

Chemical Information Bulletin
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Message from the Chair

The past ACS Spring National Meeting in San Diego was a great success with productive business meetings, stimulating and informative symposia and great networking opportunities. The CINF program schedule was packed with a large number of symposia and speakers. Of note were symposia on *Systems Chemical Biology* and *Computer-Aided Drug Design*. Both symposia were well attended and the credit goes to the organizers for putting together a stellar speaker list and a great set of talks. It was also encouraging to see a well-attended, lively CINFlash session of lightning talks. The high level of participation was also evident in the sixteen posters that were presented at the CINF Scholarship for Scientific Excellence event, hosted at the CINF Welcoming Reception on Sunday. The posters highlighted excellent work covering a diversity of topics ranging from a network analysis of retractions to reaction modeling and docking.



While business meetings are not usually exciting on Saturday, they were quite productive in San Diego. This was certainly helped by the new meeting schedule initiated by Past-Chair Gregory Banik. I expect that this schedule will be maintained for future CINF business meetings. We proposed for the Executive Committee to convene via teleconference once a month. I anticipate that this will help us keep up the momentum on multiple CINF initiatives and speed up decision-making. We also discussed how CINF could get more involved with its members outside of National Meetings. To this end, we'll be trying to organize "CINF Happy Hour" at various locations – Antony Williams is currently trying to coordinate one in the Research Triangle Park region and I will be coordinating one in the Central Connecticut region. Obviously, this doesn't cover all the areas where our members reside. So we'd be delighted to know if other members would be interested in getting involved in this effort. More generally, if you have ideas that CINF can do or should be doing to enhance the Division's utility to its members, please let us know.

Of course, all the science and business is strenuous, and that's why CINF provides ample opportunities for networking and relaxation with receptions, Harry's Party and the CINF Luncheon. For the Spring Luncheon we invited Dr. Kirsten Skogerson to speak on the "Chemistry of Wine." Audiovisual equipment hiccups notwithstanding, Dr. Skogerson gave a fascinating talk on what goes into making wines and how it all boils down to chemistry.

Attending the San Diego meeting and noting the extensive participation by old and new CINF members was really invigorating and the credit for the success of the meeting must go to the hard work of many people, especially the symposium organizers for volunteering their time and effort and the sponsors for their generous contributions supporting our program and social events.

I highly recommend attending the next meeting this fall (we have an excellent program lined up!) and I hope you'll consider getting more involved in CINF committee activities. I look forward to a great meeting in Philadelphia and I hope I will see you there.

Rajarshi Guha, Chair, ACS Division of Chemical Information

Letter from the Editor

Greetings! With great pleasure I have assembled pertinent information on the award announcements, symposium overviews, and committee updates from CINF and related matters in this issue of *Chemical Information Bulletin* for perusal by division members and friends. The Spring 2012 ACS National Meeting was the second largest in attendance for a spring national meeting since 2004, attracting 16,864 scientists to San Diego (see Councilors' Report, page 27). Similarly, the CINF technical program had the second largest number of abstract submissions, more than 130 for this meeting. This was slightly less than the record number of 140 submissions for the CINF technical program at the 2010 Spring Meeting in San Francisco, where the total attendance reached 18,076.



Among many CINF highlights in San Diego was the record number of sixteen student poster presentations at the CINF Scholarship for Scientific Excellence. In the tight competition, two students, Freya Klepsch, University of Vienna, and David Fooshee, University of California Irvine, won the \$1,000 scholarships. Bin Chen, a student at Indiana University, was selected as the recipient of the 2012 Lucille Wert Scholarship. Dr. Wendy Warr, a renowned fellow of CINF, was named to be the recipient of the 2012 Val Metanomski Meritorious Service Award. The presentation of the awards to Bin Chen and Wendy Warr will take place at the Fall CINF Luncheon in Philadelphia on August 21, 2012. Congratulations to all award recipients!

Additionally, a CINF symposium, *Drug Polypharmacology Prediction and Design*, organized by Shuxing Zhang, was spotlighted for the **Chemistry of Life** thematic program in San Diego. Go over the *CINF Technical Program Highlights* by Rachele Beinstock in this issue. Then, dip into full reports of five CINF symposia, namely, *Instructional Tools for Chemical Information* by Charles Huber, *CINFlash* by Rajarshi Guha, *Joint CINF-CSA Trust Symposium Beyond Small Molecules: Pushing the Envelope for Chemical Structure Representation* by Keith Taylor, *How Many Miles Have We Gone, InChI by InChI?* by Alex Tropsha and Antony Williams, and *Libraries and Institutional Research Evaluation* by Andrea Twiss-Brooks. Recorded content from six CINF symposia (30 presentations) will be freely available to everyone after May 8, 2012. Read on about the highly successful thematic programming in San Diego and themes for future ACS National Meetings in the *News from the Multidisciplinary Planning Program Group* by Guenter Grethe.

Furthermore, check out a welcome addition of a report from the *CINF Education Committee* by Charles Huber. With no break in programming since San Diego, the Education Committee is now looking forward to *Before and After Lab: Instructing Students In "Non Chemical" Research Skills*, a symposium organized for the Biennial Conference on Chemical Education, Penn State University, July 29-August 2, 2012 (<http://www.2012bcce.com>). Also, an invited report with highlights from the *Joint Board Council Committee on Publications* by Leah Solla is featured.

In conclusion, I would like to thank everyone who wrote articles for this issue. Many thanks to Mark Luchetti for designing the cover page, Bonnie Lawlor and Wendy Warr for proofreading this issue, and Wendy Warr for taking photographs in San Diego (<http://www.flickr.com/photos/cinf/>).

Svetlana Korolev, Editor, *Chemical Information Bulletin*

AWARDS AND SCHOLARSHIPS

2012 Val Metanomski Meritorious Service Award



The CINF Awards committee unanimously approved the nomination of Dr. Wendy Warr for the 2012 Val Metanomski Meritorious Service Award. Wendy is cited in the nominating letter “for her outstanding contributions to the CINF Division in major tasks over 26 years.” She has been a steadfast supporter of CINF in so many ways (Awards, Fundraising, Program, Publications) that her tremendous contribution to the chemical information community is indisputable. The award will be presented during the CINF luncheon at the ACS National Meeting in Philadelphia in August 2012.

2012 Lucille M. Wert Student Scholarship



Bin Chen, a graduate student enrolled in the School of Informatics and Computing at Indiana University, was selected as the recipient of the 2012 Lucille Wert Scholarship. The Lucille Wert Scholarship is an award of \$1500 to “help persons with an interest in the fields of chemistry and information to pursue graduate study in library, information, or computer science.” Bin Chen is currently pursuing a Ph.D. under the direction of Prof. David Wild.

2012 CINF Scholarship for Scientific Excellence



Accelrys sponsored two CINF Scholarships for Scientific Excellence for spring 2012. Sixteen applicants for the scholarships presented posters during the Division’s Sunday Welcoming Reception. Students from the USA, UK, Poland and Austria participated. The scholarship recipients, Freya Klepsch and David Foshee, were recognized during the Division’s Luncheon where they each received their award checks. Details of the winning presentations follow:



Structure based pharmacophore screening for new P-gp inhibitors. **Freya Klepsch**, K. Prokes, Z. Parveen, P. Chiba, G. F. Ecker, Department of Medicinal Chemistry, University of Vienna.

COBRA: Computational brewing approach to predicting the molecular composition of organic aerosols. **David Foshee**, T. B. Nguyen, S. A. Nizkorodov, J. Laskin, A. Laskin, P. Baldi, Institute for Genomics and Bioinformatics, University of California, Irvine.

Andrea Twiss-Brooks, Chair, CINF Awards Committee

TECHNICAL PROGRAM

CINF Technical Program Highlights



San Diego has been one of the jewels of CINF programming. With well over 130 submitted abstracts (and very few withdrawals and no cancelled symposia) it has been one of the largest CINF programs in recent history! (At least, since I have been Program Chair ☺).

The CINF program had a double track every day with the exception of Thursday. The meeting was extremely well attended. In fact, CINF sessions were so well attended that little room 27A in the San Diego Convention Center consistently featured every seat taken and attendees leaning on all walls. If the fire marshall had walked in, we would have been in trouble! Even our Thursday morning session with the “spunky” updated title “General Papers: Chemical Databases, Drug Discovery and Chemical Structure Representation” managed to have a nice, ample-sized audience.

Additionally, one of the CINF symposia, “Drug Polypharmacology Prediction and Design,” organized by Shuxing Zhang, was highlighted as part of the “Chemistry of Life” thematic programming in San Diego. Because there was nominal co-sponsorship between this CINF symposium and the LIFE symposium, “Chemical Networks in Biology,” the ACS special “LIFE” promotional pieces and glossy flyers distributed around the convention center listed our symposium and featured CINF prominently next to the names of Nobel Laureate Roger Tsien and MacArthur Fellows Carolyn Bertozzi and Laura Kiessling! CINF had its own celebrities too, as Chris Lipinski was one of the featured speakers in our standing-room only “Drug Polypharmacology” session. This session also featured superb presentations on polypharmacology models for large datasets (Swamidass), QSAR datasets for GPCRs (Muratov), Gaussian ensemble virtual screening methods (Perez Nueno), and other physical binding site predictive modeling and virtual screening methodologies (Varela, Chen, Zhang, Koch), as well as the use of semantic linked databases (Wild) and drug repurposing (Ekins).

Orr Ravitz (SymBioSys), Chris Corbeil (CCG) and Jason Cross (Cubist Pharmaceuticals), lined up a group of stellar experts in the field for their symposium on “Computer Aided Drug Design,” including Christine Humblet, Richard Law, Thomas Fox and Marti Head for the commercial drug development perspective, and Tudor Oprea, Chris Breneman and Jeffrey Gray for the academic perspective.

Keith Taylor (Accelrys) chaired our joint CINF-CSA Trust Symposium, “Beyond Small Molecules: Pushing the Envelope for Chemical Structure Representation,” which featured several presentations on strategies for representations and searching of complex molecules, including cheminformatics of porous materials (Martin), proteins and nucleic acids (Sayle), biotherapeutics (Villar, Taylor), Markush representation (Deng, Yerin, Walter), and PubChem representations (Bolton).

We had a record number (sixteen candidates) for our CINF Scholarship for Scientific Excellence poster session. In fact, Guenter Grethe warned me that we were reaching our upper limit of posters that could be appropriately evaluated and judged - CINF should always have a problem like this! CINF was also represented for the first time with a large SciMix poster session held on Monday evening.

“CINFlash” has found a successful home on Sunday late afternoon, so we will repeat this same time slot at the fall meeting in Philadelphia.

