlight.openmolecules.net), using Spotlight (the desktop search feature of Apple's OS X operating system) plus Open Babel[26] and about 300 lines of code. ChemSpotlight is a metadata importer plug-in for Mac OS X, which reads common chemical file formats using the Open Babel chemistry library. Spotlight can then index and search chemical data: molecular weights, formulas, SMILES, InChI, fingerprints, etc. The data are kept as native files with a separate index. The current version (with about 800 more lines of code) allows freely rotatable 3D views of molecules and 2D views of ChemDraw and molfile formats, thanks to the ChemDoodle WebComponents. Geoffrey refers to ChemSpotlight as an "undatabase" because it has no (visible) database or SQL. It stores fingerprints, and number of atoms, bonds, and residues, PDB and SDfile keywords and properties, calculation keywords, and calculation results. Geoffrey presented a new genetic algorithm approach with Spotlight for designing new molecules for organic heterojunction solar cells, by calculating electronic and optical properties, and a synthetic score, for virtual libraries of more than a million compounds. His take-home message was that "undatabases" and ChemSpotlight, integrated into user-friendly tools, work well for big data.

Brian McMahon of the International Union of Crystallography (IUCr) talked about crystallographic publishing in the semantic age. The Semantic Web adds value (and meaning) to data in IUCr journals online through linking, allowing navigation, search, provenance, accreditation and access to related data and literature. Dynamic textual annotation of IUCr article content currently gives links to the *Online Dictionary of Crystallography* and the *IUPAC Gold Book*. The layout in HTML tables implies some semantics and can communicate meaning to another application (e.g., Jmol to highlight a selected bond).

The Crystallographic Information File (CIF)[27] information interchange standard has informed the structural content of CML. CIF was designed from the outset as an extensible standard, and now covers many areas of crystallography. It forms the basis for integrated data and publishing workflows linking laboratories, data repositories, publishers and databases, and has been an important factor in improving the quality of published crystal structures. The CIF publishing editor pubCIF (http://journals.iucr.org/services/cif/publcif/) is a desktop application for formatting and validating CIFs. CIF acts as a vehicle for article submission; checkCIF (http://checkcif.iucr.org) can be used to validate the structural model. An enhanced figures toolkit (http://submission.iucr.org/jtkt) brings an article alive by creating Jmol enhanced figures. The CIFs in SI for non-IUCr articles on the Web can be loaded into the IUCr visualization tool. The metadata about instrument, refinement etc.

is available. CheckCIF can be run on the SI. Brian concluded his presentation with some charts showing where CIF sits in the data flow in crystallography and the publication flow in IUCr journals.

Kitware has developed a new open-source application, ChemData (part of the Open Chemistry project), to facilitate the exploration and analysis of large chemical datasets. Kyle Lutz described the program features of which include a variety of 2D plotting techniques, such as traditional scatter plots, parallel coordinates charts, and scatter plot matrices. Similarity relations between molecules can be explored using a range of graph-based visualization methods. Multiple querying and filtering functions allow users to locate molecular data relevant to their work.

ChemData is a native C++ application built with the user interface framework Qt (http://qt-project.org/). It uses the NoSQL database MongoDB (http://www.mongodb.org/) as a semantic data store, focusing on cheminformatics and assessment of chemical properties such as QSAR data. Computational chemistry data are stored directly in the file store, and semantic data are extracted to facilitate search and analysis. ChemData uses the Visualization Toolkit (VTK, http://www.vtk.org/) for 2D and 3D dataset visualization. Molecular structure, geometry, identifiers and descriptors are stored as a single "ChemicalJSON" object. JSON is used as the data interchange format, rather than XML/CML, because it is more compact, it is the native language of MongoDB, and it is easily converted to a binary representation. Initial work is in progress for using Web-based visualization and analysis tools. ParaViewWeb (http://paraviewweb.kitware.com/PW/) accesses the MongoDB database and will provide a collaborative remote Web interface for 3D visualization with ParaView as a server. ParaView (http://paraview.org/) is an open-source, multi-platform data analysis and visualization application.

InChI and Databases on the Web

Stephen Heller, the project manager for InChI (http://www.iupac.org/home/publications/e-resources/inchi.html), outlined the significance of this standard. InChI is a non-proprietary, machine-readable string of symbols which enables a computer to represent a compound in a completely unequivocal manner. InChIs are produced by computer from structures drawn on screen with existing structure drawing software, and the original structure can be regenerated from an InChI with appropriate software. InChI is not a registry system. It is not a replacement for any existing internal structure representations; it is in addition to what one uses internally. Its main value to most organizations is in linking information. Like a barcode, it is not designed to be read by humans. The InChIKey has been designed so that Internet search engines can search and find the links to a given InChI. To make the InChIKey the InChI string is subjected to a compression algorithm to create a fixed-length string of upper-case characters. Steve showed examples of Google searches for an InChI and an InChIKey, and of Henry Rzepa's QR smartphone app for InChI.

The InChI Trust (http://www.inchi-trust.org/), a UK charity, was formed to develop and improve on the current InChI standard, further enabling the interlinking of chemistry and chemical structures on the Web. InChI is a truly international project with programming in Moscow, computers in Germany, incorporation in the UK, and a project director in the United States. Collaborators from over a dozen countries, from academia, pharma, publishing, and the chemical information industry, have all offered senior scientific staff to develop the InChI standard. InChI is a success because

organizations need a structure representation for their content so that it can be linked to and combined with other content on the Internet. InChI provides an excellent return on investment. It is a public domain algorithm that anyone, anywhere, can freely use.

ChemSpider (http://www.chemspider.com/) would not have been possible without InChI. Valery Tkachenko of the RSC put it into perspective. We live in the world of Web 2.0; a connected world of social networks, mobile communications and Internet TV; a big data world with semantic content and new interfaces. Data is king and NoSQL is the new data model approach. Data flows in and can be structured, searched, linked and navigated. Data and code are distributed and self-sustained in the cloud. Federated systems take precedence over standalone solutions. Sophisticated human computer interfaces and pervasive machine-to-machine interfaces prevail. Yahoo, Google, Facebook and YouTube are huge islands on the Internet map; why are chemical domains so insignificant?

ChemSpider is a database and search engine for small organic molecules, their properties, names and synonyms, and spectra. It is an aggregator of information from online resources as well as a host of data extracted from RSC scientific articles. Over the past five years more than 26 million chemicals, together with a diverse array of associated data, have been deposited. The online database is open to community deposition, annotation, and curation and, as a result, has expanded into a rich resource to contribute to a Semantic Web of chemistry. ChemSpider provides access to its data *via* Web Services and as RDF. There is an extensive infrastructure: a computer farm and components. Standard interfaces such as Simple Object Access Protocol (SOAP), Representational State Transfer (REST), JSON, RDF and SPARQL are used. Automated validation and standardization procedures are now being developed. ChemSpider provides the chemistry services supporting the Open PHACTS project (http://www.openphacts.org/),[14] a semantic project serving the life sciences community to facilitate the linking of chemical and biology data and enable drug discovery.

Chemistry is also available in Wikipedia. Martin Walker of the State University of New York at Potsdam described DBpedia, a project to extract data from Wikipedia, such as the substance information in a ChemBox or DrugBox. Traditionally these boxes were used simply for cutting and pasting, but the Wikipedia team has made a machine-friendly version using formats such as SMILES and InChI. Now ChemBoxes are more like a database, and it is easier to pull data out. The InChIs for complex molecules can be very long, and this was a hindrance to their use in Wikipedia until "show/hide" became available. "Table creep" could be a problem in data pages; the answer is to put data on a supplementary data page.

Data validation lets the user know if the data are correct. Curation is the ongoing process of fixing errors. In 2008 a validation exercise was initiated and, in collaboration with CAS, 3,500 substances have been validated as having the same name, structure, and CAS Registry Number (CAS RN). Validated entries carry a green check mark. Every old version of an article, with a RevID, is preserved for posterity and can potentially serve as a permanent record of a validated version. To protect validated fields, a bot patrols the pages and logs dubious CAS RN edits, in a system developed by Dick Beetstra of Eindhoven University. Structures present more of a problem since they are loaded from an external file on Wikimedia Commons which can be "invisibly" changed, but, since fall 2010, a modified bot has been looking out for such changes.

