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Message from the Chair



Ah, New Orleans...the culinary delights, the gentle climate, the incredible opportunities to engage in the music scene, the people-watching possibilities of Bourbon Street and, let's face it, an *excellent* venue for an ACS meeting and all that CINF programming has to offer. In my short stay in the Division Chair seat I was proud to have been associated with the first of two ACS meetings. A rich and varied program packed into the week drew speakers and attendees from around the world. Our social events, despite a couple of minor hurdles, were ideal for networking, for catching up with old friends and colleagues, and for launching spirited efforts to grow our membership and reinvigorate our mission.

The invitation of a science comedian to the CINF Luncheon and to lead a session on communicating science brought to light not only how much fun science can be, but for me, the spirit of camaraderie that I feel exists across our Division. We are, one and all, concerned with, excited by, and driven to excellence in our field of expertise. So, a great conference...hopefully, you all agree.

On Saturday evening as the conference was just beginning to kick off in earnest we hosted a CINF event to garner input regarding what would help to keep us relevant, how we could expand our membership, and what we could do to grow our stature and impact. During a wonderful dinner each table was hosted by a moderator through the discussions and we left with a lot of feedback. There were some common themes: CINF is a wonderful Division to be a member of, we need to do more outside of our Division to encourage participation and engagement, and we clearly have lots of passionate people willing to share their input and energy towards helping to make CINF successful. More will follow on our actions moving forward as we distil down the outcomes from the gathering.

In New Orleans I did take the opportunity to speak in a Division of Chemical Education symposium, and after the presentation I was encouraged to make sure that CINF collaborated more with CHED. I learned a lot about their challenges and shared our activities. I think this is a common situation that we often speak within our own Division whereas so many of our users, customers, and those with the most to gain from our work are actually elsewhere in the ACS conference. I encourage you to think about speaking outside CINF at future ACS Meetings. Our relevance, stature and impact as scientists and contributors to the field of chemical information will likely increase as we share our skills outside of our existing circles and instill more interest in what we have to deliver in our field of expertise and in our Division. We have put additional work into the Indianapolis meeting to ensure co-sponsored programming with the hope that this seeds our outreach effort.

Looking forward to the next meeting in Indianapolis we have much to do. What culminates in a hectic week of activity at the ACS Meeting sits on the shoulders of a number of committees and dedicated individuals within the Division. Yes, it is work, but it is very rewarding to be a part of a team and feel partly responsible for delivering to the meeting. We are also actively working on improving access to our activities via the CINF website (<http://www.acscinf.org>) and supporting efforts in providing teaching resources for chemical information via the XCITR website (<http://www.xcitr.org>). While in New Orleans we did ask "What do you need from your Division?" I encourage you to consider "What does your Division need from you?" We need you to spread the word about CINF, encourage people to view our webinars and learn about what is new in our domain, encourage membership, participate in the programs, step up and volunteer for the committees, and be vocal about the importance of chemical information. We need you!

Antony Williams, Chair, ACS Division of Chemical Information

Letter from the Editor

Welcome to the all-around post-conference issue of the *Chemical Information Bulletin*. This issue covers a wide spectrum of the Division's activities at the most recent Spring 2013 ACS National Meeting - ranging from highlights of the impressive CINF technical program and including full reports of seven symposia, to the "bright future" of the ACS thematic program planning, from brief student scholarship winner announcements and calls for award nominations, to the detailed committee and ACS Council reports, from book reviews of "alternative information aspects of chemistry" to sponsor announcements featuring their new products. Hopefully, the readers of this Bulletin can benefit in all respects from the experiences of the meeting attendees who were willing to share their expertise, not only at the meeting, but also to write their timely reports to this publication (47 pages).



In the opening *Message from the Chair*, Antony Williams stresses that New Orleans is "an excellent venue for an ACS meeting and all that CINF programming has to offer" and the "great success of the conference" is observed by many submissions throughout this issue. Speaking of numbers and reviewing national meeting data of CINF since 2006, New Orleans 2013 saw the third highest number of CINF presentations - 124 plus lightning talks at a Spring Meeting (2010 San Francisco - 158, 2012 San Diego - 133). The previous Spring 2008 New Orleans Meeting also saw a peak of CINF presentations - 114. (Note: no location or a change of seasons could beat San Francisco. CINF usually sees more presentations, but fewer members attending, at Spring than at Fall National Meetings in the same year. This trend could be explained by the programming focus on the Herman Skolnik Award Symposium in Fall).

In the news from Multidisciplinary Program Planning Group, Guenter Grethe emphasizes that "unquestionably, part of the success was due to the location, but an excellent program with the theme **Chemistry of Energy and Food**, fittingly selected by MPPG for New Orleans, certainly played an important role." The CINF symposium *Foodinformatics: Applications of Chemical Information to Food Chemistry* organized by Jose Medina-Franco and Karina Martinez Mayorga was part of the ACS Meeting theme. Their symposium overview is included in this Bulletin, as well as those of six other symposia, namely, *Library Cafes, Intellectual Commons and Virtual Services, Oh My! Charting New Routes for Users into Research Libraries* by Teri Vogel, *Scholarly Communication: New Models, New Media, New Metrics* by David Martinsen, *Food for Thought: Alternative Careers in Chemistry* by Patricia Meindl, *Public Databases Serving the Chemistry Community* by Sean Ekins and Antony Williams, *Advances in Virtual High-Throughput Screening* by Sean Ekins and Joel Freundlich, and *Computational De Novo Protein and Peptide Design* by Rachelle Bienstock.

In conclusion, I would like to thank all authors for their generous contributions to this issue. Many thanks to Mark Luchetti for designing the cover page, to Farai Tsokodayi for providing national meeting data of CINF, to Bonnie Lawlor and Wendy Warr for proofreading this issue, to Danielle Dennie for putting it on the website, and to Wendy Warr for taking photographs at the New Orleans Meeting (<http://www.flickr.com/photos/cinf/>).

Svetlana Korolev, Editor, Chemical Information Bulletin

AWARDS AND SCHOLARSHIPS

2013 Lucille M. Wert Student Scholarship



Kristin Briney, holder of a Ph.D. in physical chemistry from the University of Wisconsin where she is currently pursuing an M.A. in library and information science, has been selected as the 2013 recipient of the Lucille M. Wert Student Scholarship. The award is for \$1500 to “help persons with an interest in the fields of chemistry and information to pursue graduate study in library, information, or computer science.” Kristin plans to combine her scientific background with her knowledge of library and information science to tackle challenges in the burgeoning field of data curation.

Andrea Twiss-Brooks, Chair, CINF Awards Committee

2014 Herman Skolnik Award Nominations: Deadline Reminder

The deadline for nominations for the 2014 Herman Skolnik Award is JUNE 1, 2013.

The ACS Division of Chemical Information established the Herman Skolnik Award to recognize outstanding contributions to and achievements in the theory and practice of chemical information science. The Award is named in honor of the first recipient, Herman Skolnik. By this Award, the Division is committed to encouraging the continuing preparation, dissemination and advancement of chemical information science and related disciplines through individual and team efforts. Examples of such advancement include, but are not limited to, the following:

- Design of new and unique computerized information systems;
- Preparation and dissemination of chemical information;
- Editorial innovations;
- Design of new indexing, classification, and notation systems;
- Chemical nomenclature;
- Structure-activity relationships;
- Numerical data correlation and evaluation;
- Advancement of knowledge in the field.

The Award consists of a \$3000 honorarium and a plaque. The recipient is expected to give an address at the time of the Award presentation.

For more information including the nomination procedure and a list of previous honorees, please visit <http://www.acscinf.org/content/herman-skolnik-award>.

Nominations for the Herman Skolnik Award should be sent to Andrea Twiss-Brooks by email (atbrooks@uchicago.edu) prior to June 1, 2013.

Andrea Twiss-Brooks, Chair, CINF Awards Committee

2013 CINF Scholarship for Scientific Excellence

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) is designed to reward graduate and post-graduate students in chemical information and related sciences for scientific excellence and to foster their involvement in CINF. The program has awarded scholarships at each of the ACS National Meetings since 2005 and has made 47 awards in total. The awards at the Spring 2013 National Meeting in New Orleans were sponsored by Accelrys.

Applicants presented their posters at the CINF Welcoming Reception and the Sci-Mix session. Two scholarships valued at \$1,000 each were presented by Dr. Keith Taylor of Accelrys to the winners at the CINF Luncheon during the same meeting.