On the educational side of things, Charles Huber organized an outstanding program on “Instructional Tools for Chemical Information” featuring several presentations on chemistry literacy and integrating chemical information into the curriculum (Mandernach, Battle, Hovland, Braendle, Galloway, Fong), XCITR (Grethe), Reaxys (Flemming), SpringerMaterials (Shaikh), CAS (Zielenbach), Chemistry Reference Resolver (Zhurakovskiy), and the role of computers and wikis (Parr, Walker). Of course, the essential role of chemical librarians in the educational process was represented in presentations by Donna Wrubewski, Valerie Tucci and Benny Chan, Judith Currano, and Jeremy Garritano.

A CINF program would not be complete now without a session on “Mobile Space and E-Books” organized by Rich Apodaca, himself a leader in the field. Steven Muskal, Woody Sherman, Alex Clark, Sean Ekins, Kevin Theisen, and Antony Williams all gave very interesting presentations on the development of chemistry-related applications for mobile devices. These apps and devices are really catching on, so after this meeting I was suffering from severe “iPad envy.”

The “InChI Symposium” organized by Alex Tropsha and Antony Williams featured all kinds of presentations on the use and development of InChI chemical representations. Steve Heller gave a nice overview of the IUPAC InChI project development, followed by presentations on using InChIs in navigating the Internet (Williams), in commercial software (Taylor), in wikis (Walker), as building block (Borodina), use at National Cancer Institute (Sitzmann), in IUPAC nomenclature (Lowe), at the Royal Society of Chemistry (Kidd), in mcule (Szalai), in UniChem (Chambers), and in the Chemistry Department at Louisiana State University (Armstrong). In short, “InChI here, InChI there, InChIs everywhere!” (Swienty-Busch and Evans).

“Beyond the Database: New Models of Scholarship in an eScience World,” chaired by Phil Bourne, featured presentations on semantic web integration of public data and other collaborative computational technologies for sharing data by David Wild, Sean Ekins, Julien Thibault, Marc Nicklaus, and Jeremy Frey.

“Recent Advances in Reaction Searching,” organized by Roger Schenck and David Evans, featured many interesting presentations on methodologies for making computer savvy synthesis (He, Eigner-Pitto, Currano, Kellett), extraction of synthetic patent data (Lowe, Zielenbach), applications for electronic laboratory notebooks (Sayle, Skinner), ChemInform Reaction Library (Stuedel) and computational reaction searching (McHale, Detering, Swienty-Busch, Johnson, and Gothard).

“Systems Chemical Biology and Other ‘Systems’ Approaches in Chemistry and Biology Research,” organized by Jan Kuras and Tudor Oprea, featured presentations on interactomes (Kouskoumvekaki, Panagiotou), small molecule inhibitor development and identification of “druggable” targets by systems methods (May, Wang, Year, Hopkins, Khasanova, Vureeva), the CARLSBAD database (Zahoransky-Kohalmi), integration of targets, drugs and outcomes (Overington, Oprea), and, of course, semantic web (Wild).

“Libraries and Institutional Research Evaluation,” organized by Leah Solla and Andrea Twiss-Brooks, featured presentations on journal article databases and research analytical tools (Brown, Wrublewski, Calton, Hook, Grecchi), and the use of social networking tools (Williams).

The Program Committee is always looking for ideas, so if you feel that you can contribute, please come to the CINF Program planning meeting on Saturday afternoon at the next conference, or email me, rachelleb1@gmail.com or our incoming chair, Jeremy Garritano, jgarrita@purdue.edu.

And, if you thought that the San Diego meeting featured a long and impressive program, then stay tuned for the next one in Philadelphia, and come celebrate with our Skolnik honorees, Henry Rzepa and Peter Murray-Rust! Hope to see you then!

Rachelle Bienstock, Chair, CINF Program Committee

Proposed CINF Program for the Fall 2012 ACS National Meeting

Chemical Space: Challengers in Visualization and Mining	Jose Medina-Franco, jmedina@tpims.org Maciej Haranczyk, mharanczyk@lbl.gov
Cheminformatics and Drug Repurposing	Jose Medina-Franco, jmedina@tpims.org Rachelle Bienstock, rachelleb1@gmail.com
Cheminformatics Opportunities in Personalized Medicine and Chemogenomics	Christoph Steinbeck, er@doktor-steinbeck.de David Wild, registrations@wild-ideas.org
CINF Scholarship for Scientific Excellence	Guenter Grethe, ggrethe@att.net
CINFlash	Rajarshi Guha, rajarshi.guha@gmail.com
Future of the History of Chemical Information	Andrea Twiss-Brooks, atbrooks@uchicago.edu Leah Solla, leah.solla@cornell.edu
General Papers; SciMix	Rachelle Bienstock, rachelleb1@gmail.com
Global Opportunities in Chemical Information	Jignesh Bhate, jignesh@molecularconnections.com Tom Blackadar, tom@binocvision.com
Hunting for Hidden Treasures: Chemical Information in Patents and Other Documents	Wei Deng, dengw2@gmail.com
Informatics Approaches to Materials Design	Maciej Haranczyk, mharanczyk@lbl.gov Ian Bruno, bruno@ccdc.cam.ac.uk
Legal, Patent and Digital Rights Management in Publishing	Judith Currano, currano@pobox.upenn.edu Charles Huber, huber@library.ucsb.edu
Open Notebook Science/Open Chemistry/Electronic Lab Notebooks	Philip McHale, pmchale@cambridgesoft.com Jean-Claude Bradley, bradlejc@drexel.edu
Science and the Law: Analytical Data in Support of Regulation in Health, Food, and the Environment	William Town, bill.town@kilmorie.com
Skolnik Symposium: Molecular Science and the Semantic Web	Henry Rzepa, rzepa@ic.ac.uk Peter Murray-Rust, pm286@cam.ac.uk
When Chemists and Computers Collide: Putting Cheminformatics in the Hands of Medicinal Chemists	Matthew Segall, matthew.d.segall@gmail.com
General Papers; SciMix	Rachelle Bienstock, rachelleb1@gmail.com

Instructional Tools for Chemical Information

This symposium, organized by the CINF Education Committee, received an excellent turnout, both of speakers and attendees and was well received by all participants. The morning session opened with the paper “Embedding chemistry information literacy skills into the curriculum at James Madison University” presented by JMU chemistry librarian, **Meris Mandernach** and chemistry faculty member, **Barbara Meisner**. They described their success in incorporating key chemical information literacy skills (as set forth in the “Information Competencies for Chemistry Undergraduates” document from the Special Libraries Association Chemistry Division and CINF) into the chemistry courses where students would be using them.

Gary Battle of the Cambridge Crystallographic Data Centre (CCDC) spoke about the Cambridge Structural Database, and, in particular, CCDC’s teaching subset of 500 crystal structures, designed to let students learn key concepts in crystallography. CCDC is also producing a growing collection of Web-based tutorials and other teaching materials that make use of this subset.

The third paper, “If they build it, will they use it: Using input from students in a chemical literature class in the redesign of the library's chemistry webpages,” highlighted another faculty-library partnership. Professor **Allen Hovland** and librarian **Rob Sloan** of St. Mary’s College of Maryland developed an innovative assignment in which undergraduate chemistry students helped design and select resources for inclusion on the library’s chemistry subject guides on the SpringShare Libguides platform.

Guenter Grethe detailed the background and goals of XCITR (eXplore Chemical Information Teaching Resources). This joint project of CINF and the Division of Computer-Information-Chemie (CIC) of the German Chemical Society is an international repository of chemical information teaching tools deposited by chemistry librarians and faculty. The tools may be freely accessed by anyone seeking resources to enhance their own chemical information instruction.

Continuing the collaborative theme, **Jessica Parr** of the Department of Chemistry of the University of Southern California, presented her work with chemistry librarian **Norah Xiao**, “Engaging the wired generation,” using lectures, interactive activities and an online tutorial to help students, faculty and staff become acquainted with the techniques and resources available to them through the library.

Martin Brändle of the Chemistry Biology Pharmacy Information Center of ETH Zurich discussed a number of projects that he and his colleagues have undertaken to improve students’ ability to meet their information needs. These include problem-solving units incorporated into laboratory courses, web guides to key resources, and individual support to end-users. One project involved students in a comparison of chemical thermodynamics entries in the German Wikipedia with those in the Römpp Online chemistry encyclopedia. A textbook portal makes use of the library’s interactive navigation tool to help students find the print resources they need.

Linda Galloway of the Syracuse University Libraries reported on her work with one-shot lectures on specific information competencies, incorporated into the chemistry undergraduate curriculum at the point of need.

Christine Flemming of Elsevier gave examples of how user feedback has helped develop Elsevier's extensive collection of training materials for the Reaxys chemistry database. She also highlighted how the Reaxys team has used social networks and online forums to help build a Reaxys user community.

Yet another collaborative venture between **Bonnie Fong** of the John Cotton Dana Library at Rutgers University and chemistry professor **Darren Hansen** has created a mini-course aimed at providing chemical information skills to beginning graduate students. The presentation described how they selected the resources to cover, and the "hot topics" to include, and how to create assignments to achieve the desired outcomes.

Mikail Shaikh provided an introduction to SpringerMaterials, the database that builds on the Landolt-Bornstein book series to provide one of the largest collections of chemical and physical property data of materials. He described how Springer Science is using a variety of tools to provide support to and obtain feedback from the SpringerMaterials user community.

The afternoon session led off with the first of two presentations by **Donna Wrublewski** of the George A. Smathers Libraries of the University of Florida. It detailed her work with the instructors of the introductory physical/biophysical chemistry laboratory course to update all the references in the course's laboratory manual, make sure that they were available in the library, and provide links to them via the library's course reserves system. An in-class information literacy lecture pointed students to the recommended references and how to access them.

Valerie Tucci of The College of New Jersey's library collaborated with chemistry faculty member Benny Chan and other TCNJ faculty to develop an undergraduate seminar series. Their presentation described the content of the series (advising in Part 1, chemical information literacy in Part 2, and good laboratory practice in Part 3), with specifics on the chemical information literacy portion of the course. The seminar uses formal instruction and assessments of students' basic skills, search techniques using SciFinder, and patent searching in the USPTO and SciFinder databases.

Peer review is a key element of the scholarly communication process, and **Judith Currano** of the University of Pennsylvania reported on an innovative use of the technique in a graduate level chemical information course. Students prepare a literature review, which is then subjected to a double-blind review by their peers in the class. This approach not only provided valuable experience in the process itself, but was found to improve the quality of the literature reviews as well.

Chemistry faculty member **Mine Ucak-Astarlioglu** of the University of Florida partnered with chemistry librarian **Donna Wrublewski** to create a chemical information component of her physical chemistry laboratory course. Students prepare two talks: one a report on a current relevant journal article, and the second on their search strategies for finding and selecting the paper covered in the first talk. Outcomes include improved student search skills and enhanced library support of the chemistry department's teaching objectives.

Kurt Zielenbach of Chemical Abstracts Service stepped in as a substitute presenter for a description of the many facets of CAS' Learning Solutions – including webinars, tutorials, online in-context

help, virtual classes, workshops and forums. All of the above and more combine to meet the goal of providing point-of-need support to the users of SciFinder and STN.