Another example of data-rich chemistry in a wiki is RSC's LearnChemistry wiki which aims to enrich RSC educational content with data from ChemSpider, and then make it open for educators to contribute their own content. ChemSpider provides data on structures, physical properties, spectra, etc. Martin and his colleagues wanted to make the data presentation more suitable for students, including high school students, and cut out all the content that beginner students would not use. LearnChemistry includes laboratory experiments, tutorials and guides, substance pages, quizzes, and project and collaboration pages. Users can share their own educational materials such as homework problems and laboratory procedures.

Conclusion

Bobbie Glen of the University of Cambridge summed up Peter and Henry's contributions to the Semantic Web of chemistry. Traditionally, science involved two main pillars: theory to generate hypotheses and experimentation to test them. In modern science, theories are complex, data volumes are large, and experimental teams are often international collaborations. We can add a third pillar, e-Science, to manage these new realities of science.[28] For e-science we need open data and standards; glue ware for computation and analysis, interfaces that encompass the "system;" access control to data and intellectual property, collaboration methods that allow analysis, dialogue and data exchange; data and data analysis tools for "big data"; scalable, physically realistic algorithms; infrastructure (networks, high performance computing, and data storage), and metadata and semantics to put it all in context. Biology, chemistry and patents have "big data," e.g., 429,512,389,024 nucleotide bases, 60,475,000 chemical substances and 150,000,000 pages of European patents. The connections present big opportunities for innovation, but also great challenges. Navigation through all this information is not easy.

Most real chemicals do not exist as connection tables; the sticky, brown stuff in the reaction vessel is not a SMILES. The next generation of chemical information tools should capture the history of the materials and the manufacturing process which went to make up the substance, as well as measured and predicted properties, and that is just a beginning. Peter and Henry's work with CML,[6,29] opens up opportunities to do just this, once we capture the data.[30] The first step is the automated lab: data capture using the human senses integrated into robotic data capture. *Everything* should be stored (minor omissions often mean an unrepeatable experiment) and a knowledge framework is needed (semantics) that gives meaning to the data: any result has to be put in the context of the experiment.

Bobby gave a few examples. The solubility of caffeine varies by orders of magnitude in the literature. Single values tell nothing useful: we need the metadata to tell us what the material was and how the solubility was measured. How flufenamic acid is made determines the aqueous solubility because there are two polymorphs, made under different conditions, with different solubilities. 6,6'-Dinitro-2,2'-diphenic acid exhibits atropisomerism (the conformation is twisted to reveal an enantiomeric structure), so how the material was synthesized needs to be included in the data. Different atropisomers of a compound have different biological activities. Some bicyclo[3.2.0]heptan-6-one derivatives have two forms in a single crystal and in solution because of transannular interactions: how should this "dynamic" molecular structure be represented? Chemistry is not best served by 20th century descriptions of molecules and materials. CML allows the addition of vital metadata within a semantic framework, which adds context, reproducibility and knowledge.

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Wendy Warr, Symposium Reporter

Global Opportunities in Chemical Information

Rachelle Bienstock kicked off the session by asking whether emerging markets will really save pharma. She cited statistics that emerging markets, currently $154B or 18% of worldwide revenue, are forecast to rise to $487B or a 37% share by 2020. *JACS* spotlights are now being translated into five languages, with Chinese at the top of the list.

Roger Sayle (NextMove Software) described his work building automatic translation of Chinese chemical names. Non-English chemistry is showing up frequently. Even some large pharmaceutical companies with ELNs that are supposed to be written in English are finding non-English pages in their archives. A Google search for "benzoic acid" hits only a few more pages than a search for the equivalent Chinese name. Patent applications now often appear first in non-English countries because of business or processing reasons.

Automated translation of Chinese is possible because IUPAC's strong morphological structuring is preserved across language. Software can identify subparts and translate them, then put it back together based on the IUPAC structuring.

In text mining the challenge is to find the beginning and the end of a chemical name. In the latest version of LeadMine using NextMove's software, 42% of simple patents written in Chinese were recognized and converted (vs. a benchmark of 86% for recognizing the original English). Image documents, however, are still not scanned successfully in most cases.

Tom Blackadar (Binocular Vision) shared his experience of living in Asia for the past 5 years. Tom began studying Chinese intensively about 2 years ago when he moved to Shanghai. He related his personal and interesting tale of the challenges and rewards of starting a small consulting company (operating as a U.S. company) to bring expert informatics practices to the developing Chinese market and link pharmaceutical companies with partners. Tom is focusing largely on western companies and Contract Research Organizations in China. He discussed many of the legal hurdles he needed to overcome. People were very impressed by his slide collection of necessary red stamped legal documents! However, Tom emphasized the need for data management and the gaps in IP and therefore the valuable niche that his company can fill in the future in China.

Brian Hitson (U.S. Department of Energy, Office of Scientific and Technical Information) talked about the efforts of worldwidescience.org to build a multilingual search system for chemistry and other sciences. OSTI provides public access to the Department of Energy's unclassified information, as well as restricted access to classified and sensitive information for appropriate people. OSTI has been a pioneer in creating "aggregators" for federated search of multiple sites. Science.gov launched in early 2000s integrates information from twelve federal agencies. Worldwidescience.org takes this to the international level, searching databases in many different countries. Started in 2007 as partnership between U.S. DOE and the British Library, it moved in 2008 to multilateral governance. The system's goal is to do true searches of the "deep web" index of other search engines that can really find most of the science.

Recent developments include multilingual translations that are the first one-to-many and many-to-one multilingual translations. One search query fires off ten different searches based on Microsoft

Translator machine translations. “Science Cinema” uses Microsoft Research Audio Visual Indexing System (MAVIS) to recognize and index audio content. Once a hit is found, the user can go directly into the place in the video where the interesting part occurred. The next step is to attack "big data." They will search the metadata and then connect the user to the landing page to explore the data in its own format.

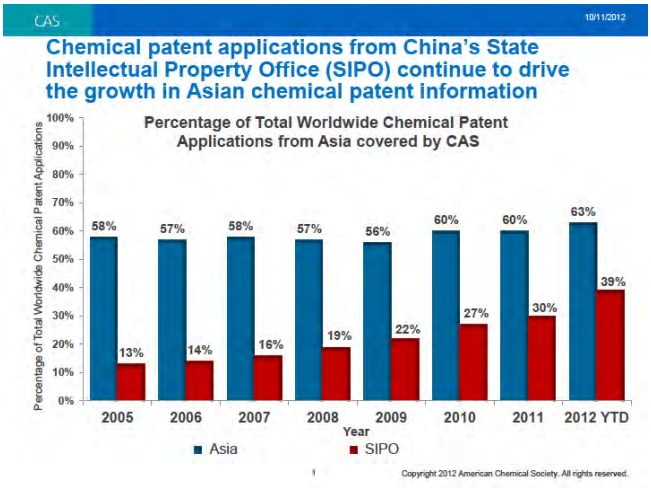
Jignesh Bhate (Molecular Connections) talked about business opportunities and challenges in India. Molecular Connections is India’s largest informatics company with over 900 employees located in Bangalore and Chennai. It focuses on indexing, abstracting, and text mining.

India is a big consumer of content, with 17% annual growth rate. The country has a huge business of service providers and multinational company sites. Indian private industry R&D spending is still only 25%, but growing rapidly. Indian research output is significant and growing, whereas US output is shrinking. Medicine and pharma are contributing over 25% of the total research output. India dominates offshoring of content production, with over 84% of the world’s total. This business generates $800M per year and is growing at 20%. The predictions are that value-add will be added to cost, with quality and TOT (terms of trade) as key metrics.

Jignesh pointed out several business challenges: India has many differences in cultures and languages; bureaucracy and corruption are significant obstacles; Indians are very sensitive to hierarchy; they focus on relationships and face-to-face contact, so phone calls get more used than email. Despite these challenges, the macro story is so compelling that you cannot go wrong. It sometimes feels like a “drunken man's stupor,” but you can get to the goal.