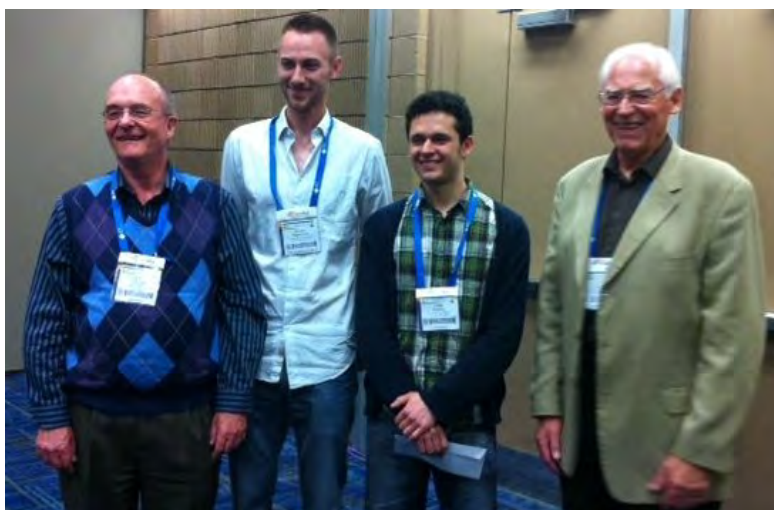
The names of the recipients and the titles of their posters were:

Julian C. Thibault, University of Utah, Department of Biomedical Informatics, Salt Lake City, UT, *iBiomes: Managing and sharing large biomolecular simulation datasets in a distributed environment with iRODS*.

Co-authors: Thomas Cheatham III, Julio C. Facelli

Amir Seddik, University of Vienna, Department of Medicinal Chemistry, Vienna, Austria, *Probing the substrate selectivity of the serotonin and dopamine transporter using structure-based techniques*.

Co-authors: Harald H. Sitte, Gerhard F. Ecker



Keith Taylor, Julian Thibault, Amir Seddik, Guenter Grethe

The next scholarships are sponsored by the Royal Society of Chemistry and will be awarded at the 2013 Fall ACS National Meeting in Indianapolis, IN.

Guenter Grethe, Coordinator, CINF Scholarship for Scientific Excellence



Chemical Structure Association Trust Grant: Applications Invited for 2014

The Chemical Structure Association (CSA) Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program and is currently inviting the submission of grant applications for 2014.

Purpose of the Grants:

The Grant Program has been created to provide funding for the career development of young researchers who have demonstrated excellence in their education, research or development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and compounds. Grants will be awarded annually up to a maximum of a total combined value of ten thousand U.S. dollars (\$10,000). Grants are awarded for specific purposes, and within one year each grantee is required to submit a brief written report detailing how the grant funds were allocated. Grantees are also requested to recognize the support of the Trust in any paper or presentation that is given as a result of that support.

Who is Eligible?

Applicant(s), age 35 or younger, who have demonstrated excellence in their chemical information related research and who are developing careers that have the potential to have a positive impact on the utility of chemical information relevant to chemical structures, reactions and compounds, are invited to submit applications. While the primary focus of the Grant Program is the career development of young researchers, additional bursaries may be made available at the discretion of the Trust. All requests must follow the application procedures noted below and will be weighed against the same criteria.

Which Activities are Eligible?

Grants may be awarded to acquire the experience and education necessary to support research activities; e.g. for travel to collaborate with research groups, to attend a conference relevant to one's area of research, to gain access to special computational facilities, or to acquire unique research techniques in support of one's research.

Application Requirements:

Applications must include the following documentation:

1. A letter that details the work upon which the Grant application is to be evaluated as well as details on research recently completed by the applicant;
2. The amount of Grant funds being requested and the details regarding the purpose for which the Grant will be used (e.g. cost of equipment, travel expenses if the request is for financial support of meeting attendance, etc.). The relevance of the above-stated purpose to the Trust's objectives and the clarity of this statement are essential in the evaluation of the application);

3. A brief biographical sketch, including a statement of academic qualifications;
4. Two reference letters in support of the application. Additional materials may be supplied at the discretion of the applicant only if relevant to the application and if such materials provide information not already included in items 1-4. Three copies of the complete application document must be supplied for distribution to the Grants Committee.

Deadline for Applications:

Applications must be received no later than March 13, 2014. Successful applicants will be notified no later than May 2, 2014.

Address for Submission of Applications:

Three copies of the application documentation should be forwarded to: Bonnie Lawlor, CSA Trust Grant Committee Chair, 276 Upper Gulph Road, Radnor, PA 19087, USA. If you wish to enter your application by e-mail, please contact Bonnie Lawlor at blawlor@nfais.org prior to submission so that she can contact you if the e-mail does not arrive.

Previous Grant Awardees:

2012

Tu C. Le: CSIRO Division of Materials Science & Engineering, Clayton, VIV, Australia. Tu C. was awarded the Grant for travel to attend a Cheminformatics course at Sheffield University and to visit the Membrane Biophysics group of the Department of Chemistry at Imperial College London.

2011

J. B. Brown: Kyoto University, Kyoto, Japan. J.B. was awarded the Grant for travel to work with Professor Ernst Walter-Knapp at the Freie University of Berlin and Professor Jean-Phillipe Vert of the Paris MinesTech to continue his work on the development of atomic partial charge kernels.

2010

Noel O'Boyle: University College Cork, Ireland. Noel was awarded the grant to both network and present his work on open source software for pharmacophore discovery and searching at the 2010 German Conference on Cheminformatics.

2009

Laura Guasch Pamies: University Rovira & Virgili, Catalonia, Spain. Laura was awarded the Grant to do three months of research at the University of Innsbruck, Austria.

2008

Maciej Haranczyk: University of Gdansk, Poland. Maciej was awarded the Grant to travel to Sheffield University, Sheffield, UK, for a 6-week visit for research purposes.

2007

Rajarshi Guha: Indiana University, Bloomington, IN, USA. Rajarshi was awarded the Grant to attend the Gordon Research Conference on Computer Aided Design in August 2007.

2006

Krisztina Boda: University of Erlangen, Erlangen, Germany. Krisztina was awarded the Grant to attend the 2006 spring National Meeting of the American Chemical Society in Atlanta, GA, USA.

2005

Val Gillet and Peter Willett: University of Sheffield, Sheffield, UK. They were awarded the Grant for student travel costs to the 2005 Chemical Structures Conference held in Noordwijkerhout, the Netherlands.

2004

Sandra Saunders: University of Western Australia, Perth, Australia. Sandra was awarded the Grant to purchase equipment needed for her research.

2003

Prashant S. Kharkar: Institute of Chemical Technology, University of Mumbai, Matunga, Mumbai. Prashant was awarded the Grant to attend the conference, Bioactive Discovery in the New Millennium, in, Lorne, Victoria, Australia (February 2003) to present a paper, The Docking Analysis of 5-Deazapteridine Inhibitors of Mycobacterium avium complex (MAC) Dihydrofolate reductase (DHFR).

2001

Georgios Gkoutos: Imperial College of Science, Technology and Medicine, Dept. of Chemistry, London, UK. Georgios was awarded the Grant to attend the conference, Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, (CMTPI-2001) in Bordeaux, France, to present part of his work on internet-based molecular resource discovery tools.

TECHNICAL PROGRAM

CINF Technical Program Highlights

I would like to thank all of the organizers, speakers, and poster presenters who contributed to the New Orleans Meeting. I heard many compliments throughout the week and hope those that attended were as equally impressed with the session line-ups as I was. I would also like to thank the many CINF sponsors whose contributions enhance our Division programming. I hope you will take the opportunity to read the various symposium reports in this issue that have been submitted by some of our New Orleans organizers.



Two of our sessions were recorded as part of the ACS Presentations on Demand program and will be made available to registered attendees soon (<http://presentations.acs.org/common/default.aspx>). The sessions were:

- Linking Bioinformatic Data and Cheminformatic Data
- Scholarly Communication: New Models, New Media, New Metrics

Looking forward to Indianapolis

As I am finishing the scheduling of symposia for the Meeting in Indianapolis this fall, we have another wide-ranging program of over 100 presentations in addition to 18 posters designated for Sci-Mix. A major highlight will be the Herman Skolnik Award Symposium in honor of Dr. Richard “Dick” Cramer on Tuesday, September 10, 2013. The symposium will proceed as follows:

Morning session **R. Cramer**, *Organizer*, **B. Masek**, *Presiding*

8:30 Introductory Remarks

8:35 Adventures in CoMFAland. **R. D. Clark**

9:05 Adventures in drug discovery: For now we see through a glass, darkly. **R. C. Glen**

9:35 Three paradigm shifts in computer-assisted drug design: The inventors and by-standers. **Y. C. Martin**

10:05 Intermission

10:20 Look back at 3D-QSAR and Dick Cramer. **A. J. Hopfinger**

10:50 Evolution of QSAR from regression analysis to physical modeling. **A. N. Jain**

11:20 Scientific analysis of baseball performance. **D. W. Smith**

Afternoon session **R. Cramer**, *Organizer*, **T. Stouch**, *Presiding*

2:00 Introductory Remarks

2:05 Synthesis planning: Something about reactions, representation, relationships, and reasoning. **W.T. Wipke**

2:35 Think local, act global: Some challenges in cheminformatics and drug research. **T. I. Oprea**

3:05 Intermission

3:20 From library design to off-target prediction: A wide array of topomer applications. **B. Wendt**

3:50 Whole template CoMFA: The QSAR grail? **R. D. Cramer**

4:35 Award Presentation.