Oleksandr Zhurakovskiy of the University of Oxford introduced Chemistry Reference Resolver, a software tool designed to assist chemists in tracking down references in the published literature. The browser plug-in can accept reference information in a variety of styles, and direct the user to the online source of the HTML or PDF document.

LibGuides is a resource now used by many academic libraries to create and host resource guides for their users. **Jeremy Garritano** of Purdue University described his use of LibGuides to enhance the chemical information literacy of the thousands of students in the freshman and sophomore chemistry lab courses at Purdue. The site was built collaboratively with input from instructors and advisors to cover communication and information-seeking skills. Usage statistics and user feedback are guiding the further development and refinement of the guides.

Martin Walker of the Chemistry Department of the State University of New York at Potsdam presented his collaboration with Aileen Day, Antony Williams and Lorna Thomson of the Royal Society of Chemistry on RSC's Learn Chemistry wiki. The wiki makes use of cheminformatics features from RSC's ChemSpider to enable educators to better share their creations (quizzes, experiments, tutorials, etc.) and incorporate chemical structures and data derived "live" from ChemSpider. The wiki not only enhances the contributed resources, but provides the educators themselves with a practical education in cheminformatics tools.

The final scheduled paper, on the ACS on Campus program by Sara Rouhi of ACS Publications had to be withdrawn due to an unavoidable schedule conflict for the presenter.

Charles Huber, Symposium Organizer

CINF Program at the 2012 Biennial Conference on Chemical Education

<http://www.2012bcce.com/>

Before and After Lab: Instructing Students in "Non Chemical" Research Skills (7/31/12)

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

CINFlash



CINFlash is an initiative that we started three meetings ago as a way to spice up the CINF program and to address some of the deficiencies of the schedule set up far in advance before the conferences take place.

The CINFlash session comprises 8-minute talks, each one strictly timed, and can be on any topic related to chemical information and cheminformatics. Given the short time period, we hope that contributors will focus on the fun aspects of their research and not necessarily provide a rigorous, comprehensive presentation of their research. In other words, if you have an off-the wall idea about something to do with chemical information, this is the place to talk about it for 8 minutes!

Most importantly, talks submitted to this session are not entered via PACS. Rather, we accept submissions by hand up until about two weeks before the meeting. This is aimed at encouraging presentations on recent ideas, rather than rehashing work performed a year or more in the past. Presently, the talks don't show up in the print or online version of the ACS meeting program, but plans are afoot to include a list of presentations in the online schedule so that it will enhance the visibility of the program.

The most recent CINFlash event held at the Spring meeting in San Diego was quite successful. It was scheduled on Sunday afternoon. We had nine speakers covering topics ranging from virtual screening pipeline and patent analytics to a philosophical discussion linking structural similarity and personal address books. With an audience of more than thirty people, it was rather well attended. I think that the idea of such lightning talks is catching on and I encourage everybody, especially students, to be on the lookout for the next CINFlash in Philadelphia – it's a low barrier to entry and a fun event where you really can talk about arbitrary topics without the complete rigor of a traditional presentation.

Rajarshi Guha, Symposium Organizer

The CINFlash experimental session is financially supported by Innovative Projects Fund for Divisional Enhancement, ACS Committee on Divisional Activities

The past CINFlash schedule of talks and presentation slides are available at:

2012 Spring Meeting in San Diego (Sunday) <http://acscinf.org/meetings/243/flash243.php>

2011 Fall Meeting in Denver (Wednesday) <http://acscinf.org/meetings/242/calls/flash242.php>

2010 Fall Meeting in Boston (Monday) <http://rguha.net/cinfTMP/flash.html>

↑Image credit: <http://calfiresandiego.blogspot.com/2010/07/lightning-safety.html>



**Joint CINF-CSA Trust Symposium
Beyond Small Molecules: Pushing the Envelope for
Chemical Structure Representation**



The scheduling of this symposium during the first session on Monday morning did not deter attendees. The session was well attended throughout with some 50-60 participants and ensured lively discussion at the end of each presentation. The topic of the symposium Beyond Small Molecules: Pushing the Envelope for Chemical Structure Representation attracted a diverse set of presentations. Abstracts (#53-60) can be found on the [CINF website](#). The session program follows:

Cheminformatics for material discovery: Representation, searching and screening of porous materials. R. L. Martin, M. Haranczyk

New strategies to normalize chemical structure representations and weed-out impractical small molecules. E. Bolton

Efficient perception of proteins and nucleic acids from atomic connectivity. R. A. Sayle

Organization and analysis of information for biotherapeutics research. H. O. Villar, M. R. Hansen, E. Feyfant

Markush structure usability in patent and combinatorial chemistry: New approaches and software tools. W. Deng, S. Csepregi

Rendering the stages of structure elucidation: ACD/Labs Markush representation. A. Yerin, I. Peirson

New developments in Markush structure searching. D. Walter

Representing and retrieving non-specific structures. K. T. Taylor

Two themes were evident: the representation of biological sequences, and Markush structure handling. The introductory presentation by **Martin** (Lawrence Berkeley National Laboratory) really took the theme to its limits. He discussed research that was seeking to characterize porous materials. While the aim of the project was to discover materials for carbon dioxide sequestration, the audience picked up on other applications with many questions ensured. **Bolton** (National Center for Biotechnology Information) discussed the problems associated with curating data obtained from public sources in order to make PubChem a reliable database of chemical structures. Curators of corporate databases overcome this problem by imposing rigorous representation standards at registration time, and they can always refer back to the chemist if there is any doubt. Bolton gave the example of the nitro group, where he has discovered over 50 representations in public sources.

There followed two papers on the representation of biomolecules. **Sayle** (NextMove Software) proposed a compact encoding that had improved processing times over the standard CTAB or SMILES encoding. **Villar** (Altoris) also discussed the challenges of encoding, particularly the

handling of non-standard residues, but most of the presentation was devoted to methods for the visualization of property data for sets of biomolecules.

Taylor (Accelrys) concluded the session with recent enhancements to the ubiquitous molfile format to encode rigorously non-specific structures, haptically bonded structures, polymers, and Markush information. He also reviewed the state of chemical representation. While the low hanging fruit is solved, there are still many challenges with Markush structures and biological materials. He also indicated that biological materials also benefit from Markush encoding; in particular antibody-drug conjugates commonly have incompletely specified connectivity for the drug.

Keith Taylor, Symposium Organizer

This Symposium was financially supported by the Chemical Structure Association Trust. The joint CINF-CSA Trust Symposium has been frequently organized for the Spring ACS National Meetings. The first symposium, [Chemical Information and E-Commerce](#), was held at the Spring 2000 ACS National Meeting in San Francisco, CA.



CSA Trustees at the San Diego Meeting, Sunday, March 25, 2012
Gunter Grethe, Dimitris Agrafiotis, Phil McHale, Peter Loew, Bob Stembridge, Martin Braendle,
Bonnie Lawlor, Peter Rusch, Grace Baysinger, Guido Herrmann
Wendy Warr and David Wild were at the meeting, but not pictured
Photo by Wendy Warr: <http://www.flickr.com/photos/cinf/>

How Many Miles Have We Gone, InChI by InChI?

How simple the communications between people of different nations would have been had we all shared the same language! The attempts to develop such a universal language adopted by the entire human population have not been tremendously successful (e.g., Esperanto), but chemists, on the other hand, have succeeded in developing a language they all understand, that of chemical structure. Chemists of all nations could easily communicate their thoughts using traditional chemical structure drawings, but this way of information exchange becomes increasingly prohibitive with the growth of chemical databases. This is when special means for compact encoding of chemical structures such as SMILES and InChI become critical, making it feasible to store and transmit huge amounts of chemical information (many current chemical databases such as PubChem or ChemSpider include many tens of millions of records). At the ACS meeting in San Diego we had an opportunity to celebrate the impact of the InChI (the IUPAC International Chemical Identifier) on the ability to communicate, link, and enhance the integration of chemistry across databases, across the Internet and in publications.

Unlike the proprietary SMILES format, InChI was designed to be “a freely available, non-proprietary identifier for chemical substances that can be used in printed and electronic data sources, thus enabling easier linking of diverse data compilations and unambiguous identification of chemical substances” (<http://www.inchi-trust.org/html/inchifaq/index.html>). Over the past decade InChI has become widely recognized and used by the chemical community to search, connect and exchange chemical structures. The first InChI symposium to be held at an ACS meeting was organized to highlight the history, recent developments, interesting applications, and current trends in InChI. The unique gist of this full day symposium in the San Diego 2012 program could probably be best summarized by the presentation title of one of the speakers, who had the title “InChIs here, InChIs there, InChIs everywhere!” (see below).

The morning session opened with **Steve Heller** presenting a brief history on how the InChI project started and an update on the present status. He emphasized that InChI was meant primarily to provide a way to link information, was an addition to what was available today, not a replacement, and is an algorithm to produce a unique label. He commented on the success of InChI with one measure being the uncoerced adoption that has been shown by publishers, database providers and software developers.

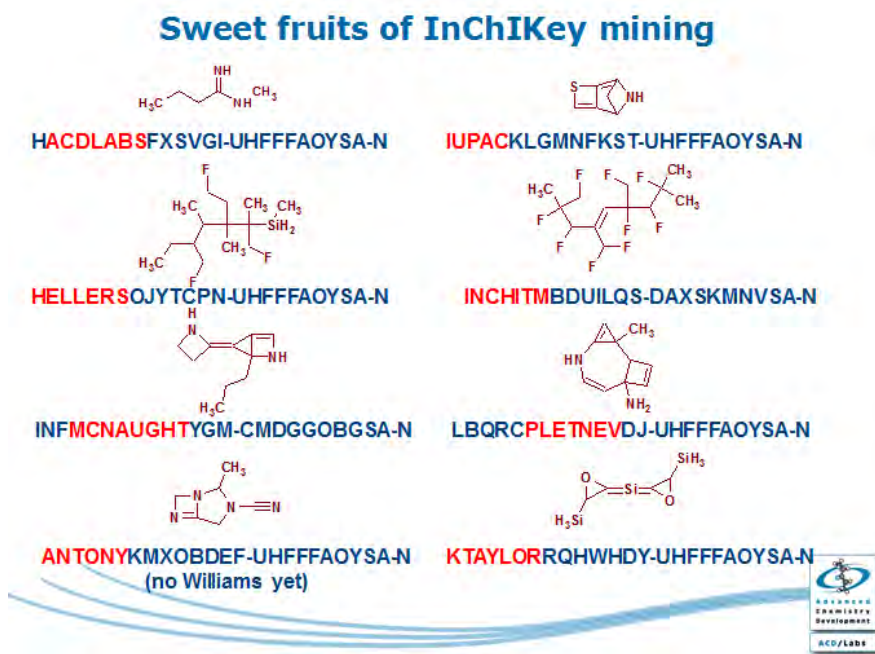
Antony Williams from the Royal Society of Chemistry Cheminformatics team, and member of the ChemSpider project, discussed the “Great promise of navigating the internet using InChIs” and reflected on what the original purpose of InChI was and how far we had come in a relatively short period of time in terms of meeting the goals. In contrast to his usual focus on data quality issues, he started by commenting that the talk was about quantity – how much data was now being linked together and could be discovered using InChI as the linker. He asked “What would be the situation if InChI never existed?” and answered with the fact that ChemSpider would never have been built without it.