Andy McFarlane (Thomson Reuters) cited that in 2011 China became #1 country in patents, with over half a million, 23% year-on-year growth. Commercial providers historically added value on top of information coming directly from the patent office. Now the information often comes through a translator or intermediator. There are challenges in scrubbing data, such as rationalizing different translations and spellings of names. India has four patent offices that issue overlapping patent numbers. Derwent World Patents Index has comprehensive English-language coverage, including Asia, with normalized company names. Thomson Reuters tries to focus on consistency of terms. Technology focus shows that India is particularly oriented towards chemistry patents.

Tom Blackadar, Jignesh Bhate and Rachelle Bienstock, Symposium Organizers



In 2009, CAS, the world’s authority for chemical information, reported that China was, for the first time, leading all nations in publication of chemical patent applications (http://www.cas.org/news/media-releases/china-leads-patents). Three years later, chemical patent information from Asia continues to be a significant source of disclosed chemistry, with patent applications from China’s State Intellectual Property Office (SIPO) still increasing. This is important to the chemical information and research communities, as CAS is reporting that in 2012, more than 70% of new substances in the literature are from patents.

Legal, Patent and Digital Rights Management in Publishing

The symposium took place on Thursday afternoon and featured five presentations. David Gange (Altimedia) gave a talk entitled "How to find references that inherently anticipate pharmaceutical patents." References that "inherently anticipate" a patent can invalidate a patent on the basis of novelty, so they are of a great interest to pharmaceutical companies, both offensively and defensively. The speaker gave examples of how broad compound claims can be affected by questions of metabolites, crystal polymorphs, hydrates, optical isomers, metabolites and other intermediates in real world patent law cases.

In her talk "Digital rights drain? Implications for library services," Leah McEwen (Cornell University) enumerated some of the many digital rights issues that impinge on libraries including problems of identifying the owners of copyright and authentication of users. One of the cases she highlighted was the problems with theses, where at many institutions thesis authors traditionally signed over reproduction rights to UMI (now ProQuest). But electronic distribution is much more "public" than microform distribution, with an impact on republication as journal articles or books. The rise of entrepreneurship among faculty and students has also complicated intellectual property questions.

Donna Wrublewski (University of Florida) in her talk "Digital rights management and e-books: Perspectives from a research library" presented on other key areas where digital rights management affects library services, including conservation and preservation of materials (can you legally copy a digital object for preservation and can you copy it into a new format?), interlibrary loan and consortial lending, and discovery services (can a library create a full-text index to a copyrighted work?). With formats evolving (and in some cases, becoming obsolete), libraries are forced into a "tech support" role. In many cases, the applicable law is too new for its interpretations as they affect libraries to be clear.

Judith Currano (University of Pennsylvania) pointed to the "problems of preserving digital content." Judith summarized the legal status of digital content preservation as "This is a gray area." Digital rights management is an addition to intellectual property law that seeks to prevent piracy and illegal copying…but it doesn't work. The combinations of hardware and software that have been tried inhibit legitimate users without stopping piracy. In the meantime, libraries are faced with changing formats, with old formats and the hardware that reads them becoming obsolete, and with license agreements that are ambiguous or over-restrictive as to what can be done.

David Parker (Momentum Press) concluded with "Finding an alternative to restrictive digital rights management: The Momentum Press approach." David reviewed some of the business models which have evolved in the transition from print publishing to electronic publishing, including various forms of open access publishing. The Momentum Press model makes e-books available for a one-time fee, with perpetual access. No third party aggregators are involved and there is no subscription or maintenance fee.

Charles Huber, Symposium Co-Organizer

Before and After Lab: Instructing Students in 'Non-Chemical' Research Skills A Symposium at the 2012 Biennial Conference on Chemical Education

Organized by: Judith Currano (University of Pennsylvania), Andrea Twiss-Brooks (University of Chicago), Grace Baysinger (Stanford University)

When students think about chemistry, one of the first things that comes to mind is the laboratory, but while the experiments done in the lab are the "meat" of the chemical research process, they are sandwiched between literature searching, reading, and acquisition of funding on one side, and publication and presentation on the other. These highly nuanced topics are frequently overlooked by educators and students alike, although they are crucial for success in both academic and industrial research. The "Before and After Lab" session at the Biennial Conference on Chemical Education, held on the campus of The Pennsylvania State University, July 29-August 2, 2012, brought together chemistry instructors to share their best practices in teaching students what to do before they enter and after they leave the laboratory. Presenters discussed how to teach students to search and read the scientific literature, to consider ethical issues inherent in scientific research, to understand the peer review process, to effectively manage literature references, and to present their work. The program with abstracts was posted: AM session, PM session. The following talks were presented during the full day symposium [links to slides are included below where available]:

- Implementation of an "Introduction to Experimental Chemistry" course. Kimberly Woznack
- An organic chemistry laboratory exercise in information literacy using SciFinder. Bonnie Swoger.
- Lost in SciFinder: Development and impact of a research-like experience in a second-semester organic chemistry lab for chemistry majors. Michael Slade
- Preparing the chemistry senior for the chemists' world – library research, method development, sample preparation, instrumentation, data analysis, and presentation. Dharshi Bopegedera
- Presentation skills for undergraduates. Adrienne W. Kozlowski
- Scandals and blunders in science: Wikipedia project. Jennifer Muzyka
- Introductory seminars to prepare students to participate in STEM research. Joe March
- Using student peer review for teaching scientific writing to first-year chemistry graduate students in a one-credit required course. Donna Hudson
- Ethical communication: Teaching students how to "behave" in the publication process. Judith Currano
- Information literacy for undergraduate chemistry students. Grace Baysinger

Andrea Twiss-Brooks, Symposium Co-Organizer

News from Multidisciplinary Program Planning Group (MPPG)

The Executive and Full Committee of MPPG, a subcommittee of the ACS Committee on Divisional Activities, met in Philadelphia during the recent National ACS Meeting to discuss the thematic programming activities of present and future ACS Meetings. For Philadelphia, the thematic organizer Xinqiao Jia, University of Delaware, did an extraordinary job in putting together an excellent program and the ACS staff again created and widely published an eye-catching logo symbolizing the meeting's theme "Materials for Health and Medicine." Divisional symposia related to the theme were advertised on flyers and in the meeting program, as were the "Kavli Foundation Innovation in Chemistry Lecture" and the Plenary Session. The Kavli lecture on "*Chemistry in medicine: From the discovery of angiogenesis to the development of controlled drug delivery systems and the foundation of tissue engineering*" was presented to a full house by Robert Langer of MIT. The plenary session, again to a standing room only audience, consisted of four presentations by eminent scientists addressing the theme of the Meeting: Jacqueline K. Barton, California Institute of Technology; Chad A. Mirkin, Northwestern University; Buddy D. Ratner, University of Washington; and John T. Santini, Jr., On Demand Therapeutics, Inc.

The future of thematic programming at ACS meetings looks bright. More and more technical divisions organize symposia related to the theme of a meeting, often co-sponsored by other divisions indicating the interdisciplinary nature of chemistry. We definitely have seen a strong upwards trend in the last few meetings. As per charter, themes for the next three years have been approved and organizers are in place for 2013 and 2014. The CINF Program Committee should look closely at the themes and available synopses to work together with the thematic program chairs to organize companion symposia. Any symposium within a given theme will provide valuable publicity to the division.

Here are the themes for future meetings:

Meeting	Dates	Theme	Program Chair
Spring 2013 New Orleans	April 7-11	Chemistry of Energy and Food	James Seiber, UC Davis
Fall 2013 Indianapolis	September 8-12	Chemistry in Motion	Robert Weiss, University of Akron
Spring 2014 Dallas	March 16-20	Chemistry of Energy/ Advanced Materials for New Opportunities	Michelle Buchanan, Oak Ridge National Lab Nitash Balsara, UC Berkeley
Fall 2014 San Francisco	August 10-14	Chemistry and Stewardship of the World	Robin Rogers, University of Alabama
Spring 2015 Denver	March 22-26	Chemical Resources: Extraction, Refining and Conservation	TBD
Fall 2015 Boston	August 16-20	History of Innovations: From Discovery to Application	TBD
Spring 2016 San Diego	March 13-17	Computers in Chemistry (tentative)	
Fall 2016 Philadelphia	August 21-25	Chemistry and Education (tentative)	

Important News: Recently, the Kavli Foundation signed an agreement with ACS to sponsor a second lecture series "The Kavli Foundation Emerging Leader in Chemistry Lecture" at future ACS National Meetings for the period 2013–2015. Divisions will be asked to nominate up to two candidates. The Kavli Emerging Leader Lecturer must be a distinguished younger scientist who is highly regarded by his or her peers for significant contributions to an area of chemistry or related multidisciplinary area. The nominee(s) have to be 40 years of age or less and fewer than 10 years after completion of his or her PhD at the time of nomination. The nominees do not have to be members of the nominating division. Division's secretaries will send out the "Call for Nomination" and submit the nominations to MPPG, who will manage the selection process. A template for nominations will be sent out by the Chair of MPPG.