Proposed CINF Program for the Fall 2013 ACS National Meeting

Back to the Future: Print Resources in a Digital World	Grace Baysinger graceb@stanford.edu
Before and After Lab: Instructing Students in 'Non-chemical' Research Skills	Andrea Twiss-Brooks atbrooks@uchicago.edu Charles Huber huber@library.ucsb.edu
Chemistry on Tablet Computers	David Martinsen d_martinsen@acs.org Martin Braendle braendle@chem.ethz.ch
CINF Scholarship for Scientific Excellence	Guenter Grethe ggrethe@att.net
Computational Profiling and Repositioning as Promising New Ways of Drug Development	Andrew Hopkins andrew.lee.hopkins@mac.com Violeta Isabel Perez Nueno pereznueno@harmonicpharma.com
Current Challenges in Cheminformatics: Exploiting Information and Knowledge in Structured and Unstructured Environments	Neil Kirby nkirby@dow.com Dirk Tomandl FreddieM007@gmx.de
Exchangeable Molecular and Analytical Data Formats and Their Importance in Facilitating Data Exchange	Antony Williams tony27587@gmail.com Robert Lancashire robert.lancashire@uwimona.edu.jm
General Papers	Jeremy Garritano jgarrita@purdue.edu
Graduate Student Research Symposium in Cheminformatics, Information Science, and Library Science	Gary Wiggins wiggins@indiana.edu
Herman Skolnik Award Symposium	Richard Cramer cramer@trupos.com
Integrative Chemogenomics Knowledge Mining Using NIH Open Access Resources	Rajarshi Guha rajarshi.guha@gmail.com Tudor Oprea toprea@salud.unm.edu Paul Clemons pclemons@broadinstitute.org
Joint CINF-CSA Trust Symposium: Semantic Technologies in Translational Medicine and Drug Discovery	David Wild registrations@wild-ideas.org Jan Kuras jankuras@hotmail.com
Role and Value of Social Networking in Advancing the Chemical Sciences	Antony John Williams tony27587@gmail.com Jennifer Maclachlan pidgirl@gmail.com
Sci-Mix	Jeremy Garritano jgarrita@purdue.edu
Science-Based Policy Development in the Environment, Food, Health, and Transport Sectors	William Town bill.town@kilmorie.com

I look forward to seeing many of you in Indianapolis. Registration and housing for the Fall Meeting will open on May 29, 2013.

Future Plans

The Spring 2014 Meeting will be held in Dallas, TX, March 16-20. The theme of the Dallas meeting will be *Chemistry and Materials for Energy*. I will be handing over the reins to Erin Bolstad of ChemAxon, CINF Program Chair for 2014, and will be assisting her in the transition. Abstract submission will most likely occur in September-November, 2013. In the coming months, we will be soliciting potential symposia organizers and session topics. If you are interested in organizing a symposium for the Dallas meeting, please feel free to contact me at jgarrita@purdue.edu.

Jeremy Garritano, Chair, CINF Program Committee

Library Cafes, Intellectual Commons and Virtual Services, Oh My! Charting New Routes for Users into Research Libraries

On April 7 we kicked off the ACS Meeting with “Library Cafes, Intellectual Commons and Virtual Services, Oh My! Charting New Routes for Users into Research Libraries,” an all-day symposium organized by Leah McEwen and Teri Vogel featuring eleven speakers, librarians and publishers who shared their knowledge and experience with creating new routes into research libraries. Most of the speakers joined us in person and several presenters delivered their talks remotely, which worked out pretty well.

Special thanks go to ACS Publications for financially supporting the symposium and to Dave Martinsen for his invaluable technical assistance with the remote presentations.

Nevenka Zdravkovska, speaking remotely from the University of Maryland, led off the morning with a discussion about the continuing trend of eliminating and/or consolidating branch libraries. She is the author of *Academic Branch Libraries in Changing Times*¹ and touched briefly on some of the research for her book, as well as some updates since. Nevenka compared the numbers of branch libraries among ARL institutions from 1983, 1999, and 2010, and in that time the number of chemistry branch libraries have decreased. Out of the 101 ARL libraries she reviewed, 20 had chemistry branch libraries, down from 37 in the 1983 survey - and there have been additional closures since. She observed that the number of music branch libraries remains strong while the chemistry libraries have closed at a faster rate. In one of the highlights of the talk, she discussed a 1949 letter from her chemistry department on why they wanted to keep the library physically located in the department. The faculty were concerned they would lose the accessibility and quality service if they lost their branch library in favor of a common science library. Nevenka also pointed out some of the reasons behind the closing and consolidation of branch libraries, citing Jeremy Garritano’s 2007 article on the state of chemistry libraries² and a 2010 ACRL committee report on academic library trends³. All science librarians at the University of Maryland are currently working on a report, *Library Services to Support Scientific Research*, due in May.

Andrea Twiss-Brooks gave us an update on how the University of Chicago is transforming space in their science libraries for scientific computing, discovery and learning. Their guiding principles: develop a programmatic framework, build partnerships, support programmatic needs, and be flexible. Earlier, they repurposed a microform reading room into the Kathleen A. Zar Room, a teaching and meeting space with movable furniture. Another project, though not in her library, was the TECHB@R, collaboration with campus IT to provide technical support beyond what the library staff can offer to users. They have a circulation terminal to check out equipment, and both the groups use the space for workshops. More recently, they upgraded the Zar Room to serve as a Research Computing Center Visualization Laboratory. This is a new program, and Andrea’s library provides a space to help support it while also enhancing their campus visibility. They added high

¹ Zdravkovska, N. *Academic Branch Libraries in Changing Times*; Chandos Publishing, Oxford, 2011.

² Garritano, J. R. Current and future status of chemistry collections and chemistry libraries at ARL institutions. *Iss. Sci. Tech. Librar.* **2007**, 50. DOI: 10.5062/F4222RQP (accessed online April 26, 2013).

³ ACRL Research Planning and Review Committee. 2012 top ten trends in academic libraries: a review of the trends and issues affecting academic libraries in higher education. *Coll. Res. Libr. News.* **2012**, 73 (6). 311-320. URL: <http://crln.acrl.org/content/73/6/311.full> (accessed online April 26, 2013).

performance computing and a 3D projector for data set visualizations, and introduced a library-hosted lecture series. Space also opened up in the library with the reduction of the reference collection and transfer of all print journals that were online to the new Mansueto Library. This created an opportunity for what Andrea highlighted as the final library-campus collaboration, a computer science instructional lab. It is modular to allow flexibility for the space to be configured into larger or smaller classrooms.

University of Washington's **Susanne Redalje** presented on her campus efforts to connect with users and bring them into the library. Libraries want to leverage innovation, technological advances, and opportunity, and also continue to demonstrate relevance and meet needs identified by any reports or assessments. The UW Libraries are creating spaces and services designed to bring users back, and Susanne shared several of those projects with us. The first was the Research Commons, a space to meet faculty and student needs for support of data-driven research, interdisciplinary studies, and digital scholarship. The space is flexible: everything moves and the configuration of individual and group stations changes daily. Graduate funding information, a design desk, rooms for group study reservation and presentation spaces, and data services are among the services offered. Librarians and researchers are also using the space for events, including instruction sessions (some recorded). One such event, Scholars' Studios, has students giving five-minute lightning talks around themes like "sustainability" or "northwest." From their assessment to date, feedback has been positive though they do not yet have a "normal": the group and quiet spaces are a premium and partnering with Graduate Services has been valuable. Susanne also told us that the graduate students appreciate the networking opportunities and diversity of services the Research Commons has provided, and that additional services may be needed for international students. Though one goal of the space was to support the interdisciplinary work, the chemistry people were just forced to use it after closing of the chemistry library. She also told us about the three new interactive classrooms for the undergraduate library. They have been designed to support active learning, and faculty can request the space for individual sessions up to the entire quarter. Again, response has been mostly positive, though there are concerns about ongoing costs, including staff, equipment, and time, as well as communicating with users. They are also applying what they have learned to improve spaces in other campus libraries.