Keith Taylor from Accelrys provided an overview of why Accelrys supports InChIs in their cheminformatics toolkit despite having their own unique identifiers already. He emphasized it was because the community asked for InChIs and found them to be valuable. He provided examples of

how different online systems used InChI and what the results were when Accelrys tools were used to perform searches against the online databases.

Martin Walker from the State University of New York at Potsdam presented on the use of InChIs in Wikipedia and their use in ChemBoxes and DrugBoxes. He also discussed how InChIs became an important part of the RSC Learn Chemistry wiki, an open website hosting educational content and encouraging educators to contribute their own data. The site hosts chemical data for over 2,100 common chemicals and uses InChI and InChIKeys to facilitate structure searching across the site and as the basis of interactive quizzes.

Andrey Yerin from ACD/Labs gave a fascinating presentation regarding InChIKey collisions and how to experimentally estimate the rate of their occurrence using algorithmically-generated structure libraries. His conclusion was that InChIKeys do have a very low rate of collision as the degree of randomness, as expected by the design of the InChIKey, is very high. He did provide some very amusing examples of InChIKeys that contained “hidden words” and examples are shown in the figure below.



As a final talk in the morning session **Juergen Swienty-Busch** presented on where InChIs are, i.e. “here, there and everywhere” as commented earlier. He showed how InChIs continue to proliferate in popularity across chemistry databases on the web and how Elsevier now includes them in their Reaxys database as well as in their publications, associated with data. Reed-Elsevier looks forward to further advances in InChI. Elsevier Properties SA is a board member on the InChI Trust and Elsevier is involved as members of three of the working groups. This indicates their belief in the standard.

The discussion of InChI continued in the afternoon. **Yulia Borodina** (FDA) discussed the challenges facing the FDA Substance Registration System when dealing with complex compounds such as biopolymers or synthetic polymers. Standard InChI is not designed to handle such structures, but it could be used to describe monomers and other building blocks of these complex structures.

Marcus Sitzmann from NCI discussed how InChI/InChIKeys are used within the NCI Chemical Identifier Resolver to annotate more than 80M unique chemical structures.

Daniel Lowe from NextMove Software addressed features in IUPAC nomenclature that cannot be addressed by standard InChI such as accurate representation of tautomers and mixtures of stereoisomers. These cases require special treatment.

In a flash talk, **Richard Kidd** discussed the use of InChI within the Royal Society of Chemistry and RSC's contribution to the development of InChI standards.

Ferenc Szalai from Mcule (Budapest, Hungary) highlighted the importance of InChI for unified annotation of chemical structures in aggregated databases that is independent of drawing conventions, tautomeric states, and other features such that each unique chemical structure is annotated only once. He stated that InChI provides the best solution for this problem.

Jon Chambers from EBI (Cambridge) made similar observations based on their group experience in assembling data in the ChEMBL database from different sources. He described their UniChem system that uses the standard InChI as a means of normalizing between different sources of chemical structures.

Bill Armstrong from Louisiana State University shared his experience in creating a teaching methodology to help researchers understand InChI as a unique, non-proprietary tool for identifying chemical structures.

Jason Wilde from the Nature Publishing Group (London) described the efforts of the InChI Trust to support the development of a nonproprietary InChI standard and discussed the ongoing efforts to provide technical solutions to develop standard InChI for difficult cases of complex structures such as polymers and mixtures.

Steve Boyer from IBM (San Jose, CA) described recent efforts of their group to employ InChI for annotating chemical structures in patents as part of chemical name to structure conversion. Their approach replaces chemical names in patent documents by InChI, enabling the search for chemical structures within certain textual content in the patents and patent literature.

In the final talk of the symposium, **Laura Croft** from Nature Publishing Group (London) described the launch of *Nature Chemistry* as part of nature.com and emphasized the utility of InChI to increase the discoverability of chemical structures and related information on nature.com and on the web in general.

This brief summary of presentations at the InChI symposium underscores the importance of InChI as universal identifier of chemical structures. InChI continues to proliferate in various areas of a chemical research and to serve as a critical means of chemical information dissemination and exchange. The anticipated new developments will likely warrant a new InChI symposium within the next couple of years.

Alex Tropsha and Antony Williams, Symposium Organizers

Libraries and Institutional Research Evaluation

Introduction

Many institutions are demanding evidence of impact for their individual researchers as well as for their overall research programs. Various indicators of research quality and impact are in use or under consideration for use, including levels of competitive funding received, international collaborations, successful patent applications, appearance in social media venues and a variety of bibliometric techniques. There is also rich literature available in this field, and I encourage you all to read more.

How do we measure the impact and/or value of the research done at our institutions? University administrators, funding review bodies and other stakeholders are turning to libraries and librarians to assemble evidence and help select tools that demonstrate this value and impact. At this symposium, we heard several talks from librarian, scientist, and vendor perspectives, and were introduced (or re-introduced) to a number of different approaches and tools for evaluating research output. Abstracts can be found on the CINF website at <http://bulletin.acscinf.org/node/285> (Abstracts 121-125/Wednesday PM Section B). The presentations were as follows:

Finding the future: Using research analytical tools with journal article databases and social media data to identify high-impact research leaders and programs / Elizabeth A. Brown (Binghamton University) [[Slides from presentation](#)]

Providing comparative data on published research impact (internally and externally) / Donna T. Wrublewski, Denise B. Bennett, Valrie I. Davis, Michelle Leonard (University of Florida) [[Slides from presentation](#)]

Social networking tools as public representations of a scientist / Antony J. Williams (Royal Society of Chemistry) [[Slides from presentation](#)]

Next era of research productivity evaluation: A multidimensional research assessment framework / Daniel Calto, Atyab Tahir (Elsevier) [[Slides from presentation](#)]

Measuring research: Beyond H / Daniel Hook (Symplectic Ltd.)

Methods and solutions for measuring and benchmarking the impact of research / Daphne Grecchi (Thomson Reuters) [[Slides from presentation](#)]

Bibliometrics

Bibliometrics (a set of methods to quantitatively analyze scientific and technological literature) have been known and used at least since the 1960's. All of the speakers cautioned against too heavy a reliance on any one bibliometric measurement, instead promoting a more comprehensive view of research output and impact. **Hook** pointed out that a measure like author h-index varies with the age and specific field of author, and tends to reward popular, but not necessarily good research. He also pointed out that stakeholders (like university administrators) like simplicity, but the usual metrics

generally lack context and tend to hide the underlying distribution of citations. While many scientists and librarians caution against too heavy a reliance on bibliometric measurements such as journal impact factor, author h-index and other indicators that reduce “value” to a single number, there is no doubt that university administrators rely on these types of measures to aid in making decisions about faculty tenure and promotion. **Wrubleski**¹ and **Brown** described approaches to providing an evaluation of research activities that are partially based on citations to work by individual faculty at their institutions. **Brown** cautioned that information from indexing and citation databases is just one of the “islands” of analytical data available, and needs to be combined with other sources of information, including research analytical/visualization tools and more informal measures of scholarship (e.g., social media profile). **Wrubleski et al.** first investigated various databases that provide citation information to determine which would best suit the need to evaluate a set of engineering faculty. The team considered both breadth and depth of subject coverage, types of research publications included in the database, and the comprehensiveness of coverage for citing/cited article references. SciFinder, Web of Science and Scopus were all considered, and a selection of a tool was made after weighing the strengths and weaknesses of each database. **Wrubleski** also provided some helpful tips and tricks for searching for citation data.

Tools for making sense of the metrics

Data analysis, presentation, and visualization are keys to extracting the most use out of bibliometrics and other research output and impact measures. **Brown** provided examples using various tools, including semantic clustering of institutions by research groups in SciVal, institutional comparison using InCites, and the presentation of publishing (books and articles), citations, awards, and grant funding in [Academic Analytics](#). **Tahir** provided in-depth exploration of the features of Elsevier’s [SciVal Spotlight](#) and [Strata](#). SciVal services are based on the concept of a “multi-dimensional research assessment framework” with different products addressing evaluation at different levels of the institutions. For example, SciVal Strata can help assess productivity/impact at the research group level. **Grecchi** provided information on a continuum of tools and services, ranging from out-of-the-box solutions to custom analytical reports like [InCites](#). Their bibliometrics refinements include methodology for normalizing citation impact across disciplines based on expected citation rates. [Research In View](#) is an institution-wide system that aggregates, standardizes, and links data from multiple sources and formats to provide a database and analytic interface for viewing, searching and reporting on faculty service, teaching, research expertise, and accomplishments. **Hook** presented in part on [Symplectic Elements](#), a research management system that includes data on faculty/researcher publications, professional activities, grants, equipment, projects, organizational structures and events.

The Role of Social Media

Several speakers addressed the emerging role of social media in research evaluation. **Brown** pointed out that researcher profile networks are becoming ubiquitous and that researchers are increasingly using social media like collaborative authoring sites/tools and conferencing in their work. **Hook** stated that traditional bibliometrics usually show the space in which the authors are

¹ Denise Beaubien Bennett, Michelle Leonard, Donna Wrublewski. “Comparing Engineering Departments Across Institutions: Gathering Publication Impact Data in a Short Timeframe,” *Issues in Science and Technology Librarianship*, Winter 2012. <http://www.istl.org/12-winter/refereed2.html>

publishing, not how important the papers are, but maybe where they feel their work best fits. **Williams** appeals to all scientists, particularly young scientists at the beginning of their careers, to develop their public face through social networking. While social networking activities are booming among scientists, it's not yet clear how we will be measuring the impact of research based on these various forms of social media. Several speakers mentioned the AltMetrics (<http://altmetrics.org/manifesto/>) site for discussion of new models of tracking impact of different types of scholarly publications (e.g., datasets, code, experimental designs, nanopublications, blogging).

What else?

When considering the construction of an institution-wide research evaluation, there is a wide variety of metrics that can be considered. Other measures that were mentioned by one or more presenters include institutional repository depositions, use of materials in institutional repositories (citations, links, and/or downloads), statistics collected for reporting and accreditation purposes and used for benchmarking in academic institutions (e.g., ACRL/NCES), research funding, patents granted, social bookmarking/sharing sites (e.g., Mendeley, CiteULike, etc.), blogs, levels of intra- and inter-institutional collaboration, technology transfer activities, publication of datasets and their subsequent use by others, faculty profile systems, and Twitter activity by scientists. **Tahir** observed that the future of research assessment lies in the intelligent combination of tools with peer review. Certainly there is no lack of data to feed the tools, but we do have to select the data that best answers the needs of the stakeholders who will use the information and insights generated through the use of research evaluation tools.