Feel free to contact me at ggrethe@att.net if you have any questions regarding MPPG.

Guenter Grethe, Member, Executive Committee Multidisciplinary Program Planning Group

Join Us Again in New Orleans

Image credit: New Orleans Spring 2013 ACS National Meeting

Registration/Housing for the Spring 2013 ACS National Meeting

Opens December 2012

COMMITTEE REPORTS

CINF Communications and Publications Committee

CINF website and the new Drupal implementation

Danielle Dennie reported that content is being transferred over from the CINF to the Drupal websites. It's going surely but slowly because of the "meetings" content, which is long and has many inconsistencies. It will be done by mid-October (at the earliest). If not, we may need to consider hiring someone else to do this painstaking work. Aside from the "meetings," most of the content has been transferred.

The "Contact" module is also being installed, both on the CINF and CIB sites. It aims at helping with spam as the emails will be hidden and a contact form will open up for email to be sent to a person. Within our hosting service, the spam filtering option and settings were also changed to "ultra aggressive" so that spam emails are sent automatically to the "deleted items" folder rather than to the inbox.

Chemical Information Bulletin

Judith Currano reported that the Spring 2012 issue was challenging because many of our long-standing writers, Svetla Baykoucheva (interviews), Bob Buntrock (book reviews), and Song Yu (literature digests), were not able to contribute at this time. As a result, the issue had a single feature about the 2012 SLA Conference by Sue Cardinal.

For future issues it would be helpful to recruit some individuals who wish to serve as regular columnists. Perhaps we could get a second literature reviewer. Martin Braendle indicated his interest in writing occasional database or product reviews. He was not able to contribute to this issue. Judith will ask Martin again for the next Spring issue.

Bill Town started a nice trend of symposium organizers writing descriptive pieces about their upcoming symposia. Judith would like to highlight one or two symposia each fall/spring issue, perhaps looking at themes that would appeal to a broader base of our membership or symposia of "lower profile" compared to a high profile Herman Skolnik Award Symposium.

Judith would like to introduce a "Member News" section with announcements about people who received awards, or have changed jobs or responsibilities. She would also like to publish the names of CINF new members and brief member profiles (e.g. one new member and one member of longer standing, specifically members who do not regularly attend ACS meetings, so that we can get to know more division members). Getting information about members has not been easy. This would involve close work with the Membership Committee.

The Spring 2012 issue was organized as follows: Chair's Message, Editorial, Features, Governance information, Sponsor News, Symposium Overview, Technical Program Schedule (CINF first, then COMP, then SCHB), Abstracts, Officers and Functionaries.

Schedules for all symposia in which CINF was a primary or a secondary sponsor were obtained. The program was divided up by primary sponsor, putting the CINF ones first and then everything else in alphabetical order. This year, it was also not possible to get the session letters (e.g., "Sunday Morning: CINF Session A"). All Technical Program listings were grouped together. Thus, anyone who wanted to print the program part, could simply print one block of pages. It was decided to include only the CINF-primary symposia abstracts in the interests of space (the issue was almost 90 pages!). Points of discussion for the Committee are: whether or not we want to include the co-sponsored symposia in future issues, whether the current organization of the technical program makes sense, and whether or not we want to include the abstracts for the co-sponsored symposia.

Concerning hyperlinks from the table of contents in the PDF version, the only way with Acrobat 7.0 Professional is to add the links manually so far. The following points need to be discussed: is there a way to automate this process that we did not find? If there is no way to automate the process, since we estimate that it is going to take a fair amount of time to do it manually, what is the value versus the time commitment? Right now, we are essentially building two separate publications. In some cases we need to actually change the text of the content to make sense for the format. The organization of both may be slightly different, too. We need to set our priorities for the two documents as a Committee, leading to a final decision once and for all.

Committee membership

David Martinsen will become Committee Chair for 2013-2015.
Graham Douglas will become Committee Assistant Chair for 2013.
Svetlana Korolev has renewed her committee membership and will continue as Editor of the Summer and Winter issues of CIB.
Judith Currano has been chosen as the 2013 CINF Division Chair-Elect and will not be able to continue as CIB Editor after the Spring 2013 issue, which she hopes to have time to co-edit with a new CIB Editor.

Other committee members: Svetla Baykoucheva, Bonnie Lawlor, Carmen Nitsche, Sara Rouhi, Song Yu.
Ex Officio: Gregory Banik (Membership Chair), Susanne Redalje (Bylaws & Procedures Manual), Fundraising Chair 2013 (TBD).

ACS Network

Graham Douglas reported on the continuing problems with the ACS Network.

Procedures manual

Work on this is still outstanding.

Bill Town, Chair, CINF Communications and Publications Committee

CINF Education Committee

The Education Committee met on Saturday, August 18, from 1:00 PM - 3:00 PM, in Philadelphia Convention Center, Room 118A.

Attended: Chuck Huber (Committee Chair), Grace Baysinger (upcoming Committee Chair 2013-14); Adrienne Koslowski (consultant). Donna Wrublewski (guest).

Review of the Fall 2012 ACS National Meeting in Philadelphia: The Education Committee was directly involved with the Thursday afternoon symposium "Legal, Patent and Digital Rights Management in Publishing" (Judith Currano, presiding; Judith Currano and Chuck Huber, organizers). The full day symposia "Hunting for Hidden Treasures: Chemical Information in Patents and Other Documents" (Sunday) and "Future of the History of Chemical Information" (Monday) were also recommended for their educational relevance.

Report of the Biennial Conference on Chemical Education (BCCE), Penn State, University Park, PA, July 29–August 2, 2012: About 1500 chemical educators attended this year's meeting. An all-day symposium "Before and After the Lab" was organized by several Education Committee members and former members: Grace Baysinger, Judith Currano, Andrea Twiss-Brooks and Adrienne Koslowski. It featured nine speakers, a mixture of librarians and chemistry faculty, and attracted thirty attendees at its peak. Presentations included: "Wikipedia in a Writing Assignment," "Collaboration between Faculty and Librarians," "Presentation Skills for Undergraduates," "Ethical Issues" and "Chemical Information Literacy." The latter, by Grace Baysinger, delved into the recommendations for chemical information literacy for undergraduates endorsed by CINF. (More information about BCCE 2012 is provided by Andrea Twiss-Brooks in this Bulletin).

Looking ahead to the Spring 2013 New Orleans ACS Meeting, April 7-11: Theme: *Chemistry of Energy & Food.* Symposia of interest include: "What Chemists Need to Know about IP/Author Rights," "Food Safety Information" (organizer: Andrea Twiss-Brooks), "Library Spaces" (organizer: Andrea Twiss-Brooks), and "Public Chemistry Databases" (organizer: Antony Williams). A symposium "Print Resources in the Electronic Era" (organizer: Grace Baysinger), originally slated for New Orleans, has been moved forward to the Fall 2013 Indianapolis Meeting.

Fall 2013 Indianapolis ACS Meeting, September 8-12: Theme: *Chemistry in Motion.* Symposia of interest include: "Print Resources in the Electronic Era" (see above), "Education for Cheminformatics" (suggested by the proximity of the Indiana University's Cheminformatics Program, possible organizer: Jeremy Garritano), "Digital Archiving" (possible organizer: Andrea Twiss-Brooks), and a student-only session (whether poster or oral to be determined). A symposium "Chemical Information for Small Teaching Colleges," originally slated for Indianapolis, has been deferred to the Fall 2014 San Francisco Meeting.