Instead of space changes, **Erja Kajosallo** focused on the librarian-centered changes they have made with their transition at MIT Libraries from a traditional library organization to a more functional model. They reorganized in 2010, moving away from the hierarchical branch library silos. There were catalysts for the change. The research had become increasingly interdisciplinary, most of the faculty and students regularly use more than one campus library, and the collection expenditures shifted from mostly print to mostly, but not entirely, digital in a relatively short period of time. And like many other libraries, budget cuts were another driver for the reorganization, which is complete but still evolving. There are now five functional groups, including "Liaisons for Departments, Labs and Centers." The liaisons are covering more areas, including the many interdisciplinary labs and centers on campus, and there are multiple models in play. Some liaisons do not cover collections development for their areas, while a group of liaisons might support a particular department/lab/center. There are currently 14 FTE for liaisons, but 27 librarians that have liaison assignments. Erja reported on the successes and challenges of their new model of split assignments. It has improved service and allows them to focus on library strategic initiatives and institutional priorities, and they also have a user experience group and assessment team in place now. However,

with no heads of libraries anymore, there are sometimes questions about who to contact when certain issues arise. While there is more collaboration among liaisons and they can leverage the shared needs and values of their user groups, there has also been less face-to-face contact with users, and scheduling time for liaison collaboration has been more difficult.

In a slides-free presentation, **Kiyomi Deards** spoke about some of the approaches she has taken for reaching out to her departments at the University of Nebraska Lincoln, which weren't well served in previous years. Her focus has been on building relationships with her user groups, so even if someone doesn't need her services now, they will remember her if they need in the future. To this end, she tries to attend at least one department seminar a quarter to help maintain a presence. She also has lunch with the undergraduate and graduate recruiters once or twice a year to keep up with what's going on the departments. One thing that Kiyomi has noticed in our profession is the amount of librarian self-doubt, something she never saw when she was working as a chemist. She advises that librarians with subject expertise not hide it, and in fact that they make sure that their users groups are aware of that expertise.

The closing of the Physical Sciences Library at Cornell (PSL) has been discussed at previous meetings, and at this symposium we had two presentations, both remote, on some of the recent service and website innovations at PSL. The challenge, as **Jill Wilson** noted, was how to still be relevant without a physical library. The redesigned website focuses on the essential services and resources, with new features. One of these is the Virtual Shelf Browser (VSB) (<http://stackview.library.cornell.edu>), a reinvention of a "classic" that was lost when the books were moved out. For their ACS on Campus program (<http://acsoncampus.acs.org/past-events/#cu>) a small group of faculty and graduate students were involved in customizing the modules. Along with a la carte services like instruction, consultations, open-ended hospitality events ("Cookies with Grads"), and embedded librarianship, the PSL is developing new services to meet the needs of their users. A current focus has been around issues of scholarly communication that go "beyond the article." The librarians hosted a 2-day workshop on speaking skills, bringing in experts to work with students on techniques like developing elevator speeches. Graduate student input has also been incorporated into an upcoming event on public communication for graduate students that will cover elevator speeches, poster presentations, etiquette, dressing for conferences and business dinners, and more. While the first workshops were created for the chemistry students, PubCon (The Public Speaking Development Conference for Graduate Students at Cornell) will be open to all graduate students.

The morning sessions concluded with a talk from ACS Publications' **Steve Hansen**, who was presenting in place of Sara Rouhi. Steve highlighted their outreach efforts to libraries and academic departments, and the shared service missions of their organization and libraries in supporting research, scholarship, and teaching. As part of their effort to broaden information competency skills, they have made the ACS Style Guide⁴ (not just the Reference section) available online (<http://pubs.acs.org/isbn/9780841239999>) for their Publications and Academic Core+ customers as well as for their ChemWorx users. They are also in the process of digitizing the Supporting Information from the 1970-1995 content that was previously available only in microform: more than 800,000 pages for more than 50,000 articles. It should all be online by the end of 2013, and there will not be an added charge for current Legacy Archives customers. Steve also talked about the just-

⁴ Coghill, A. M.; Garson, L. R. Eds. *The ACS Style Guide*; American Chemical Society: Washington, DC, 2006. URL: <http://pubs.acs.org/isbn/9780841239999> (accessed online April 26, 2013).

launched ChemWorx (<http://www.acschemworx.com>), a tool to keep track of references, collaborate, and share documents. While these services exist elsewhere, ACS wanted to create something that would integrate them within a single interface. On the teaching and learning front, ACS launched their Publishing Your Research 101 (<http://pubs.acs.org/page/publish-research/episode-1.html>) video series in May 2011, and, 60,000 video views later, are about to release the tenth and final video. Steve concluded the presentation with a mention of ACS on Campus (<http://acsoncampus.acs.org>), which many in the audience had already hosted on their campus. In 2012, more than 2600 students and 100 faculty members attended one of the 23 campus visits.

The afternoon session focused on online information tools to reach research and teaching libraries. **Susan Henderson** started off with an overview of the Cambridge Crystallographic Data Centre (CCDC) (<http://www.ccdc.cam.ac.uk/pages/Home.aspx>). They continue to heavily subsidize the cost of Cambridge Structural Database (CSD) for academics (<http://www.ccdc.cam.ac.uk/Solutions/CSDSystem/pages/CSDSystem.aspx>), and more libraries have adopted site-wide licenses since the introduction of WebCSD, which does not have the installation requirements of the DVD version (<http://www.ccdc.cam.ac.uk/Solutions/CSDSystem/Pages/WebCSD.aspx>). They also offer free software and services like Mercury for crystal structure visualization, and anyone can have access to the original deposited crystal data regardless of subscription. CCDC is in the process of replacing their current CSD format (ASER), legacy data, and systems. This will reduce the amount of developer time spent on redundancies and maintaining their homegrown software. Also on the horizon is a major upgrade to the WebCSD database that will add new search functionality. Once the ASER format is replaced, it will enable CCDC to make further improvements to CSD that should improve the user experience and provide better, faster data. Another feature that Susan highlighted is CSD X-Press, a WebCSD service that offers early access to newly published crystal structures prior to being fully curated by the CCDC editors. They are also linking to other collections of chemical data; ChemSpider and PubChem substances have links back to WebCSD if they are in the database, and links from RSC, IUCr, and Elsevier journal citations to the CCDC structures. Also coming soon is CSD-searching integrated into Wavefunction's [iSpartan](#) molecular modeling app for iOS devices.

The ChemEd WikiHyper glossary (WHG) (<http://whg.chemeddl.org>) was the topic of **Robert Belford's** (University of Arkansas at Little Rock) presentation. He gave a brief history of Information and Communication Technologies (ICTs), their development in the digital age from the World Wide Web to social web to semantic web, and the challenges that free agent or DIY learners face. The WHG is a glossary-generating program that uses social semantic information literacy technology to query terms in a document and return data from external sources like ChemSpider, ChemEd DL, and the Protein Data Bank. Canonical definitions are coupled with social definitions; there may be a non-editable IUPAC definition, along with up to four wiki-generated definitions that can be tailored for specific audiences. Appropriate background knowledge can be embedded for reading comprehension. Robert showed some videos to give us a better sense of the WHG in action. You choose a glossary, select text or a URL, and your document is returned with links to definitions, or links to ChemSpider.

In his talk about wiki-based chemistry resources **Antony Williams** (Royal Society of Chemistry) started off by asking how many of those in the audience have managed wikis, or created or edited

content. Beyond the basic definition, wikis can be a place to connect and collaborate, for discussion and constructive conflict, and for community engagement. With one project to curate the Wikipedia entries for the 200 top selling drugs, Antony and others involved came across errors with structures and names, incorrect associations with names or structures, incorrect database links, property data errors, and CAS Number validation issues. They ran into challenges with CAS over using SciFinder to validate the Registry Numbers, but after some discussion CAS gave the dataset to Wikipedia to validate the numbers for the chemicals and drugs. This was a beneficial outcome for all involved. As part of the curation process, once the ChemBox or DrugBox for an entry has been validated, robots on the site will prevent further editing by automatically reverting back to the validated data. There are also gaps in the chemical information on Wikipedia; entries for drugs, but not necessarily for the scientists who developed them, for example. Because of Wikipedia's rules about conflicts of interest and notability, Antony noted that adding porn stars to Wikipedia can be easier than adding scientists. He concluded with an overview of other chemistry wiki projects. There is work to expand Wikipedia content for minerals, polymers, and reactions. ChemSpider Reactions is in development, and it will integrate ChemSpider SyntheticPages (<http://cssp.chemspider.com>) and several RSC databases. ScientistsDB (<http://www.scientistsdb.com>) is a wiki that allows scientists to create and maintain their own wiki pages and use widgets to embed content from YouTube, Twitter, Facebook, Mendeley and other sites that make up their profile. There are also related wikis for science databases and mobile applications, and the RSC Learn Chemistry (<http://www.rsc.org/learn-chemistry>) wiki for secondary and undergraduate education resources is another one that is looking for more content. It includes substance pages with a simpler interface than ChemSpider, plus teaching resources like lab experiments, tutorials, and quizzes. They are also working on a chemical structure collection that they will donate to anyone who wants to link to Wikipedia by a chemical (and you should contact Antony if you are interested).