Final thoughts

There is no single metric that can or should be used to measure research impact. **Wrubleski** reminded us that we need to consider what our communities are asking for vs. what they really want. Anyone who is embarking on a project to evaluate research impact or value needs to be aware of all the commonly reported measures, understand the underlying methodologies on which each measure is based, and have a firm sense of the strengths and weaknesses of each approach. Institutional research evaluation should be thought of as a multi-faceted problem, and an assemblage of complementary data is needed to provide a more complete picture of any institution's research program. In the future, providing a comprehensive picture will probably require the use of less traditional measures of less traditional research output, like scientific blogging and other social networking activities. We will also have to balance the need for detail in the evaluation data with the resources required to assemble that data. Although there are tools that can help, the process can be both time consuming and expensive. Finally, the development of research evaluation metrics and frameworks need to be aligned with the goals of the institutions whose research programs are being studied and the needs of the stakeholders who will make use of the data.

Resources and readings

Elizabeth Brown's Social Disruption blog: <http://www.science3point0.com/socialdisruption/>

Sources from Brown's presentation:

Where is the library in the digital workflow of research? Research in the age of Social Media, Swets/Mendeley, 2012. <http://www.swets.com/Research-in-the-age-of-social-media-whitepaper>

Angela van Barneveld, Kimberly E. Arnold and John Campbell, Analytics in Higher Education: Establishing a Common Language, ELI Paper 1: January 2012. <http://www.educause.edu/Resources/AnalyticsinHigherEducationEsta/245405>

Using Bibliometrics: A Guide to Evaluating Research Performance with Citation Data, Thomson Reuters, 2008. <http://ip-science.thomsonreuters.com/news/2008-07/8465001/>

Co-Citation Analysis: The Methodology of SciVal Spotlight, Elsevier, June 2009. <http://www.info.scival.com/resource-library/white-paper-co-citation-analysis-methodology-scival-spotlight>

Kristen Fisher Ratan, Metrics: The New Black?, PLoS, NFAIS 2012. <http://www.slideshare.net/kristenratan/metrics-the-new-black>

Jennifer Howard, Tracking Scholarly Influence Beyond the Impact Factor, *Chronicle of Higher Education*, February 28, 2012. <http://chronicle.com/blogs/wiredcampus/tracking-scholarly-influence-beyond-the-impact-factor/35565>

Advanced Computing Infrastructure: Vision and Strategic Plan, National Science Foundation Cyberinfrastructure for 21st Century Science and Engineering (CIF21), February 2012. http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf12051

Paul Wouters and Rodrigo Costas, Users, Narcissism and Control – tracking the impact of scholarly publications in the 21st Century, SURF foundation, February 2012. <http://www.cni.org/news/surf-report-users-narcissism-and-control/>

Social Media and research workflow, CIBER, University College London, December 14, 2010. www.ucl.ac.uk/infostudies/research/ciber/social-media-report.pdf

Denise Beaubien Bennett, Michelle Leonard, Donna Wrublewski. “Comparing Engineering Departments Across Institutions: Gathering Publication Impact Data in a Short Timeframe,” *Issues in Science and Technology Librarianship*, Winter 2012. <http://www.istl.org/12-winter/refereed2.html>

Antony Williams’ ChemConnector blog <http://www.chemconnector.com/>

SURF report: Users, Narcissism and Control: Tracking the Impact of Scholarly Publications in the 21st Century <http://www.surffoundation.nl/nl/publicaties/Documents/Users%20narcissism%20and%20control.pdf>

Andrea Twiss-Brooks, Symposium Co-Organizer

Recorded content from six CINF symposia held at the Spring 2012 ACS National Meeting is at: <http://edmc.acs.org/Common/session.aspx/Spring2012/CINF>

Multidisciplinary Program Planning Group (MPPG)



Since its inception in 2007, thematic programming at ACS National Meetings has made large strides and most divisions recognize its importance by working closely together with the Thematic Program Chairs. Theme-related divisional symposia get additional exposure and advertising, thereby enhancing recognition of the respective divisions. Themes are now being developed by MPPG three years in advance, giving divisions sufficient time to organize symposia under the theme. Marketing of a given theme by the dedicated staff at ACS has vastly improved and has proved to be very successful. This was very much in evidence at the Spring National ACS Meeting in San Diego. The beautiful logo of the theme “Chemistry of Life” could be seen everywhere, at banners at the Convention Center and throughout town, on meeting programs and on flyers. One of CINF’s sponsored symposia, “Drug Polypharmacology Prediction and Design,” organized by Sean Ekins and Shuxing Zhang was one of five symposia highlighted on the official flyer giving CINF additional exposure.

The Thematic Program Chair, Peter Senter, VP of Seattle Genetics and Senior Editor, *Bioconjugate Chemistry*, put together a highly-successful program. The Plenary Symposium on Sunday afternoon in front of a large, standing-room-only audience featured four eminent speakers: Roger Tsien, Howard Hughes Medical Institute, lectured about “Molecules to image biology and disease in living color;” Samuel Stupp, Northwestern University, discussed “Chemistry for regenerative medicine;” Laura Kiesling, University of Wisconsin-Madison, described her research in her presentation on “Building the cell’s sugar coat;” and J. Craig Venter, J. Craig Venter Institute, talked about “From reading to writing the genetic code.” The large audience, made up to a large degree of young scientists, was treated to excellent and highly interesting presentations. Peter Senter also was involved in the selection of the lecturer for “Kavli Foundation Innovations in Chemistry” session. Carolyn Bertozzi’s, University of California Berkeley, presentation, again to a standing-room-only audience, was entitled “Bioorthogonal chemistry: Chemistry for life...literally.” These presentations together with the many outstanding divisional symposia addressing the theme “Chemistry of Life,” made for a highly successful National Meeting.

Now we are looking forward to Philadelphia in August where the theme of the meeting is “Materials for Health and Medicine.” Based on recent advances in molecular biology and genomics/proteomics that significantly influenced the design and application of biomaterials, the Philadelphia meeting again promises to be of high interest. The Thematic Program Chair, Xinqiao Jia, University of Delaware, is working with divisions to organize interesting interdisciplinary symposia. The speakers for the Plenary Session are: Jacqueline Barton, California Institute of Technology; Buddy Ratner, University of Washington; Chad Mirkin, Northwestern University; and John Santini, Jr., On Demand Therapeutics, Inc. The speaker of the Kavli lecture will be Robert Langer, MIT.

In 2013, the National ACS meetings will take place in New Orleans in Spring and Indianapolis in Fall. The themes for these meetings are “Chemistry of Energy and Food” organized by James Seiber, University of California Davis, and “Chemistry in Motion” organized by Robert Weiss, University of Akron. Preparations for these meetings are well under way. I will provide more details about the planned thematic programming after the Philadelphia meeting. Looking further ahead, the themes for 2014 have been approved, organizers have been selected and work has been

started. The 2014 meetings and themes are: Spring, Dallas with “Chemistry of Energy/Advanced Materials for New Opportunities,” and Fall, San Francisco with “Chemistry and Stewardship of the World.”

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

Future Thematic Programming at ACS National Meetings

Meeting	Dates	Theme	Organizer
Fall 2012 Philadelphia	August 19-23, 2012	Materials for Health and Medicine	Xinqiao Jia
Spring 2013 New Orleans	April 7-11, 2013	Chemistry of Energy and Food	James Seiber
Fall 2013 Indianapolis	September 8-12, 2013	Chemistry in Motion	Robert Weiss
Spring 2014 Dallas	March 16-20, 2014	Chemistry of Energy/ Advanced Materials for New Opportunities	to be announced
Fall 2014 San Francisco	August 10-14, 2014	Chemistry and Stewardship of the World	to be announced

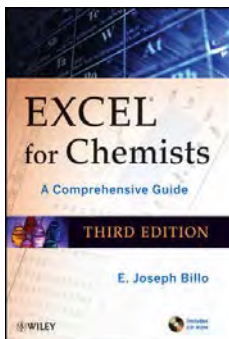
Join Us Again in Philadelphia



Registration & Housing for the Fall 2012 ACS National Meeting Open May 8

Image credit: <http://acswebcontent.acs.org/newsletter/SD2012/120413.html>

Two Brief Book Reviews



Billo, E. Joseph. *Excel® for Chemists: A Comprehensive Guide 3rd ed.*; John Wiley, Hoboken, US. \$59.95 (Softcover) 732 pp. ISBN: 978-0-470-38123-6.

Since I'm a spreadsheet "dummy," I was quite happy to review this book and have already put to use a reference. The 1st edition (1997) was reviewed in *J. Chem. Educ.* in 2000, but no reviews of subsequent editions have been published in ACS journals. Since the 2nd edition in 2001, three new versions of Excel for the PC have appeared: 2003, 2007, and 2010. This edition covers both the familiar 2003 version as well as the 2007/2010 versions.

New chapters have been added. Twenty three chapters are organized within five sections covering basics, advanced spreadsheet topics, spreadsheet math, Excel Visual Basic for applications (VBA), and applications of VBA. There are eleven appendixes and a CD that contains most of the worksheets in the text.

This excellent resource should be on the desktop of anyone using or creating scientific spreadsheets, not just for chemical applications.



Judson, Philip. *Knowledge-Based Expert Systems in Chemistry: Not Counting on Computers*; RSC Publishing: Cambridge, UK. £121.99 (Hardcover). 211 pp. ISBN: 978-0-85404-160-2.

This interesting book takes the reader on a foray into Artificial Intelligence (AI) whether the reader realizes that they've likely already been there. The cryptic subtitle becomes clearer in the introductory discussions of qualitative vs. quantitative results; the former may be more practical than the latter (including for QSAR). Knowledge-based systems don't discover rules; they just apply those that are input. Expert systems can generate their own models using statistical methods, but can't explain themselves. A waggish definition heard at a conference is "An expert system is one that gives the answers an expert would give, including the wrong ones." More than philosophical, most of the book describes practical programs in synthesis planning (LHASA, SECS, SYNGEN, etc.), structure representation (Wiswesser, Smiles, chemical markup, etc.), substructure searching (Morgan names, InChI, Markush, etc.), and predicting toxicity, metabolism, and biodegradation. The book closes with a discussion of the future, including assimilation of results and predictions, not only by scientists, but by the public.

The practical applications discussed illustrate the relevance of this book to the readers of *Chemical Information Bulletin* and related publications. Recommended.

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COMMITTEE REPORTS

CINF Education Committee

The CINF Education Committee met on Saturday, March 24, 2012, in San Diego, CA. The following items were discussed:

1) The committee reviewed its plans for current and future programming:

ACS National Meeting, San Diego: A symposium “Instructional Tools for Chemical Information” received eighteen submissions (one subsequently withdrawn) and was scheduled for morning and afternoon sessions on Sunday, March 25.