Spring 2014 Dallas ACS Meeting, March 16-20: The Committee deferred further program planning until the theme is known. (Theme: *Chemistry of Energy/Advanced Materials for New Opportunities* was made known to the Committee after 08/18/12).

BCCE 2014, Grand Valley State University, Annandale, MI, August 3-7, 2014: The theme for this meeting is "Sustainability: Greener on the Grand." The conference website is: http://148.61.114.203/bcce/dates.html. The call for workshops begins June 3, 2013 and for symposia, August 1, 2013. The deadline for abstract submissions for both is December 2, 2013. The committee will try to recruit a local liaison in the Michigan area for CINF. A complicating factor is how close BCCE 2014 is on the calendar to the San Francisco ACS National Meeting (the latter begins only a few days after the former ends).

Fall 2014 San Francisco ACS Meeting, August 10-14: The symposium "Chemical Information for Small Teaching Colleges" has been deferred to this meeting. As San Francisco Meetings are usually highly attended, the Committee wants to prepare many programs once the theme is available. (Theme: *Chemistry and Stewardship of the World* was made known to the Committee after 08/18/12).

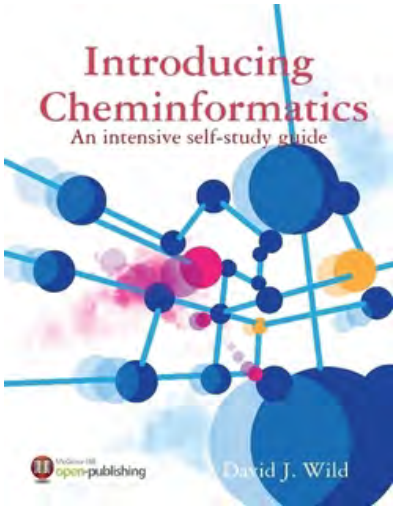
Information Competencies for Chemistry Undergraduates: Grace Baysinger will add a link to the current version of the document from the CINF website. The committee will inform the ACS Committee on Professional Training (CPT) to get them to link to the document.
The Wikibooks link for the document is:
http://en.wikibooks.org/wiki/Information_Competencies_for_Chemistry_Undergraduates

Information Competencies for Chemistry Graduates: Judith Currano has prepared an outline. Grace Baysinger will post it to the Education Committee group on the ACS Network.

XCITR: All agreed that we need to encourage more of our colleagues to deposit teaching materials (or links to teaching materials) in XCITR. How best this might be accomplished was not resolved.

Committee Membership: Selection of the Assistant Chair of the Education Committee was deferred to the Spring 2013 New Orleans Meeting.

Chuck Huber, Chair, CINF Education Committee



ebook (PDF) 59 pages $29.00

Report from the ACS Council Meeting

The Council of the American Chemical Society met in Philadelphia, PA on Wednesday, August 22, 2012 from 8:00am until approximately 12:15pm in the Grand Ballroom A - F of the Philadelphia Marriott Downtown Hotel. It opened with a resolution and moment of silence for deceased Councilors, a vote to accept the minutes of the Council meeting held on March 28, 2012, an announcement that Dr. Peter Stang will be awarded the Priestley Medal, and an announcement that after 36 years Rudy Baum will be leaving *Chemical & Engineering News,* where he currently serves as Editor-in-Chief. The highlights of the meeting are as follows:

Nominations and Elections

Council Policy Committee: Council voted to fill four slots on the Council Policy Committee. There were eight nominees as follows: Frank D. Blum, Mary K. Carroll, Joseph A. Heppert, Martha G. Hollomon, Lee H. Latimer, Willem R. Leenstra, Carolyn Ribes, and Ellen B. Stechel. By electronic ballot, the Council elected Frank D. Blum, Mary K. Carroll, Lee H. Latimer, and Carolyn Ribes for the 2013-2015 term.

Committee on Committees: Council voted to fill seven slots on the Committee on Committees. There were fourteen nominees as follows: Spiro D. Alexandratos, G. Bryan Balazs, Christopher J. Bannochie, Arindam Bose, Dawn A. Brooks, Michelle V. Buchanan, Alan B. Cooper, Judith Currano, Warren D. Hull, Jr. David J. Lohse, Christopher J. Masi, Ingrid Montes, Jason R. Ritchie, and Ralph A. Wheeler. By electronic ballot, the Council elected G. Bryan Balazs, Dawn A. Brooks, Michelle V. Buchanan, Alan B. Cooper, and Ingrid Montes for the 2013-2015 term; and Spiro D. Alexandratos and Judith Currano for the remainder of a two-year (2013-2014) term.

Committee on Nominations and Elections: Council voted to fill five slots on the Committee on Nominations and Elections. There were ten nominees as follows: Cherlynvaughn Bradley, Dwight W. Chasar, Catherine E. Costello, Milagros Delgado, Kevin J. Edgar, Carol B. Libby, Les W. McQuire, Donivan R. Porterfield, Robert A. Pribush, and Steven W. Yates. By electronic ballot, the Council elected Cherlynlavaughn Bradley, Milagros Delgado, Carol B. Libby, Les W. McQuire and Donivan R. Porterfield for the 2013-2015 term.

The committee on Nominations and Elections announced the names of candidates for national office that will appear on ballots that will be mailed in October. These are as follows: *Candidates for the 2013 President-Elect:* Dr. Thomas J. Barton, Distinguished Professor, Iowa State University, Ames, IA and Dr. Luis A. Echegoyen, Robert A. Welch Professor, University of Texas at El Paso, El Paso, TX; *Candidates for Directors-at-Large 2013-15:* Ms. Carol A. Duane, President, D&D Consultants of Mentor, Mentor, OH, Ms. Valerie J. Kuck, Retired, Lucent Technologies (Bell Labs), Murray Hill, NJ, Ms. Helen (Bonnie) A. Lawlor, Executive Director, National Federation of Advanced Information Services (NFAIS), Philadelphia, PA, and Dr. Ingrid Montes, Professor, University of Puerto Rico, Rio Piedras Campus, San Juan, PR; *Candidates for District I Director 2013-15:* Dr. Thomas R. Gilbert, Associate Professor, Northeastern University, Boston, MA and Dr. Neil D. Jespersen, Professor of Chemistry, St. John's University, Queens, NY; and Candidates for District V Director 2013-15: Dr. John E. Adams, Curators' Teaching Professor of Chemistry, University of

Missouri, Columbia, MO and Dr. Peter K. Dorhout, Dean, College of Arts & Sciences, Kansas State University, Manhattan, KS.

Society Estimated Financial Results for 2012 Looking Positive

The Committee on Budget and Finance presented estimated year-end results for 2012. They estimate that total revenues will be $491.6 million ($7.1 over budget) and expenses will be $474.2 million ($5.5 over budget), giving a net from operations of $17.4M. If the estimate is correct, the year-end net will be $1.6M favorable to the budget.

Senior Chemists Committee to be Created upon Board Approval

Council approved a recommendation from the Committee on Committees to create a Senior Chemists Committee as a Joint Board-Council Committee. It will be established upon approval of the ACS Board of Directors. The mission of this committee will be to enrich the educational, technical, and cultural lives of the ACS Membership by ministering to and employing the talents of senior ACS members by: sharing with ACS members of all ages a rich variety of personal experiences and expertise gained over many years of professional service; fostering interest and participation in the science of chemistry through community outreach, especially in grades K-12; acting as science advisors/ambassadors for the purpose of cultural exchange at home and abroad; providing senior ACS members with challenging, diverse, and enjoyable professional experiences that enable them to contribute to the cultural experiences of their communities; and recommending policies that address issues of interest to senior chemists. The committee is aimed primarily at members over 60 years of age.

Other Committees

Council voted to accept the recommendation put forth by the Committee on Committees (ConC) to authorize the continuation of the Committee on Chemists with Disabilities and the Committee on Professional Training.

ConC honored all committee chairs and members who will reach their statutory limit of service this year and also recognized Councilors who have reached significant anniversaries of years of Council service.