Dianne Dietrich at Cornell University closed out the presentations with her talk about more of the work on the technical side of the Physical Sciences Library (PSL) (<http://physicalsciences.library.cornell.edu>). One of their most significant projects has been CuLLR, short for Curated List of Library Resources, the librarians' tool to display key resources for astronomy, chemistry and physics, divided by sub discipline. Dianne and Leah McEwen have separate pages set up on the PSL homepage to retrieve annotated lists of databases, e-book collections, and e-journals. Work on the library website is iterative and done in programming sprints. Every six to eight weeks, the PSL librarians "borrow" a programmer from the Libraries IT Division for a three-day sprint, at which time he essentially belongs to PSL to work on their projects.

We concluded the symposium with an open discussion and Q&A on several topics, including Wikipedia and web discovery systems. Thank you to everyone who attended and participated.

Slides for some presentations are posted at: <http://bulletin.acscinf.org/node/413#Sc>

Teri Vogel, Symposium Co-Organizer

Scholarly Communication: New Models, New Media, New Metrics

The Symposium on “Scholarly Communication: New Models, New Media, New Metrics” featured twelve speakers all presenting a perspective on different aspects of the evolving world of scholarly communication. This symposium was organized by David Martinsen, Colin Batchelor, and Bill Town.

Bob Belford from the University of Arkansas at Little Rock kicked off the symposium with a description of the online ConfChem conferences developed by the Division of Chemical Education's Committee on Computers in Chemical Education (CCCE). These conferences started pre-web, with papers posted on a gopher server, and discussions via a listserv. In more recent times, the conferences migrated to a Drupal environment, with discussions appended to the papers as comments. Two new and ongoing projects were presented, a social tagging infrastructure to enable folksonomy indexing of the archives, and an intercollegiate OnLine Chemistry Course (OLCC) in Cheminformatics that will be offered in 2014. This will be the 6th OLCC since 1996 and although an OLCC can be massive, they are a different paradigm for online education than the Massive Open Online Courses (MOOCs) that are currently garnering so much attention. With the Cheminformatics OLCC the CCCE will be pioneering new ways to utilize social and semantic web technologies for intercollegiate teaching and learning.

Colin Batchelor of RSC (Royal Society of Chemistry) gave a nice picture of the tools and technologies the RSC is using to enhance the RSC archive with the same semantic and structure enrichment as is done with the current content. Using Hadoop methods, they are able to process the content and apply the technologies in a reasonable amount of time. These techniques will work nicely on the born-digital material, but the tools will need to be refined to be applied to the scanned pages.

Several talks could be grouped under the topic of quality assessment of research data and enabling reproducibility of experiments, both wet labs and *in silico* experiments. **Rob Chirico** from NIST/Boulder discussed the enhancements to the ThermoML data checking techniques, an environment that, through cooperation with several publishers and journals, discovers potential problems and ultimately improves the quality of published thermodynamic measurements. **Greg Landrum** of Novartis presented a survey of recent publications and stories around experimental methods that could not be reproduced, and urged journal publishers to take steps to improve the reproducibility of published results through more publication of data and use of cheminformatics techniques to evaluate the results, as appropriate. **Gerhard Klimeck** from Purdue University described NanoHUB, a platform that allows researchers to post data and algorithms in order to promote both reproducibility and reuse of data. Researchers can analyze posted data with their own algorithms, and can also use published algorithms to check their own data. The site is used in both teaching and research settings. Finally, **David Martinsen** from American Chemical Society described the work of the NISO/NFAIS Supplementary Journal Article Material Working Groups, who established recommended practices for publishing supplemental materials. High on the list of recommendations were metadata to enable association of the supplemental material files with the associated articles, to indicate whether or not the material had been peer reviewed, as well as to develop plans for preservation/archiving of the files.

Daphne Grecchi from Thomson Reuters described the new *Data Citation Index* (DCI). This Index is one of the new metrics emerging in scholarly communication. Receiving appropriate credit for their contributions is seen as one of the motivations for researchers to publish their primary research data. Archiving and sharing the data outputs of grant-funded research is beginning to be mandated by a number of funding agencies worldwide. If scientists saw a data metric, akin to the impact factor or H-index, they might be more willing to publish their primary data. Thomson Reuters is working with a number of established data repositories to register their existence in the DCI, and then to count citations to the data repositories, and specific data in the data repositories. Thomson Reuters will use the insights learned in handling the initial data to inform the incorporation of additional repositories in the future.

Judy Chen of American Chemical Society described some of the ways in which ACS surveyed active researchers, including graduate students, postdocs, faculty and scientists, through campus visits, through hosting of researchers at its headquarters in Washington, DC, and through online surveys, to help determine the features and functionality of the new workflow tool, ACS ChemWorx that was launched on March 27th. ACS ChemWorx provides a unified environment that facilitates the research process by providing tools to import, manage and search one's existing reference library; store, markup, and highlight PDFs; manage research activities via groups, projects, tasks and calendars; share one's reference citations and files with collaborators; cite references without leaving Microsoft Word or LateX; and track citations of articles. The tools provide some interesting functions not available previously through the ACS Publications website, such as usage metrics on an author's published ACS journal articles and free full-text access to the *ACS Style Guide*.

Matt Straiges of the Royal Society of Chemistry discussed the RSC Gold-for-Gold program. This Open Access program is designed to allow subscribers to the Gold subscription package for RSC journals to credit the entire subscription fee against the author publication charges (APCs) to pay for open access for their RSC articles. In 2012, the UK pilot was a way for institutions to encourage researchers to begin to comply with the Finch Report recommendations for Gold Open Access in the UK. Recently, the program has been expanded to all other areas of the world.

Roger Schenck from CAS (Chemical Abstracts Service) presented a talk entitled "We're not in Kansas anymore." After first assuring the audience that CAS and SciFinder are indeed still available in Kansas, he described how CAS has adjusted as the model of scholarly communication has changed. As more articles are published in different versions (accepted, ahead of print and traditional journal issues), as more patents are being published worldwide, and as more substances are covered in each patent, CAS has leveraged new algorithms and new workflows to enable the scientists curating the databases to keep up with the flow of information.

Antony Williams of Royal Society of Chemistry described some of the new metrics that are emerging to assess the contributions of scientists to the scientific enterprise. Companies like Altmetrics, Plum Analytics, and ImpactStory seek to measure blog, twitter, and news media references to journal articles. Where available, article usage from the publisher website can be included as well. In this new world, Williams encouraged scientists to take advantage of social media to establish reputations via these alternate metrics. In order to encourage community contributions to ChemSpider they will begin to offer badges to top contributors. Tony also

mentioned #RealTimeChem, a twitter hashtag to network with other chemists, as well as a weeklong contest, beginning on April 22, #RealTimeChemWeek.

In past CINF symposia about scientific communication, we have usually focused on publication-based communication and social media. We have largely ignored the art of oral presentations. **Brian Malow**, a science comedian, gave a special presentation at the end of the day. He described how he has used humor to communicate science to scientists and non-scientists alike, and offered tips to audience members as they think about communicating science in oral presentations. Knowing your science is paramount, but understanding your audience, translating your science to terms that can be understood by them, and practicing your presentation are all important aspects of communication. This was a welcome, entertaining ending to a long day of intensive presentations.

David Martinsen, Symposium Co-Organizer



Introduces New Chemical Intelligence Capabilities for Accelerating the Lead Discovery Process

Lead Discovery for TIBCO Spotfire Software Provides Extensive Chemical Structure Searching & Visualization for Finding Promising Compounds Faster

[PerkinElmer, Inc.](#), a global leader focused on improving the health and safety of people and the environment, is introducing the newest version of Lead Discovery for the TIBCO Spotfire software platform. PerkinElmer's [Lead Discovery 5.1](#) enhances the [TIBCO Spotfire](#) software data analysis capabilities with new functionality built specifically with chemists in mind. Based on PerkinElmer's industry-leading [ChemDraw](#) drawing tool, the chemical intelligence in Lead Discovery provides scientists using TIBCO Spotfire software with extensive chemical structure searching and visualization. Now scientists are able to dynamically filter their experimental data sets by chemical structure and pinpoint promising structural features and scaffolds in the output from their medicinal and combinatorial chemistry programs. The new technology enables users to mine their chemical databases to identify more compounds that have similar chemical structures, broadening their potential pool of candidates based on known properties and shortening their time to discovery of a viable candidate or lead.