Biennial Conference on Chemical Education (BCCE), Penn State University, July 29-August 2, 2012: The committee has organized a symposium “Before and After Lab,” consisting of ten presentations and two panel discussions.



ACS National Meeting, Philadelphia, Fall 2012: Nothing specifically attached to the committee is scheduled. (Editor’s note: see other symposia below).

ACS National Meeting, New Orleans, Spring 2013: Symposia in the areas of interest to the Education Committee include: “What Chemists Need to Know about IP/Author Rights,” “Food Safety Information” (organizer: Andrea Twiss-Brooks), “Print Resources in the Electronic Era” (organizer: Grace Baysinger), “Library Spaces” (organizer: Andrea Twiss-Brooks), and “Public Chemistry Databases” (organizer: Antony Williams).

ACS National Meeting, Indianapolis, Fall 2013: Several possible symposium topics were proposed, including “Education for Cheminformatics” (suggested by the proximity of the Indiana University cheminformatics program (possible organizer: Jeremy Garritano), “Chemical Information for Small Teaching Colleges,” “Digital Archiving” (possible organizer: Andrea Twiss-Brooks), and a student-only session, whether poster or oral to be determined.

ACS National Meeting, Dallas, Spring 2014: Nothing planned at present.

Biennial Conference on Chemical Education (BCCE) 2014 will be held at Grand Valley State University, Allendale, MI. Ye Li (chemistry librarian at the University of Michigan) will be our local point person. We plan to organize at least one symposium, but no topics were proposed.

ACS National Meeting, San Francisco, Fall 2014: The committee will organize something for this meeting, but further discussion was deferred to the Philadelphia meeting, where the theme for the San Francisco meeting will be announced.

2) Information Competencies for Chemistry Undergraduates

The history of the document was reviewed. Plans for future publicity (Special Libraries Association 2012, BCCE 2012) were discussed, as well as suggestions to publicize it to the Association of

College and Research Libraries (ACRL) and the ACS Chemical Education Division (CHED). The team who prepared it hopes to review it annually, and call for suggestions for new sections.

3) Information Competencies for Chemistry Graduate Students

After considerable discussion, it was decided that we would work on a single document, with one general section applying to all graduate students, and several sections focusing on specific areas of chemistry. Among the topics we believed all graduate students needed familiarity with were: flow of information, scholarly communication (organization, copyright, open access, data management, mandates, ethics, titling publications, other publishing), searching techniques (including finding an expert in your field), staying up to date, patent literature, health and safety, finding commercial availability, impact metrics, grant process (e.g. PubMed Central IDs), and networking (professional organizations, social networking, mentoring and “chemical genealogies”).

Areas of chemistry meriting their own sections included: organic, inorganic and organometallic, physical chemistry/chemical physics, analytical, materials chemistry, polymer chemistry, nanoscience, biochemistry/biophysics/chemical biology.

4) Other topics

Grace Baysinger volunteered to fill the vice-chair (Assistant Chair) vacancy of the CINF Education Committee. A vice-chair for 2013 will be selected at the Philadelphia meeting. Terms for the current members were resolved. We decided to hold at least one virtual meeting between San Diego and Philadelphia, the method (Skype, Google+) for which will be explored.

The chair will contact Richard Love about having recordings of past CINF symposia presentations archived on the CINF site after they pass off the main ACS page.

Chuck Huber, Chair, CINF Education Committee

Other Philadelphia Symposia

What You Need to Know About the New U.S. Patent Laws (SCHB)	Jeffrey Bergman, bergman@oshaliang.com Carlyn Burton, burton@oshaliang.com
Mobile Devices, Augmented Reality, and the Mobile Classroom (DCHE)	Harry Pence, penche@oneonta.edu Antony Williams, antony.williams@chemspider.com
Communicating Chemistry and Public Engagement: Celebrating the 25th Anniversary of National Chemistry Week (PRES)	Bassam Shakhashiri, bassam@chem.wisc.edu
Chemistry Books Edited by E. F. Smith (HIST)	Ned Heindel, ndh0@lehigh.edu
Beyond the Bench: Non-Traditional Careers in Chemistry (CHAL)	Justin Hasford, justin.hasford@finnegan.com Krista Bianco, krista.bianco@finnegan.com
Young Investigator Awardee Forum: Views on Hot Topics in Research (COMSCI)	Tina Nenoff, tmnenof@sandia.gov

Report from the ACS Council Meeting

The Council of the American Chemical Society met in San Diego, CA on Wednesday, March 28, 2012 from 8:00am until approximately 12:00pm in the Marriott Hall of the San Diego Marriott Marquis & Marina 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 August 31, 2011, and approval of interim action by the Council Policy Committee to elect Carolyn Ribes as its Vice Chair. The highlights of the meeting are as follows:

Nominations and Elections

President-Elect: The Committee on Nominations & Elections (N&E) put forth for Council vote four nominees for the office of 2013 ACS President-Elect: Thomas J. Barton, Luis A. Echegoyen, William A. Lester, Jr., and Barry M. Trost. The four nominees answered questions at the Town Hall meeting that was held on Sunday, March 25th and each gave a three minute presentation at the Council meeting. Council voted to select Thomas J. Barton and Luis A. Echegoyen as the final two candidates whose names will appear on the fall ballot.

Other Elections

The Committee on Nominations and Elections announced the list of nominees to represent District I and District V on the Board of Directors for the term 2013-2015. Nominees for District I include Barbara J. Garrison, Thomas R. Gilbert, Neil D. Jespersen, and Julianne M. D. Smist. Nominees for District V are John E. Adams, Frank D. Blum, Peter K. Dorhout, and Frankie K. Wood-Black. Ballots have been mailed to Councilors in the two districts. The final ballots with two candidates for each district will be mailed on or before October 10 to all members in District I and District V for election of a Director from each District.

The Committee on Nominations and Elections also announced the selection of the following candidates for Director-at-Large for a 2013-2015 term: Carol A. Duane, Valerie J. Kuck, Bonnie Lawlor, and Ingrid Montes. The election of two Directors-at-Large will be conducted in the fall. Ballots will be mailed to the Council on or before October 10, 2012.

ACS Dues for 2013

Council voted to approve the recommendation from the Committee on Budget and Finance with regard to the 2013 membership dues (an increase of \$3.00 - from \$148 to \$151). The increases to ACS dues are based upon an escalator defined in the ACS Bylaws (Bylaw XII, Section 3,a). The dues are calculated by multiplying the base (current) rate "by a factor which is the ratio of the revised Consumer Price Index for Urban Wage Earners and Clerical Workers (Service Category) for the second year previous to the dues year to the value of the index for the third year previous to the dues year, as published by the United States Department of Labor, with the fractional dollar amounts rounded to the nearest whole dollar".

Base rate 2012: \$148.00

Change in the Consumer Price Index, Urban Wage Earners, Services Category:

December 2011 CPI-W Services:	262.954
December 2010 CPI-W Services:	257.382
Change in CPI-W Index:	2.16%

2013 Dues, fully escalated:	$\$148.00 \times 1.0216 =$	\$151.20
2013 Dues, Rounded:		\$151.00

Report from the Committee on Budget & Finance

Despite the sluggish economy, ACS generated strong operating results in 2011. Total revenue was \$472.0 million, up +1.8% over 2010. The Net from Operations was \$20.9 million, or \$7.7 million favorable to budget. This result was attributable to better-than-expected performance by the ACS Publications Division and careful expense management across the Society. While operating results were favorable, Unrestricted Net Assets declined from \$130.5 million to \$102 million. The decline was primarily due to a sizable accounting charge related to the Society's closed postretirement benefit plans. ACS ended the year in compliance with four of the five Board-established financial guidelines. The slides presented at the meeting can be accessed at:

http://portal.acs.org/portal/PublicWebSite/about/governance/committees/budget/CNBP_029717.

Change in Committees

After a regular performance review, the Committee on Committees (ConC) put forth a recommendation for the continuation of Project SEED and Council approved. The Committee on Project SEED sets policy for all Project SEED programs, including review of Project SEED I and II program applications for student research projects, funding decisions, and Project SEED college scholarship applications.

Approval of Chemical Professional's Code of Conduct

Council voted to accept the newest edition of the *Chemical Professional's Code of Conduct* (last revision was in 2007). The changes are minor. A statement that says "comply with safety policies and procedures" has been added to the section on the responsibilities of chemical professionals to their employers. In the section on responsibilities of chemical professionals to their employees, the wording now reads "respect the professionalism of their subordinates and have concern for their well-being..." Other minor changes address the environment and respect for colleagues despite their level of education and whether they come from government, academia or industry or from other scientific and engineering disciplines.

Meeting Attendance

As of the evening of Tuesday, March 27th, the spring national meeting had a total of 16,864 attendees as follows:

Regular:	8,933
Guests:	386
Students:	5,727
Exhibitors:	1,065

Exhibit-only: 753

Spring meeting attendance since 2004 is as follows:

2004: Anaheim, CA:	14,141
2005: San Diego, CA:	15,385
2006: Atlanta, GA:	12,546
2007: Chicago, IL:	14,520
2008: New Orleans, LA:	13,454
2009: Salt Lake City, UT:	10,668
2010: San Francisco, CA:	18,076
2011: Anaheim, CA:	14,047
2012: San Diego, CA:	16,864 (as of Tuesday, March 27 th)

A total of 11,716 papers were presented at the Spring 2012 meeting.

ACS Membership at Record Level

As of December 31, 2011, ACS membership totaled 164,215 - the highest number in ACS history. The Society lost 23,145 members, but gained 24,249 (16,092 Regular Members and 8,157 Undergraduate Members). There are 16,500+ student members in 1,000+ student chapters.

Chemistry Job Outlook

It was reported that as of March 1, 2012 the unemployment rate for chemists was 4.6% - the highest in 40 years! There were 943 job seekers at the job fair held at the conference. They were competing for 85 positions being offered by 31 employers. A virtual job fair held earlier attracted 2,673 job seekers and 14 employers. A column on career tips will be included in *Chemical & Engineering News* beginning in April.

Chemistry Teacher's Association Approved

The Society Committee on Education supported the recommendations from a task force to create a stand-alone association for chemistry teachers housed within ACS, supported by professional staff and governed by a volunteer board of association members.

Local Sections Reach Milestone Anniversaries

The following Local Sections are celebrating their 100th Anniversary in 2012: Detroit, Lexington, Maine, New Haven, Oregon and Rochester. The Orange County Local Section is celebrating its 50th Anniversary this year.