Proposal to Transfer Two Local Sections Approved

The Committee on Nominations and Elections (N&E) recommended that the Hampton Roads and Western Maryland local sections be shifted from District II to District III. The background on this recommendation is the following: N&E is responsible for annually reviewing the distribution of member population within the six electoral districts to assure that the districts have equitable representation. According to Bylaw V, Section 4a, the member populations of each district must be within ten percent of the result of dividing by six the number of members whose addresses lie within these districts. During its meeting in March 2012, N&E learned from year-end 2011 membership figures that the total membership in one electoral district was below the permissible minimum (the permissible range is 21,038–25,714). The District III population was 140 members below the permissible minimum and N&E must recommend to Council a redefinition of District boundaries to

bring District III member population back into compliance with the Bylaw provision regarding population. The two local sections agreed to the shift.

The Council voted 58% to 42% (via clicker vote) to approve the shift. However, there was quite a bit of discussion on this issue with the net result that N&E has been asked to conduct a comprehensive review of the optimal alignment of local sections within districts.

Two Petitions Voted Down

Council voted on two petitions for changes to the ACS Bylaws. The first was a *Petition on Candidate Comment in C&EN.* The wording to BYLAW V, Section 13 was recommended to have the following added with the objective of avoiding an unfair campaign advantage to incumbents who may choose to make official statements on their task force or committee activities prior to elections.

"Other than official position statements provided for in election procedures, the official organ of the SOCIETY shall not publish without charge any written material under the name of a candidate for any position on the Board of Directors, including President-Elect, at any time after May 1 in the year of the election."

Council voted against the petition.

The second petition was a *Petition on International Chemical Sciences Chapters Funds*. This petition sought to clarify that the Board of Directors may grant funds to international chapters for specific purposes. The proposed wording of BYLAW IX, section 4 was as follows:

"An International Chemical Sciences Chapter shall receive no allotment of funds from the SOCIETY and shall not be entitled to elected representation on the Council. However, the Board of Directors may grant funds to a Chapter for a specific SOCIETY activity in which participation of the Chapter is deemed necessary for carrying out that SOCIETY activity effectively."

The Council voted not to approve this petition as well (64% to 36% via clicker vote).

Bylaw Changes for Consideration Only

Petition to Amend National Election Procedures

The increasing demands of recent campaigns for electing the President-Elect of the Society have made it ever more difficult to recruit leaders in the chemical community to accept nomination. The problems are increased substantially by the process used to choose candidates from among nominees, as otherwise potentially excellent candidates are often voted off the ballot because they are not well known to Councilors. Serving many years in ACS governance is not, and should not be, a pre-requisite for serving as President-Elect.

The proposed change will charge N&E to find two candidates for President-Elect. Others, as now, may be nominated by members by petition, and procedures for preferential balloting remain unchanged. All candidates could then be invited to a public forum, such as a Town Hall meeting, at

the Fall National Meeting, and would appear on the ballot. This process would shorten the campaign period, allow all candidates to be seen by Council and other members, and ease the burden on N&E.

The financial impact is still being assessed and the petition will appear on the Council agenda in the spring of 2013.

Distribution Formula for Local Section Allotments Delayed

The Committee on Local Section Activities (LSAC) had reported that they believe there is a deficiency in the current formula used to distribute the ACS Local Section annual allotments (LSAC reviews the calculations every three years or sooner, if deemed necessary). Their concern is that the total allotment for distribution will be greater than the funds available to distribute and they had planned to recommend a formula at this Council meeting to correct this deficiency for the 2013 allotments with a recommendation for a long-term solution coming in 2013. However, the Council Policy Committee (CPC) voted to remove this item from the agenda for this meeting and put it on the 2013 spring agenda.

Chemists' Employment Issues

The Committee on Economic and Professional Affairs (CEPA) reported that the unemployment rate for chemists has declined slightly – from 4.6% to 4.2%, but that 8.2% of those unemployed report being in that position for four months or more. There were 999 job seekers at the job fair held at the conference. They were competing for 148 positions being offered by 45 employers. A virtual job fair held earlier attracted 1,499 job seekers, 13 employers, and only 41 positions. It was also reported that the salaries of PhD and MS chemists have declined in real dollars, but that the salaries of BS chemists have held the line.

Divisional Activities

The Committee on Divisional Activities reported that the Program and Abstract Creation System (PACS) will no longer be supported after December 31, 2012 and ACS will have to find a new vehicle for the submission of papers for the National Meetings.

Fall Meeting Attendance

As of August 22, 2012, the ACS Fall National Meeting had attracted 13,320 registrants. Totals in select categories are as follows: Regular attendees 7,817; Students 3,177; Guests 337; Exhibit Only 740 and Exhibitors 1,249. The history of attendance at ACS fall national meetings since 2004 is as follows:

2004:	Philadelphia, PA	14,025
2005:	Washington, DC	13,148
2006:	San Francisco, CA	15,714
2007:	Boston, MA	15,554
2008:	Philadelphia, PA	13,805
2009:	Washington, DC	14,129

2010: Boston, MA	14,151
2011: Denver, CO	10,076 (decline assumed to be due to timing - the week before Labor Day)
2012: Philadelphia, PA	13,251

Special Discussion Item

A special discussion item was put on the Council agenda for this meeting. ACS President Bassam Shakhashiri presented and moderated a discussion on "What major efforts should ACS pursue to help alleviate water and other global challenges?" Members of the ACS feel a responsibility as scientists and citizens to help address global challenges facing society in the 21st Century to help sustain Earth and its people. These challenges include increasing population growth, limited natural resources, malnutrition, disease, climate change, violence and war, and the denial of basic human rights, including the right to benefit from scientific and technological progress. This discussion focused primarily on the crisis of available water suitable for drinking, agriculture and industry. Following the presentation, more than 30 Councilors engaged in a discussion of this global challenge and others and offered numerous suggestions. Councilors are invited to continue discussion of this topic within the ACS Network Councilor Group (https://communities.acs.org/groups/councilor-group) at https://communities.acs.org/message/11677.

Resolution to Honor the Memory of Glenn T. Seaborg in the Centennial Year of His Birth

The Council passed a resolution to honor the 100th anniversary of the birth of Glenn T. Seaborg, Chemistry Nobel Laureate and past ACS President.

Update on ACS vs. Leadscope Litigation

The Chair of the Board gave an update on the ACS vs. Leadscope litigation. As of this meeting, there was still no opinion announced by the Ohio Supreme Count on ACS's appeal in this case, despite the fact that oral arguments were presented nearly a year ago. ACS has no information on when an opinion might be delivered.

Update on September 18, 2012: Statement on ACS vs. Leadscope decision from the Supreme Court of Ohio from Dr. William F. Carroll, Jr., Chair, ACS Board of Directors, on its behalf

The Supreme Court of Ohio today issued its decision in the case of ACS v Leadscope, Inc., originally filed in 2002. It is a complex decision and ACS needs to carefully review and assess the decision over the next several days.

Based upon initial review, the ACS Board of Directors is gratified that the Court, in a 5-2 vote, found that ACS did not defame the defendants and vacated the lower court's award of damages on that issue, which constituted the majority of the damages award in this case.

As to the defendants' claim of unfair competition, the Court acknowledged ACS' First Amendment right to seek judicial review of its original claims. Although the Court also agreed with ACS' legal arguments that the trial court had improperly instructed the jury on that claim, the Court, in a 4-3 vote, affirmed the lower courts' decisions.

Today's ruling will not impact ACS member dues; ACS products, programs or services; ACS staffing levels; or the ability of ACS to achieve its mission.

ACS also appreciates and acknowledges the strong support it received from the Ohio Attorney General, the Ohio Chamber of Commerce, the Ohio State Bar Association, the Ohio Manufacturers' Association and the Ohio Council of Retail Merchants – all of which submitted briefs supporting ACS to the Supreme Court of Ohio.

To review the Supreme Court of Ohio decision click here:
http://www.supremecourt.ohio.gov/rod/docs/pdf/0/2012/2012-ohio-4193.pdf

To read a summary of the case prepared by the Supreme Court of Ohio's Office of Public Information click here: http://www.courtnewsohio.gov/cases/2012/SCO/0918/101335.asp

Actions of the Board of Directors

(This portion of the report is taken verbatim from the Councilor talking points provided by the ACS, for which this author is most grateful.)