In addition to dynamic, structure-based filtering, another key functionality of Lead Discovery 5.1 is that it automatically analyzes and displays R-groups (group side chains in chemical structure diagrams) or substituent variations on similar chemical scaffolds. These chemical variations have significant impact on dose response and side effects as they affect how the molecule interacts with a target. Using the new informatics tool, scientists can quickly isolate the variables to identify and optimize promising compound candidates.

For more information, please see a [press release](#) (May 8, 2013).

Food for Thought: Alternative Careers in Chemistry

This session, organized by Donna Wrublewski, Patricia Meindl, and Dana Antonucci, had seven speakers who ranged from librarians to publishers to grant workers. One common theme was how all of these presenters took a hard look at their skills during their graduate studies and took control of their futures.

Vincent Scalfani from the University of Alabama first did a PhD in block copolymers, but decided that his future did not necessarily include a lab. He looked at the skills he had learned during his schooling and found that while chemistry and lab techniques were important skills, he had also developed technical writing, teaching, literature search and problem solving skills as well. He has turned all of his skills into valuable assets as a Science Librarian. He understands the research cycle and can bring that into how he deals with his liaison duties promoting data management or bringing new technologies into the library and his university.

Lily Khidr did a PhD in biochemistry, but then decided to pursue a job in publishing instead of staying in her field. She first worked for Nature Publishing and learned quite a bit about the editing and the publishing cycle. Her skill set includes a broad scientific background, outreach and communication to the public, leadership skills, and the ability to work in cross-matrix groups. She now is a publisher at Elsevier and enjoys the challenges of bringing new products to the market and dealing with all the demands this brings. This makes me think of the Queen in *Through the Looking Glass* who says “sometimes I’ve believed as many as six impossible things before breakfast” - although I think Lily actually does those six impossible things!

Colin Batchelor was our third speaker and he brought his perspective as a cheminformatics specialist. He began with a PhD in molecular Rydberg dynamics and found his transferable skills to be the ability to communicate his science to the public as well as diverse programming skills. He began his post PhD career at the Royal Society of Chemistry as a technical editor on *Physical Chemistry Chemical Physics* (PCCP) and *Faraday Discussions* which included copy editing, proofreading, and issue mockup. Then he moved on to become a Senior Informatics Analyst helping bring Project Prospect to life. Colin is now working with ChemSpider and OpenPhacts, advancing publishing to include not only the journal articles, but also the data behind them to the researchers.

Svetla Baykoucheva began her education in Bulgaria and during her PhD studies she started translating various materials from English into Bulgarian to make them more available to the scientists there. Among her translations were some of Eugene Garfield’s *Current Contents* essays as well. She had a varied research career working at labs in France and the US. Svetla went back to school while working at Kent State University and got her MLIS in 1997. She worked as a reference librarian at the ACS library and was the editor of the *Chemical Information Bulletin* for 6 years. Svetla is now Head of the White Memorial Chemistry Library at the University of Maryland where she can use her extensive knowledge to help her researchers navigate the rising tide of information.

Our last two speakers each went a different way even though they were friends at university! **Rebecca Boudreaux** was very proactive during her undergraduate years expanding her knowledge out of the classroom: she did departmental research projects, NSF sponsored programs, and summer jobs at Princeton and MIT. These opportunities helped her decide more clearly what she wanted to

do for her PhD. During her PhD studies she switched supervisors and learnt to take control of her own career. She applied for scholarships that would teach her new skills such as finance. While in grad school, she and some grad colleagues started a biotech firm. She was the CFO for 4 years and needed to learn many new skills and a different language: accounting! Then she went back to school to finish her PhD, but found that she really had enjoyed building the company and the problem solving that went along with it. So she began to work as a consultant to other companies. Eventually, she worked with Oberon Fuels who produce dimethylether as an alternative fuel source. She is now the President of the company! Her message to our attendees was “You are the CEO of your career.” Find ways to develop more than just your science skills – seek professional development opportunities, build and maintain your network, give back to the community (sometimes this can also give back to you in unexpected ways) and be persistent. She also recommends two books:

1. *Strengths based leadership: great leaders, teams, and why people follow.*
By Tom Rath and Barry Conchie. 2008. ISBN: 9781595620255.
2. *What I wish I knew when I was 20: a crash course on making your place in the world.*
By Tina Lynn Seelig. 2009. ISBN: 9780061735196.

Our final speaker (via Google chat) was **Ticora Jones** who is now a Program Coordinator for United States Agency for International Development (US AID). She enjoyed doing science as a graduate student, but knew she was also interested in people and how systems transform. So she looked for activities outside the lab that she could get involved in such as public policy and career development for grad students. Once she graduated and did a postdoc, she applied for a congressional fellowship and was thrust into the world of politics during an election: “like drinking from a fire hose.” After that heady experience she applied for a US AID fellowship that helped people define problems and work to solutions. Her field was creating science and technology programs: some of which have grown from two people to an office of forty! She is now a program coordinator and finds a key skill is to be able to define problems tightly and to get people to the table to work on these. Other skills include listening and being flexible, being able to develop relationships, ability to communicate and to bring food: everyone loves cookies! To be successful in this area of international development, you really need to know yourself and be a people person. She encourages everyone to go look for fellowships or volunteer opportunities to find out more about who you are and to hone new skill sets. Oh, and get involved!!

Patricia Meindl, Symposium Co-Organizer



FoodInformatics: Applications of Chemical Information to Food Chemistry



The symposium took place on Monday, April 8, 2013 from 1:30 PM until approximately 5:30 PM in the New Orleans Morial Convention Center. The symposium was part of the ACS Meeting theme: **Chemistry of Energy & Food**. The main goal of the symposium was to continue encouraging the application, i.e., “repositioning” of chemoinformatic methods, commonly used in the pharmaceutical industry, to the food chemistry field. This goal is in line with the expansion of the boundaries of chemical information and the repurposing of food chemical databases for health-related benefits. The symposium was divided in two major parts: 1) theory and scope of chemical information and 2) food chemistry applications using chemoinformatic tools. Eight speakers from academia, industry and other research groups shared their leading expertise and vision of this emerging and promising area with about 40 attendees.

Gerald Maggiora (University of Arizona and the Translational Genomics Research Institute, United States) opened the symposium with an overview of chemical informatics pointing out that many applications have been focused for pharmaceutical research. Dr. Maggiora covered the general approaches to represent molecules and emphasized the major impact of molecular representation on many applications and interpretations of chemical information. He raised the important point that some descriptors are not amenable to describe numerical or categorical variables and the prominent examples are descriptors related with food chemistry such as taste and flavor. Dr. Maggiora mentioned that fuzzy methods can be conveniently applied to describe odors and fragrances, which are very complex in nature.

Jean-Louis Reymond (University of Berne, Switzerland) presented an approach to define the chemical space of flavors and fragrances. First, he summarized advances in the development and visualization of the Chemical Universe Database GDB, an impressive collection of virtual compounds well-known in the drug discovery field. Then, Dr. Reymond presented the major results of a chemoinformatic analysis of Superscent and Flavornet using the same approaches that his group has employed to navigate through GDB. In particular, he discussed an analysis of atom count and visualization of the chemical space covered by FF (Flavor and Fragrances) compounds.

Alberto Del Rio (University of Bologna, Italy) highlighted the significant role of food component natural compounds in epigenetic and metabolic pathways. Dr. Del Rio presented the concepts of nutriepigenomics and nutrimetabolomics, providing specific examples of dietary components that after metabolism are implicated in epigenetic events. He discussed ongoing efforts in his lab to use computational approaches with emphasis on pharmacophore-based techniques to systematically track molecular mechanisms involved in nutriepigenomics and nutrimetabolomics. In conclusion, Dr. Del Rio emphasized the need for comprehensive public databases of food chemicals that are readily accessible for drug discovery projects.

Quoc-Tuan Do (Greenpharma, France) explained the concept and principles of reverse pharmacognosy, highlighting the crucial role of chemoinformatic techniques, such as inverse screening to speed up the process of identifying the specific molecule (or molecules) responsible for the biological activity of an organism. Dr. Quoc-Tuan presented two successful examples of reverse

pharmacognosy using Selnergy, a tool developed at Greenpharma to predict interaction energies of a ligand with a target protein based on docking. From his presentation it was clear that the principles of reverse pharmacognosy can be adapted to identify potential health-related benefits of food supplements.