Petition on Market Data Collection

Council voted to approve a petition related to market tests for data collection. This petition seeks to add a provision to the ACS Constitution and Bylaws to allow for recommended controlled market

testing to collect data before the Society changes benefits, dues or membership categories. The Committee on Budget and Finance could not assess with reasonable accuracy the range of potential costs that would result from the implementation of this petition as they have no idea how many market tests may ultimately be conducted. The petitioners added additional wording that will impose limits on the size and length of tests. The wording is as follows:

“The Committee on Membership Affairs may conduct membership recruitment and retention market testing of SOCIETY memberships, services, and benefits, including special dues categories, to provide data as the basis for recommendations to the Council. The number of individuals included in any test related to dues discount shall not exceed a number equal to 10% of the total membership. Each test shall be limited to three years’ duration unless granted prior approval by Council. All test results will be reported to Council at least once a year.”

The Board of Directors will vote within 90 days on whether to ratify the approved petition.

Petition to Amend Recorded Vote Request Procedure

Council also voted to approve a change in wording to BYLAW III, Section 4, regarding recorded votes taken at Council meetings. The wording is as follows:

“Any member of Council may call for a recorded vote on the current action before the Council, other than an election, at any time before voting using a method from which it can be determined how each Councilor voted has commenced.”

This wording was introduced as Council now uses “clickers” for voting. The computer that totals the votes can list votes by clicker number from which it can be determined how each Councilor voted. The petition has no impact on the finances of the Society. The Board of Directors will vote within 90 days on whether to ratify the approved petition.

Petitions for Consideration Only

The following petitions were listed in the Council Agenda Book for consideration only. They will be voted upon at the 2012 fall meeting in Philadelphia, PA.

Petition on Candidate Comment in C&EN

The wording to BYLAW V, Section13 is recommended to have the following added:

“A candidate for election to the Board of Directors may not publish an ACS Comment in *C&EN* six months before the ballots are mailed for the corresponding election.”

This is to avoid an unfair campaign advantage to incumbents who may choose to make official statements on their task force or committee activities prior to elections.

Petition on International Chemical Sciences Chapters Funds

The proposed revised wording of BYLAW IX, Section 4, is as follows:

“An International Chemical Sciences Chapter shall receive no allotment of funds from the SOCIETY and shall not be entitled to elected representatives on the Council. However, the Board of Directors may allocate 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 financial implications of this petition are still being assessed.

Special Discussion Item

A special discussion item was put on the Council agenda for this meeting. ACS President Bassam Shakhshiri presented and moderated a discussion on “What is your reaction to the proposed topics for the ACS Climate Science Toolkit?” President Shakhshiri’s working group on ACS Climate Science has developed a preliminary web-based toolkit that ACS members can use as a resource for understanding and communicating basic climate science. Following the presentation, Councilors engaged in a robust discussion on the proposed toolkit, and offered numerous suggestions for consideration.

ACTIONS OF THE BOARD OF DIRECTORS

At this meeting, the ACS Board of Directors considered a number of key strategic issues and responded with several actions.

The Board’s Committees

The Committee on Grants and Awards presented the Board with a screened list of nominees for the 2013 Priestley Medal, Charles Lathrop Parsons Award, and the Award for Volunteer Service to the ACS. The Board VOTED to approve the screened lists, and will now vote on, and announce, the winners of these three awards after its June meeting. The Board also VOTED to approve a Society nominee for the National Medal of Science.

On the recommendation of the Committee on Executive Compensation, the Board VOTED to approve several actions relative to compensation for the Society’s executive staff. The compensation of the Society’s executive staff receives regular review from the Board of Directors.

The Executive Director/CEO Report

The Executive Director/CEO and several of her direct reports updated the Board on the activities of CAS (Chemical Abstracts Service), the ACS Publications Division, and the Society’s General Counsel.

ACS vs. Leadscope Litigation

The General Counsel report included a briefing on the ACS vs. Leadscope litigation. As previously reported, ACS has appealed to the Ohio Supreme Court, and the Court agreed to hear the case. Briefs have been filed in support of our position by several prestigious organizations, including the

Ohio Attorney General, the Ohio Chamber of Commerce, the Ohio Manufacturers' Association and the Ohio State Bar Association. On September 7, the Supreme Court heard oral arguments in the case, and a [link](#) to the arguments can be found on acs.org. A ruling has not been issued but could come at any time. A more detailed report appears in the most recent edition of the Councilor Bulletin. Please contact the Office of the Secretary if you would like a copy.

Other Society Business

The Board received the following:

A briefing on current virtual and hybrid meeting strategies using the Virtual Career Fair and Virtual Exposition. A report from the Committee on Professional Training-Committee on Education (CPT-SOCED) Task Force on the American Association of Medical Colleges and the Howard Hughes Medical Institute report *Scientific Foundations for Future Physicians*, wherein the CPT-SOCED task force is considering the implications of chemistry-related recommendations contained in the report. And a report from the President-Elect on plans and priorities during her presidential year; and a discussion on presidential succession budgets, particularly in light of increasing international and domestic travel demands.

The Board approved:

The 2015 Pacifichem budget and authorized reimbursement, on a pro rata basis, to the participating ACS Divisions for expenditures in support of the Pacifichem program and activities; changes to Board Regulations regarding the composition of the Planning Committee and the appointment of canvassing and award committees; a proposal to administer and present the AkzoNobel North American Science Award as recommended by the Committee on Grants and Awards; and proclamations recognizing the 100th Anniversary of the South African Chemical Institute and the 80th anniversary of the Chinese Chemical Society.

The Society's International Activities and its Open Session

The Board welcomed and received reports from several international guests representing the following scientific societies: the Canadian Society for Chemistry, the German Chemical Society, the Hungarian Chemical Society, the International Union of Pure and Applied Chemistry, the Mexican Chemical Society, and the Royal Society of Chemistry.

The Board held a lively, well-attended open session which featured a special forum on "The Future of Graduate Education and Research in the Chemical Sciences." Members attending this standing-room only session received an overview and update from the chair and executive director of the ACS Presidential Commission on Graduate Education in the Chemical Sciences. The commission is addressing two major questions: "What are the purposes of graduate education in the chemical sciences?" and "What steps should be taken to ensure that important societal issues, as well as the needs and aspirations of students, are addressed in graduate school?" Members discussed how the Society might offer greater assistance on this very important and timely topic.

ADDITIONAL INFORMATION

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

Safety

safety@acs.org: email address for sharing ideas on “How can ACS best cultivate a culture of safety in US universities and colleges?”

www.acs.org/safety: information on the Committee on Chemical Safety including “Creating Safety Cultures in Academic Institutions”

Employment/Careers

www.acs.org/careers: information on ACS career resources

www.acs.org/ei: information on the ACS Entrepreneurial Initiative (Training and Resources)

Local Section Resources

www.acs.org/getinvolved: grant information, important deadlines, officer resources

www.acs.org/forms: submit annual reports, record meetings, activities and events year round

speakers@acs.org: nominate speakers for the Online Speaker Directory

Other

www.acs.org/strategicplan: information on the new ACS Strategic Plan for 2012 and Beyond

www.acs.org/bulletin5: location of the Society’s governing documents and unit bylaws, and information on the petition process to amend the Society’s governing documents

bylaws@acs.org: email address for questions to the Committee on Constitution and Bylaws

www.acs.org/climatescience: information on the Climate Science Toolkit

Bonnie Lawlor and Andrea Twiss-Brooks, CINF Councilors

Council Committee on Nomenclature, Terminology and Symbols

The Committee continued to monitor developments in the redefinition of the SI (International System) Base Units. Of particular interest to the Committee and the SOCIETY are the redefinitions of the kilogram and the mole. The 24th quadrennial CGPM (General Conference on Weights and Measures) met in October, 2011. At the meeting, Resolution 1, “On the possible future revision of the International System of Units,” was adopted accepting the proposed “fixed constant” definitions and encouraging further cooperation on their development.

It remains for CODATA (The Committee on Data for Science and Technology) to publish the best, accepted values for the Planck constant (defining the kilogram) and the Avogadro constant (defining the mole). Once available, the fixed values of the constants will be inserted in to the definitions that will be presented for adoption by the next CGPM to be held in 2015.

The Committee has continued its reflections upon and consideration of its duties and how they may be more actively pursued.

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

Highlights from the Joint Board Council Committee on Publications

The Joint Board-Council Committee on Publications (JBCCP) assesses the editorial quality and content of the publication program of the Society; serves as a channel among Society members, users of the Society's publications, and the ACS governing bodies; advises on copyright policy and recommends actions to protect ACS copyright. Leah Solla, also CINF Secretary (2010-2014), is a member of JBCCP and the associated Copyright Subcommittee and the *Chemical and Engineering News* Editorial Board. Highlights of the open portion of the publications committees at the 243rd National Meeting in San Diego are summarized below:

- In 2011 ACS Editors-in-Chief handled nearly 100,000 manuscript submissions through the editorial peer review process and ACS Publications published more than 36,000 accepted articles. In 2011 the global scientific community accessed and downloaded a record 77 million COUNTER-compliant full-text downloads from the ACS Publications Web Editions platform, an 8% growth over 2010.
- Improvement of ACS branding and impact at the ACS National Meetings included a combined ACS Central booth featuring 11 separate ACS units, including ACS Publications, Chemical Abstracts Service, and Membership & Scientific Advancement. In total, ACS Publications exhibited at 55 scientific and library conferences in 2011.
- The “Why I” campaign focused on using real customer testimonials and images to help engage the community and echo the voices of actual researchers reinforcing ACS Publications' leadership position.
- A new educational, web-based video series is designed to support researchers with the process of writing, reviewing, submitting and editing original scholarly research for publication in peer reviewed articles. Episodes released in 2011 include:
 - ***How to Write a Paper to Communicate Your Research***, Prof. George Whitesides (Harvard)
 - ***Writing your Cover Letter***, Prof. Paula Hammond (MIT & Assoc. Editor *ACS Nano*); Prof. Tim Lodge (Univ. Minnesota & Editor-in-Chief, *Macromolecules*), *et al*
 - ***Selecting Peers to Suggest to Reviewers***, Prof. Richard Eisenberg (University of Rochester & Editor in Chief, *Inorganic Chemistry*), *et al*
 - ***Submitting your Manuscript using the ACS Paragon Plus Environment***, Dr. Sarah Tegen (Director Editorial Operations, ACS Publications)
- The development and publication of five new journals, including *ACS Catalysis* and *ACS Medicinal Chemistry Letters* in 2011 and early editorial and marketing launch of *ACS Macro Letters* and *ACS Synthetic Biology* (formal launch in 2012) was reported. Approval was secured from the Governing Board for a new journal in the area of green chemistry and sustainability, planned for publication in 2013.



A number of new subscription assortments and pricing plans were introduced, including *ACS Lab Packs*, the *ACS Academic Core+*, the *ACS Metered Access Program*, and streamlining of *ACS Articles/Issues on Command*.