The Board's Committees and Working Groups

The Board of Directors received reports from its committees on Grants and Awards (G&A), Executive Compensation, and Budget and Finance (B&F); and from its working group on Society Program Portfolio Management.

On the recommendation of the Committee on Grants and Awards, the Board VOTED to approve Society nominations for the Perkin Medal and the National Science Board Public Service Award. The Perkin Medal is the highest honor in American industrial chemistry, and the National Science Board Public Service Award honors individuals and groups that have made substantial contributions increasing public understanding of science and engineering in the US.

The Board received a briefing and approved a recommendation from its Committee on Executive Compensation. The compensation of the Society's executive staff receives regular review from the Board.

On the recommendation of the Committee on Budget and Finance (B&F), the Board VOTED to approve an advance member registration fee of $370 for national meetings held in 2013. The Board also considered program funding requests, and on the recommendation of B&F VOTED to reauthorize funding for inclusion in the 2013 proposed budget the *ACS Science Coaches* program and the *ACS Global Research Experiences, Exchanges, and Training Program (GREET).*

The Board of Directors considered two other recommendations from the Committee on Budget and Finance and VOTED that an in-depth review of the expectations for the financial goals for National Meetings be performed, and that a financial plan for the long-term viability of the *ACS Presentations on Demand* program (formerly known as Electronic Dissemination of Meeting Content) be developed and shared with B&F at its 2013 spring meeting.

The working group on Society Program Portfolio Management briefed the Board on its activities. The working group is charged with recommending a process for portfolio management of Society programs in the divisions of Membership and Scientific Advancement, Education, the Office of Public Affairs and pilot programs.

The Executive Director/CEO Report

The Executive Director/CEO and her direct reports updated the Board on the following: security threats faced by the Society's information technology systems and the measures in place to protect against them; a recommendation from the 2011 Financial Planning Conference that ACS identify additional revenue sources; and the activities of CAS (Chemical Abstracts Service), the ACS Publications Division, and the Society's General Counsel. The General Counsel report included an update on the ACS vs. Leadscope litigation. As a follow-up to the Publications report, the Board VOTED to approve several journal editor re-appointments.

Strategic Assessment of ACS Information Services Divisions

As a result of the 2011 Financial Planning Conference, the ACS Board of Directors requested that the ACS Executive Director and Chief Executive Officer carry out a strategic assessment of the ACS Information Services Divisions. As a practical matter, these studies have been conducted approximately every three years to ensure that our information services divisions, CAS and ACS Publications are fulfilling ACS's strategic goals. The study was conducted over a period of nine months, with the ACS Board of Directors and the Governing Board for Publishing discussing the study at key milestones along the way. The study affirmed the robust operating performance of CAS and ACS Publications, from both mission and financial viewpoints. It commended the increasing collaboration between the divisions and their global presence, and identified areas of synergy where additional opportunities for innovation and growth should be explore.

Presidential Symposia at Philadelphia

ACS President Bassam Z. Shakhashiri hosted several well attended symposia under the presidential theme, "Advancing Chemistry and Communicating Chemistry": a plenary lecture on "Chemistry and Climate Change" delivered by Nobel Laureate Mario Molina; the 25th anniversary of National Chemistry Week; "Communicating Controversial Science" honoring Rudy Baum on the occasion of his retirement as Editor-in-Chief of C&EN; and "150 Years of Chemistry at Land Grant Institutions: The Past as a Prelude to the Future" honoring the sesquicentennial of the Morrill Land Grant Act.

Other Society Business

The Board received reports from the Presidential Succession on their current and planned activities for the remainder of 2012 and 2013; approved the appointment of Dr. Jerauld Skotnicki as the Coordinating Editor, ACS Presentations on Demand; and welcomed and received reports from international guests representing the Canadian Society for Chemistry, the German Chemical Society, the Chemical Society of Japan, and the Royal Society of Chemistry.

The Board held a well-attended open session which featured a special forum titled "What are the 'real world' ethics issues faced by students and practitioners of chemistry?" Members attending this standing-room only session offered personal observations about ethical issues they have observed or been challenged by and possible options to address them.

The ACS Leadership Institute will be held in Dallas, Texas, January 25-27, 2013, for new committee, local section, and division chairs, and other volunteer governance members.

In order to increase the available time for abstract submission for the ACS National Meetings, the Committee on Meetings and Expositions will be studying the feasibility of eliminating the print version on-site program books with a target of the 2013 fall national meeting in Indianapolis.

The 25th anniversary of National Chemistry Week will be celebrated October 21-27 with the theme, "Nanotechnology – The Smallest BIG Idea in Science!" All local sections are encouraged to participate in NCW and plan an event that will recognize their coordinators.

The 10th anniversary of Chemists Celebrate Earth Day will be celebrated in 2013. All local sections are encouraged to participate.

ADDITIONAL INFORMATION

The following is a list of URLs and email addresses presented on slides at the Council meeting. You will find the information noted on these cites helpful.

www.acs.org/ChemistryAmbassadors - Information on the Chemistry Ambassadors program
www.facebook.com/ChemistryAmbassadors - Chemistry Ambassadors group on Facebook
www.acs.org/getinvolved - Details on Innovative Project Grants through the Committee on Local Section Activities
www.acs.org/climatescience - Information on the ACS Climate Science Toolkit
outreach@acs.org - Contact email for more information on the Coins for Cleaner Water initiative
www.acs.org/bulletin5 - The ACS governing documents including certification information on unit bylaws
bylaws@acs.org - Contact email for submitting petitions and other questions regarding the governing documents
www.acs.org/ei - Information on the ACS Entrepreneurial Initiative
careers@acs.org - Email address for forwarding revisions on the Academic Professional Guidelines
www.acs.org/cpc - Information on the Council Policy Committee including the Councilor Handbook and Strategy Café Toolkit
www.acs.org/councilreports - Location for committee reports posted following the Council meeting

Bonnie Lawlor and Andrea Twiss-Brooks, CINF Councilors

Council Committee on Nomenclature, Terminology and Symbols

The Committee on Nomenclature, Terminology and Symbols held its open meeting on Monday, August 20, 2012. We received a report on the discovery of two new elements: number 114 and 116. The Committee found that the proposed names and symbols follow a long tradition of selecting element names from geographic place names. Thus, the names Flerovium (element 114; symbol Fl) and Livermorium (element 116; symbol Lv) honor the two laboratories that cooperated in the discoveries. They join other elements named for other laboratories such as: Berkelium (element 97), Dubnium (element 105), Darmstadtium (element 110).

In previous reports from this Committee, Council was informed regarding the redefinition of the kilogram and the mole. The Committee on Nomenclature, Terminology and Symbols began its work with two goals: 1) to understand what is being done; and 2) to understand what it means to the practice of chemistry.

At its meeting in October 2011, the General Conference on Weights and Measures endorsed the concept of re-defining all of the SI Base Units on physical constants deemed "invariants of nature." The proposed new definitions, however, were not adopted. Instead, the Conference encouraged further work on the values of the physical constants to reach a target uncertainty of 20 parts per billion. Presently, the Planck constant that will define the kilogram has an uncertainty of 44 parts per billion.

The re-definition of the *mole* will be based on the Avogadro constant causing the mass of Carbon-12 to be determined experimentally and no longer be defined as 12.0 exactly. Presently, the uncertainty in the Avogadro constant is also 44 parts per billion.

The next General Conference on Weights and Measures is scheduled for 2014 rather than after the normal four-year interval that would place it in 2015. Provided the target uncertainties of the physical constants have been met, the new definitions should be adopted at that time.

The Committee has begun preparation of a series of descriptions of the new definitions of SI Base Units. These descriptions are designed to address the chemical education needs of different grade levels and will be available on the Committee's web site.

Peter Rusch, Chair, Committee on Nomenclature, Terminology and Symbols

Highlights from the Joint Board-Council Committee on Publications

The open session of the ACS Joint Board-Council Committee on Publications (JBCCP) is usually scheduled on Friday afternoon before the national meeting commences and is open to any society members. Brian Crawford, President of the ACS Publications Division, presented an update to the ACS Joint Board-Council Committee on Publications and the ACS membership. Slides are posted here. Leah McEwen, Committee Member and CINF Secretary, provides the summary below. Questions may be directed to the Committee Chair, Ned D. Heindel, email: ndh0@lehigh.edu.