Sebastian E. Ahnert (University of Cambridge, United Kingdom) could not present his paper due to unavoidable travel conflicts.

Christina L. Cole (United States Pharmacopeial Convention) described the major features of the Food Chemicals Codex (FCC), which is an online resource that puts together more than one thousand international standards for the identity and purity of food ingredients. She also elaborated on the integration of the information of the Reference Standards of the United States Pharmacopeia (USP) into the monographs of the Food Chemicals Codex. Dr. Cole presented an appealing spectrum and interplay between foods, food additives, functional food ingredients, dietary supplements, excipients and drugs. FCC is a clear example of the integration of compound database management of food chemicals.

David Evans (Elsevier, Switzerland) spoke about the progress in the development of the Reaxys database with particular emphasis on the retrieval of information related to food chemistry. Starting from a case study of food chemistry literature, Dr. Evans showed the features of Reaxys to extract information pertinent to chemical structures, physicochemical properties, chemical reactions, spectra, use and handling of chemicals. He also presented the visualization tools in the database to filter the information and links to external databases either public or in-house.

Helene Hopfer (University of California Davis, United States) provided an example of the application of multivariate statistical and visualization methods to analyze trace metal compositions in wine storage at different packing configurations and temperatures. Sensory, chemical and physical properties were analyzed. Just as in pharmaceutical applications, these data were analyzed with multivariate statistical methods. Canonical variate analysis plots of sensory data, such as aroma and flavor, were presented. Her talk was an excellent example of food chemistry that uses principal component analysis as a data visualization tool.

Piotr Minkiewicz (University of Warmia and Mazury in Olsztyn, Olsztyn, Poland) closed the symposium presenting the results of a bioinformatics study aimed at analyzing the distribution of epitopic fragments of the chicken egg allergens in the universal proteome. The rationale of this work was that the existence of common epitopes in proteins of different species can cause the appearance of cross reactivity. The BIOPEP database was used in this study. This comprehensive sequence database, developed by Dr. Minkiewicz and collaborators, can be searched online (<http://www.uwm.edu.pl/biochemia/index.php/pl/biopep>). This study exemplifies one of the most active research areas in food chemistry that uses bioinformatics and cheminformatics tools, namely the identification of allergenic proteins in foods.

Our goal of bringing together experts from chemical information and food chemistry fields was fully accomplished. The presenters and attendees interacted and initiated potential collaborations, making this symposium a seed in the development of the FoodInformatics field.

José Medina-Franco and Karina Martinez-Mayorga, Symposium Organizers

Public Databases Serving the Chemistry Community

How do you find a reaction of interest? How do you find a molecule that may have activity against a target you are working on? How do you synthesize that molecule? How do you find the sequence of that target? How do you find a crystal structure or NMR spectrum of a compound? It seems that almost every day biologists and chemists increasingly make use of public resources on the Internet to answer these and many more questions. These resources are likely predominantly databases. How, you might add, would we survive (or at least do our jobs) if we did not have access to these resources? At the ACS Meeting in New Orleans we had the opportunity to meet many of the people involved in developing and maintaining such databases, as well as those thinking beyond what we have now and addressing such topics as quality, the future, and new technologies.

The morning session was opened with **Evan Bolton** (National Center for Biotechnology Information, NIH, United States) presenting “PubChem: A community driven resource.” He described how [PubChem](#) is an open archive that is used globally for people to push data whether small molecules or increasingly RNAi’s. To date there are 47 million CIDs (PubChem Compound Identifiers), and 650,000 assays and 1.8 million molecules have bioactivity results. PubChem is also accessible via the PUG ([Power User Gateway](#)) and has various widgets for mining data.

Markus Sitzmann (National Cancer Institute, NIH, United States) then presented on “NCI/CADD chemical structure Web services.” He described the chemical ID resolver launched in 2009 which is most widely used by Eli Lilly. The NCI chemical structure database has 84.6 million unique structures and they are working on a new database with 141.7 million unique structures. In addition, the group is working on several web apps that will be accessible by iPad.

In the talk titled “ChemSpider: Disseminating data and enabling an abundance of chemistry platforms” **Antony Williams** (Royal Society of Chemistry, United States) described the many projects which his group is involved, in ranging from mobile apps to consortia projects providing resources for the chemistry community both in the UK and elsewhere. These initiatives include [Open PHACTS](#) which is a triple store registering public and private facts, PharmaSEA which is a project to de-replicate natural products, and the [National Chemical Database Service](#), which is a UK project providing access to a series of commercial databases and prediction services and will ultimately deliver a repository for data generated by the UK academic community. ([slideshare](#)).

Yanli Wang (National Center for Biotechnology Information, NIH, United States) then provided an overview of “PubChem BioAssay: A public database for chemical biology data.” She showed the growth in records and reported over 40,000 compounds with bioactivity <1 uM. To date 177 chemical probes have been identified. The [database](#) covers 8000 targets and 2000 organisms.

Gary Battle (European Bioinformatics Institute, United Kingdom) then presented “Chemistry-related resources at the Protein Data Bank in Europe.” He described the [Protein Data Bank](#) in Europe and how they have a strong focus on ligands and tools for chemists. He gave examples of molecules with incorrect ligand geometry and also cited a recent paper that described 20% of structures as having geometric errors (The good, the bad and the twisted: a survey of ligand geometry in protein crystal structures. *J. Comput.-Aided Mol. Des.* **2012**, 26, 169-183).

Egon Willighagen (Maastricht University, The Netherlands) then presented “Architecture for an open science molecular compound database.” He described Open Notebook science, RDF graphs and Nanopub.org. ([slideshare](#)).

The afternoon session began with **Julien Thibault** (University of Utah, United States) speaking on “Local and remote tracking of molecular dynamics data for global dissemination,” which described the [iBiomes](#) integrated biomolecular simulator and the iRoDS rule-orientated data management system.

In the next presentation titled “Chemical science that underpins the Reaxys database” **Juergen Swienty-Busch** (Elsevier Information Systems, Switzerland) discussed the recent advances they have made in order to support the daily workflow of a research chemist. The database started from the early publication of Beilstein in 1881 which collated 1,500 compounds over 2,200 pages and is now the Reaxys database covering chemical reactions from over 16,000 periodicals.

Valentina Eigner-Pitto (InfoChem, Germany) then described “ChemReact: A free database containing more than 524,000 reactions available at your fingertips.” She explained how this represents the most comprehensive free resource available today, and on a Mobile App! Interestingly, a plot that showed the reaction type with frequency appeared to show a power law. During discussions it was found that this was something that other groups had noticed, but it has not been widely disseminated.

Sean Ekins (Collaborations in Chemistry, United States) then delivered a lecture on behalf of **Christopher Southan** (TW2Informatics, Sweden) “Navigating between patents, papers, abstracts, and databases using public sources and tools.” He described how such navigation was possible due to ChEMBL’s capture of SAR from journals, the deposition of three major automated patent extractions (SureChem, IBM and SCRIPDB) in PubChem for over 15 million structures, open tools such as chemicalize.org, OPSIN, and OSCAR, which enable the conversion of IUPAC names or images to structures, and the indexing of chemical terms (e.g. InChIKeys) that turn Google searches into a merged global repository of 40 to 50 million structures. ([slideshare](#)).

Colin Batchelor (Royal Society of Chemistry, United Kingdom) then described “ChemSpider reactions: Delivering a free community resource of chemical syntheses.” This was a work in progress report regarding the work of the Royal Society of Chemistry to create an online resource of hundreds of thousands of reactions. The original source data that is to be unveiled will result from the PhD research of Daniel Lowe (originally at the University of Cambridge, Unilever School of Informatics and now at NextMove Software). ([slideshare](#)).

Michael Kappler (Roche, United States) presented the final talk of the day on “Intuitive and integrated browsing of reactions, structures, and citations: The Roche experience.” He described how they could not get data out of their CambridgeSoft ELN and created instead a unified data model leveraging Pipeline Pilot and Reaxys. He mentioned how they had 27 informaticians at Roche working on the project, and it took seven months to migrate 99.5% of all reactions.

Day 2 began with **Noel O'Boyle** (NextMove Software, United Kingdom) "Universal SMILES: Finally, a canonical SMILES string?" He discussed how to use the InChI's canonical labels to derive a canonical SMILES string in a straightforward way and the performance of these methods. ([slideshare](#)).

Next, **Laura Guasch** (National Cancer Institute, NIH, United States) talked about "Analysis of tautomerism in databases of commercially available compounds." She reported on the tautomerism analysis in a large database of commercially available compounds to investigate how many cases there are of the same chemical being sold as different products (at possibly different prices), and to test the tautomerism definition of the widely used cheminformatics toolkit, CACTVS. She reported on thousands of cases where at least two products are listed as different compounds in the Aldrich Market Select (AMS) database from ChemNavigator/Sigma-Aldrich.