- Leading scientists were selected by Editor Search committees in accordance of the bylaws, appointed by the Board of Directors and contracted by ACS Publications management:
 - **Jonathan Sweedler**, University of Illinois Urbana Champaign, new Editor of *Analytical Chemistry*;
 - **Chris Voigt**, Massachusetts Institute of Technology, new Editor of *ACS Synthetic Biology*;
 - **Gunda Georg**, University of Minnesota, and **Shaomeng Wang**, University of Michigan, new Co-Editors of *Journal of Medicinal Chemistry*.
- ACS Publications worked closely with JBCCP in undertaking formal editorial monitoring studies and reports for journals across the ACS portfolio, and deliberated regarding several editorial reappointments and recommendations to the ACS Board.
- The “**Most Trusted**” brand was enhanced by joining the Committee on Publishing Ethics (COPE) to provide all ACS Editors-in-Chief and Publications Staff access to a network of like-minded editors and publishers to discuss ethical issues and fully utilize the Committee’s guidelines for handling ethical disputes; pilot implementation of *CrossCheck*, a cross-publisher initiative to detect plagiarism in journal articles as part of the peer review and publication process; and updating the ACS Publications “Ethical Guidelines to Publication of Chemical Research.”
- The mobile program to the Android environment was extended. ACS Mobile now delivers about 50,000 abstract downloads and 7,500 *C&EN* news feeds a month with the 10,000+ user base. A free dedicated *C&EN* Mobile app was also introduced for iPhones, iPads, and Android mobile devices. Subscription access to *C&EN* content via *C&EN* Mobile is a new, free ACS member benefit; members can access all new *C&EN* issues on their smartphone or tablet at no charge.
- Completion of the first phase of the *C&EN* Publishing Automation Program (CPAP 1.0) to create a digital, end-to-end workflow, including rendering all *C&EN* content in high-quality XML. Introduction of the **Biological SCENE** and the **Materials SCENE**, two new syndication channels to provide content from *C&EN* and papers in ACS journals. *C&EN*’s twitter feed (@cenmag) has more than 3,600 followers. *C&EN*’s Facebook page (<http://facebook.com/cenews>) added 1,207 “likers” this year, bringing the total to nearly 3000.
C&EN’s YouTube channel (<http://www.youtube.com/cenonline>) contains about 100 *C&EN*-created videos and has received more than 122,500 views altogether; the videos are embedded by other major media outlets, such as the *Wired* and *BoingBoing* blogs.

- ACS Publications celebrated the International Year of Chemistry (IYC) with publication of the *ACS International Year of Chemistry Virtual Journal* with other ACS offices and programs, highlighting health, environment, energy and materials research from a number of ACS Publications. The journal published 12 issues in 2011 and received approximately 10,000 downloads.



C&EN contributions included:

- The cover story of the June 27, 2011 issue, “Celebrating IYC 2011”;
 - Series of “IYC Profiles” of ACS members native to foreign countries where there are very few ACS members, including Cuba, Fiji, Lebanon, Burkina Faso, Moldova, Azerbaijan, Vietnam, Ghana, Mauritius, Bosnia, Mongolia, and Honduras;
 - The CENtral Science IYC 2011 blog, which chronicled events associated with the celebration throughout the year.
- ACS Publications worked closely with CAS to experiment with a number of features that utilize and expose CAS SciFinder tools within the ACS Web Editions platform, and vice versa:
 - **Patent Limiter** allows users to launch a SciFinder patent-only search within any of the journal or eBook articles on the ACS Web Editions site.
 - **CAS Section Subject Index** allows users to search, browse and discover content with CAS subject taxonomy on the ACS Web Editions site.
 - **ACS Reference Quick view** allows users to quickly access multiple publisher article abstracts and metadata for references found in ACS journal articles without leaving the ACS Web Editions platform.
 - **CAS SciFinder** allows users to display a graphical abstract and table of contents elements from ACS Journals within CAS records, and to easy access reaction narratives and other experimental procedures from selected journals.
 - A new ACS Member Subscription Benefit program offers every ACS member immediate and universal access to the entire portfolio of ACS’s journal and book publications, including access to the ACS Legacy Archive and the recently released *C&EN Archive*. 25 full-text articles may be downloaded annually by each member. End-users can also register for ACS IDs to opt in to a range of content and news alerts. There are more than 166,000 ACS ID registrants, up 30% over 2010, and less than 25% of these are paid ACS members, making this cohort an attractive audience to whom the benefits of ACS membership can be promoted.

For more information or to contact JBCCP, please see:

<http://portal.acs.org/portal/PublicWebSite/about/governance/committees/jbccp/index.htm>

Leah Solla, Member, Joint Board Council Committee on Publications

CINF Social Networking Events

The Division of Chemical Information was pleased to host the traditional CINF social networking events at the ACS National Meeting in San Diego, California. The division depends on generous contributions by our sponsors to support symposia and social gatherings where the chemical information community gathers to converse, connect, and celebrate. Fun photos from the CINF events are at <http://www.flickr.com/photos/cinf>.

The **CINF Sunday Welcome Reception** was supported by four repeat sponsors joining an exceptional blend of about 100 chemical information devotees from the extended continuum of CINF activities. The group rubbed elbows while nibbling delicious fare and engaging in friendly chat to kick off the San Diego meeting. Many thanks to our reception supporters: **ACS Symposium Series**, **InfoChem**, **Thieme Publishers**, and the *Journal of Chemical Information and Modeling*. The **CINF Scholarships for Scientific Excellence** poster session at the Sunday Reception featured a record sixteen poster presenters. Our generous sponsor, **Accelrys**, provided two \$1,000 scholarships to our poster winners, David R. Fooshee from the Institute for Genomics and Bioinformatics, University of California Irvine, and Freya Klepsch from the University of Vienna. Please let your students and interns know about future scholarships <http://www.acscinf.org/awards/sciexcel.php>.

Harry's Party, again hosted by **FIZ CHEMIE Berlin** on Monday evening, reunited the CINF kindred in a view suite at the Manchester Grand Hyatt. About 70 CINF functionaries, friends and family enjoyed a beautiful view of San Diego; and snacks, drinks and conversation with familiar and fresh friends. If you missed Harry's Party in San Diego, please join us in Philadelphia this fall.

The **CINF Tuesday Luncheon** provided delicious fare and an educational wine tasting to about 60 diners who were educated by Dr. Kirsten Skogerson, an Analytical Biochemist at Monsanto and PhD holder from the UC Davis Department of Viticulture & Enology. Dr. Skogerson presented on "*The Chemistry of Wine*" covering chemical interactions at all stages of wine making with commentary on the complimentary wine tasting of selected California Cabernet Sauvignon and White Zinfandel. This informative event was made possible through the exclusive sponsorship of **RSC Publishing**.

The **CINF Tuesday Reception in support of the CINF InChI Symposium** was attended by almost 100 CINF members and affiliates in the Manchester Grand Hyatt. The occasion of the *CINF InChI Symposium* on Wednesday added a diverse group of open-access aficionados to the reception mix for informative discussions. CINF thanks the **ACS Division of Chemical Information**, **Accelrys**, **ChemAxon**, **PerkinElmer** and *Nature Communications* for teaming up to support this event.

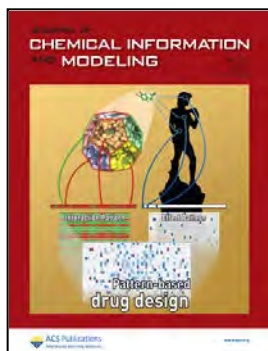
In addition, speaker support for the *Computer-Aided Drug Design* symposium was provided by the **Chemical Computing Group**, **OpenEye**, and **SimBioSys**. Speaker support for the *CINF InChI Symposium* was also provided by the **InChI Trust**.

The ACS Division of Chemical Information 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, Fundraising Committee

SPONSOR ANNOUNCEMENTS

News from the *Journal of Chemical Information and Modeling*

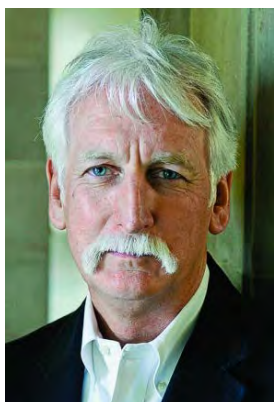


The *Journal of Chemical Information and Modeling* (JCIM) publishes papers reporting new methodology and/or important applications in the fields of chemical informatics and molecular modeling. Specific topics include the representation and computer-based searching of chemical databases, molecular modeling, computer-aided molecular design of new materials, catalysts, or ligands, development of new computational methods or efficient algorithms for chemical software, and biopharmaceutical chemistry including analyses of biological activity and other issues related to drug discovery.

To learn more about *Journal of Chemical Information and Modeling* please visit the journal website at pubs.acs.org/jcim

[View a free sample issue of the journal](#)

JCIM Editor-in-Chief Wins Award

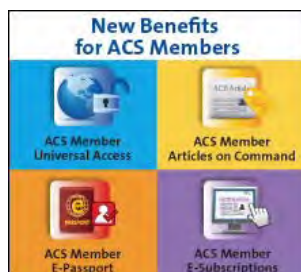


William L. Jorgensen, a Sterling Professor of Chemistry at Yale University, was the recipient of the Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids.

Jorgensen has been a key figure during chemistry's dramatic computational evolution over the past few decades. In 2004, he became editor of what was then the American Chemical Society's *Journal of Chemical Information & Computer Sciences*, which he split into two separate publications: the chemical-informatics-focused [Journal of Chemical Information & Modeling](#) and the [Journal of Chemical Theory & Computation](#), which focuses on computational chemistry.

Jorgensen presented the award address before the ACS Division of Physical Chemistry at the Spring ACS National meeting, March 27, 2012.

[Read more](#) in *Chemical & Engineering News*, [90\(7\)](#), February 13, 2012



Expanded Access to ACS Journals

ACS members now have expanded access to over 1 million articles and book chapters from ACS publications. This new benefit is offered exclusively to ACS members.

[Read more about new benefits for ACS Members](#)

SPRESImobile App successfully released



InfoChem is pleased to announce the successful release of the SPRESImobile App in March. This new App for iPhone, iPod touch, and iPad enables users to perform structure and reaction searches on their mobile devices. The App, developed in cooperation with [Eidogen-Sertanty](#), can be downloaded free of charge on iTunes (<http://itunes.apple.com/app/spresimobile/id505308290?mt=8>).

The free App gives access to approx. 400,000 unique chemical reactions, a subset of the SPRESI reaction data ([ChemReact](#)). With SPRESImobile, InfoChem is one of the first companies supporting reaction searches on mobile devices.

For more information about SPRESI^{web} click [here](#) or visit www.spresi.com.

InfoChem Raffle during the ACS Exhibition in San Diego

The puzzle quiz organized together with [Thieme](#) and [Oakwood Chemicals](#) during the Exhibition at the ACS Meeting in San Diego has a winner. Chelsea Modafferi from the College of Mount Saint Vincent in New York is the happy owner of a brand new iPad 3.

Please feel free to [contact us](#) for more information about InfoChem, our current research projects and our products.



Photos from the Spring 2012 ACS National Meeting are at <http://www.flickr.com/photos/cinf/>

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