Highlights from the ACS Publications Division operations included the following:

- Several new journal publications on track for 2012-2014 and Editor-in-Chief search committees are underway for several key journal titles.

- Maureen Rouhi has been promoted to the Editor-in-Chief of *C&EN*. Former *C&EN* Editor-in-Chief Rudy Baum retired on September 14. A symposium in his honor was held at the Fall Meeting http://portal.acs.org/portal/PublicWebSite/pressroom/newsreleases/CNBP_030555.

- Web article requests are up 7% on an YTD basis; ACS articles have been downloaded over 40 million times at the mid-year point. The increased member access benefits are so far a success.

- New technical development efforts are focused on web and mobile product innovations, CAS collaborations, and infrastructure enhancements.

- The ACS Publications Division is focusing outreach to graduate students and post docs through the ACS on Campus program and its Graduate/PostDoc Summer Institute.

- The Division's expanded presence in China includes the hiring of CINF member Norah Xiao to the Editorial Development team in the newly-created position of Manager, Editorial Development (Asia). Xiao will pursue new publishing opportunities in Asia, as well as the strategic development of an expanded cadre of expert scientists to serve as trained peer reviewers and candidate editorial advisory board members and Associate Editors for ACS journals. The division is also planning expanded customer and user help capabilities for Asia.

A strategic assessment of the ACS Publications Division and CAS was recently conducted by the ACS Board. It indicated robust operating performance on mission and financial fronts, and encouraged increased collaboration between the two publishing arms and with the technical divisions. ACS Publications is also monitoring open access (OA) initiatives in the US and beyond, and engaging in outreach and advocacy. The ACS Governing Board approved a pilot project to explore a cross-publisher content linking initiative with the Department of Energy as alternative to government-mandated centralized deposit. Alternative business models regarding ACS journals and open access will also be evaluated.

Crawford presented some background on the OA landscape in publishing from the ACS Publications Division perspective. The two primary forms of OA are "Green" where the authors are able to self-archive a version of their published articles in an institutional repository, and "Gold" where the journals themselves are OA. Many society publishers support Green OA and some have been experimenting with Gold. Many commercial publishers also offer Gold OA journals. 6,000 journals were surveyed in 2010, and 25% offer some form of OA, predominately in some hybrid form (89%). There are very few established OA publishers. Springer now has an OA publishing arm. There are many new OA entrants: 2.6 new journals launched each day; over 7,000 available, but very few are proving to be successful. eLife (http://www.elifesciences.org/) is a new joint initiative between the Howard Hughes Medical Institute, the Max Planck Society, and the Wellcome Trust. ACS Publications is concerned that it will be difficult for the public to distinguish "wheat from chaff,"

and JBCCP plays a crucial role through membership involvement to keep the ACS reputation high as a purveyor of quality information.

The political climate is currently in a perfect storm around OA: the Research Works Act backlash, the failure of the Stop Online Piracy Act (SOPA) and the Protect against Internet Piracy Act (PIPA), the reintroduction of the Federal Research Public Access Act (FRPAA), a pending report from the White House Office of Science and Technology Policy (OSTP), a petition to the White House and Obama administration for response, institutional mandates and faculty engagement, and the recent Finch Report in the UK. The Finch report recommends a policy direction for research publishing in Europe towards more OA and hybrid journals through article publishing charges. A survey of the publishing industry conducted by the Association of American Publishers (AAP) in 2010 indicating the vast majority of revenues comes from paid circulation to institutions suggests the cultural magnitude of such a shift. ACS authors are roughly divided in thirds between the United States, Europe and Asia (East Asia & Pacific) with the remaining 10% distributed across the rest of the Western & Eastern Hemispheres. OA developments worldwide impact not only the publishers in regions creating publishing policies, but also authors who publish across international boundaries.

ACS Publications is monitoring these developments to consider policies that funding bodies should advocate, and emerging balanced and sustainable approaches to cultural change through close contact, dialogue, and thorough and reasoned study. JBCCP and all ACS members are encouraged to read the report: http://www.researchinfonet.org/wp-content/uploads/2012/06/Finch-Group-report-FINAL-VERSION.pdf. Currently on the OA front, the ACS offers: ACS articles on Request, ACS Author Choice (minimal uptake <1%), updated Journals Publishing Agreement, facilitation of NIH Public Access Policy, custom licensing agreements with the Wellcome Trust and other funding agencies, society position statement and advocacy regarding unfunded public mandates and trade association engagement.

Question from the floor: The NSF requirement for data management plans is another unfunded mandate. Is ACS Publications taking any action?

Crawford: Data can be divided broadly into two groups – the first is the raw output of the research process and the second is that which is published along with journal articles. A task force of ACS editors is investigating a possible role for the Society regarding data management support for investigators. This group is also coordinating with CAS. The Association of American Publishers (AAP) is in the process of reviewing potential intellectual property issues associated with published and processed data and it is generally recommended that researcher-validated primary data be made openly available. The White House Office of Science and Technology Policy (OSTP) is also considering issues around the public availability of published and primary data.

Suggestions from the floor: ACS Publications should ask authors to supply links to their primary data. Thomson Reuters is planning to launch the Data Citation Index later this year (see: http://wokinfo.com/products_tools/multidisciplinary/dci/).

Leah McEwen, Member, Joint Board Council Committee on Publications

CINF Social Networking Events

The Division of Chemical Information hosted a fantastic set of social networking events at the recent ACS National Meeting in Philadelphia. The division was fortunate to receive several generous contributions from our sponsors to foster successful symposia and social gatherings where division members and associates gather, mingle, commune and link. Please see event photos at http://www.flickr.com/photos/cinf or at the Division of Chemical Information group on the ACS Network.

The **Science and the Law Symposium**, co-hosted with the Division of Chemistry and the Law, was heavily attended and a great success on Sunday. Many thanks to **Kilmorie Clarke** for snacks and refreshments.

The **CINF Welcoming Reception** was supported by five helpful sponsors drawing a varied group of almost 100 chemical information devotees to enjoy the fare and conversation, and to inaugurate the Philadelphia meeting on Sunday. Many thanks to our host of supporters: **Bio-Rad Laboratories**, **InfoChem, Optibrium, PerkinElmer,** and ***ACS Sustainable Chemistry & Engineering***. The **CINF Scholarship for Scientific Excellence** poster session at the Welcoming Reception provided $1,000 awards to three student winners by our generous scholarship sponsor, **FIZ CHEMIE Berlin**. Please let your students and interns know about these prizes at http://www.acscinf.org/awards/sciexcel.php.

Harry's Party, also hosted by **FIZ CHEMIE Berlin** on Monday evening, rejoined the chemical information cast in the Governor Suite at the Sheraton Philadelphia City Center with great views of the Philadelphia Library and other sites. A crowd of comrades and acquaintances enjoyed excellent food and drink while renewing old friendships and building new rapport.

The **CINF Tuesday Luncheon** offered tasty fare and an engaging presentation to about 80 diners. Dr. William Brock spoke to *The Case of the Poisonous Socks: Tales from Chemistry*, a collection of anecdotes regarding chemistry and forensics. CINF thanks **RSC Publishing** for sponsoring this fun event again.

The **Herman Skolnik Award Reception honoring Dr. Peter Murray-Rust & Prof. Henry Rzepa** followed a well-attended Herman Skolnik Award Symposium and was visited by at least 100 division members and affiliates at the Chemical Heritage Foundation. The museum was open for viewing and the food and drink were well received. It was fantastic to see the old and new faces enjoying a great celebration. No one wanted to leave. Many thanks for the support of our diverse group of co-sponsors: **Imperial College**, **Microsoft Research**, **Schrodinger**, **Unilever** and the ***Journal of Cheminformatics***.

The CINF Division would not be able to host these social networking events without the generous support from all our sponsors to whom we extend our sincere thanks.

Graham Douglas, Chair, CINF Fundraising Committee

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