Colin Batchelor (Royal Society of Chemistry, United Kingdom) reported on the RSC's Chemical Validation and Standardization Platform (CVSP) and their efforts to use algorithmic checking on chemical compound representations to try and provide a potential path to quality-conscious databases. The CVSP platform checks chemicals using a set of rules such as hypervalency, charge-imbalance, absent stereo, etc. and uses algorithms to convert submitted structure representations into standardized representations such as those expected by the FDA for their substance registry system. The system, when released, will be available for the community to use. ([slideshare](#)).

Sean Ekins (Collaborations in Chemistry, United States) then elaborated on "Challenges and recommendations for obtaining chemical structures of industry-provided repurposing candidates." He described recently published efforts (*Drug Discovery Today* **2013**, *18*, 58-70) to find the structures for repurposing candidates provided by the pharmaceutical industry to the National Center for Advancing Translational Sciences (US) and Medical Research Council (UK) initiatives. He also described efforts to make the structures identified available publically and analyze them *in silico* to identify new uses. ([slideshare](#)).

Juergen Swienty-Busch (Elsevier Information Systems, Germany) then reviewed "One size fits all or how to find the needle in the haystack?" He described a workflow that used Pathway Studio, Reaxys medicinal chemistry to design molecules with good ADME properties, and PharmaPendium to prioritize the drug pipeline. He also mentioned that Reaxys and PubChem overlap by 20%.

Alex Clark (Molecular Materials Informatics, Canada) presented the final talk entitled "Pistoia Alliance AppStore: Apps for life sciences R&D." The app strategy of the Pistoia Alliance was introduced: the precompetitive organization is exploring ways to encourage the uptake of mobile apps for life sciences R&D, and has released its own catalog of relevant apps. Future directions for the project were discussed. ([figshare](#)).

In summing up, the presentations described a broad array of databases and efforts that are enriching the chemistry community and will likely be a starting point for future ACS presentations and research.

Sean Ekins and Antony Williams, Symposium Organizers

Advances in Virtual High-Throughput Screening

Virtual high-throughput screening is widely used in drug discovery to identify potential molecules to test from the massive drug-like chemistry space. Approaches may be structure- or ligand-based, and increasingly tools are being developed to facilitate and validate such strategies. At the ACS meeting in New Orleans we had the opportunity to meet many of the people involved in developing and applying such virtual high-throughput screening approaches.

The session was begun by **Carsten Detering** (BioSolveIT, United States) who described “Setting up a discovery pipeline in KNIME and PipelinePilot: High-throughput de novo design utilizing gigantic virtual chemistry spaces.” He described a ROCS shape search of 1.2×10^7 compounds in a minute and a Pfizer virtual screen of 3×10^{12} molecules in 10-15 minutes. An additional example was provided with Bayer, in which 116 of 172 molecules were plant-active compounds.

Frank Boeckler (Eberhard Karls University, Germany) discussed “New targets addressed by DEKOIS 2.0: Demanding evaluation kits for objective in-silico screening.” This automated process enables creating tailor-made decoy sets for any given sets of bioactives. It facilitates a target-dependent validation of docking algorithms and scoring functions, helping to save time and resources (www.dekois.com).

Evan Bolton (National Center for Biotechnology Information, NIH, United States) lectured on “PubChem3D: A virtual screening platform.” PubChem3D is an extension of PubChem resources to include a 3D layer, providing users with new capabilities to search, subset, visualize, analyze, and download data. With the ability to uncover latent structure-activity relationships of chemical structures while complementing 2D similarity analysis approaches, PubChem3D represents a new resource for scientists to exploit when exploring the biological annotations in PubChem.

Sean Ekins (Collaborative Drug Discovery, United States) then presented “Dual-event machine learning models to accelerate drug discovery.” He described how cytotoxicity and bioactivity data were combined to produce dual-event Bayesian models (using Discovery Studio) for identifying compounds with activity against *M. tuberculosis* and a relative lack of cytotoxicity versus Vero cells. Over 38,000 compounds were virtually screened from different libraries and 17 of 106 predicted hits were empirically shown to be active. In one example, a GSK antimalarials library was virtually screened and 5 of 7 predicted hits were active versus *M. tuberculosis*, leading to one molecule being tested *in vivo*. ([slideshare](#)).

Vladimir Poroikov (Orekhovich Institute of Biomedical Chemistry, Russian Federation) subsequently presented “Virtual high-throughput screening of novel pharmacological agents based on PASS predictions.” The robustness of the PASS algorithm for heterogeneous datasets has been shown widely. PASS is used to estimate qualitative (yes/no) predictions of biological activity spectra for over 4000 biological activities.

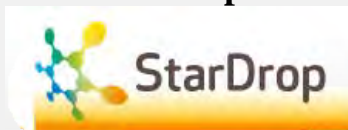
Finally, **Simon Krige** (Cresset Biomolecular Discovery, United Kingdom) discussed “How GPUs can find your next hit: Accelerating virtual screening with OpenCL.” He described how OpenCL is about 40 times faster for a GPU versus a CPU and 25 times cheaper. For example, a single NVidia or AMD graphics card can be used and has the same screening performance as more than 40 modern

CPU cores. Such a dramatic speed increase means that screening a few million compounds can be done overnight using a single desktop box with 4 GPUs, compared with using a Linux cluster. A small cluster equipped with GPU coprocessors can be used to screen virtual libraries of tens or hundreds of millions of molecules. Such databases were previously accessible only to 2D methods.

These presentations by virtual screening software developers and scientists involved in applications of these technologies suggest that virtual high-throughput screening may be increasingly utilized to accelerate drug discovery efforts.

Sean Ekins and Joel Freundlich, Symposium Organizers

New bioisosteric transformations and predictive toxicity capabilities in



Optibrium's StarDrop software platform guides decisions in drug discovery to quickly identify chemistries with a high chance of success. StarDrop's unique probabilistic scoring approach to multi-parameter optimization intuitively integrates predicted and experimental data to guide the design and selection of compounds that balance the many requirements for a high quality lead or candidate drug.

The release of StarDrop version 5.4 will introduce new modules to the suite of plug-ins that extend StarDrop's core capabilities. The addition of the new Derek Nexus module, developed in collaboration with Lhasa Limited, will provide access to the world-leading technology for knowledge-based prediction of key toxicities in over 40 endpoints including mutagenicity, hepatotoxicity, and cardiotoxicity.

The capabilities of StarDrop's existing Nova module will also be expanded by the addition of the BIOSTER database from Digital Chemistry to simulate the search for high-quality compounds by generating relevant compound ideas prioritized against a project's property requirements. The BIOSTER module contains a unique compilation of over 20,000 precedented bioisosteric transformations, manually curated from the literature. The combination of Nova and BIOSTER will enable the application of this comprehensive database to generate novel structures with a high likelihood of biological activity and synthetic accessibility.

The combination of these technologies with StarDrop will enable chemists to intuitively design high-quality compounds, balancing the reduction of toxicity risk with all the other requirements for a successful, safe, and efficacious drug in hit-to-lead and lead optimization.

If you would like to know more, please download a brochure from <http://www.optibrium.com/stardrop/brochure.php>, visit www.optibrium.com or email info@optibrium.com to arrange a demonstration or free evaluation.

Computational De Novo Protein and Peptide Design

Although this symposium was scheduled for Wednesday afternoon, we had sizeable interest and attendance due to the significance of the topic and excellence of the speakers. The emphasis on the development of biologics as drugs has increased dramatically over the last few years. In fact it is well accepted that biologic drugs will drive pharmaceutical future market growth. For example, biologics represent over 30 percent of Abbott's development pipeline, while Roche, obtained two-thirds of its pharma sales in 2010 from biologics (a report by [MedCity News](#), November 20, 2012).

Biologics are specifically being developed for use in cancer, diabetes, rheumatoid arthritis, and orthopedics. Examples include Abbott's Humira, Amgen's Enbrel, and Biogen Idec's Rituxin as representative best-selling biologics.

It is with this in mind that **Francisco Hernandez-Guzman** (Accelrys, United States) began our session with "Novel in silico prediction algorithms for the design of stable and more effective proteins." Dr Hernandez-Guzman discussed new computational tools available from Accelrys to calculate the energetic effects of mutations on protein stability and protein-protein binding affinity including pH dependence, and use of these methods for successful protein design. He presented a validation example for the method examining binding affinity of OMTKY3 inhibition of proteinase B residues with 19 P1 residue mutations, and an in silico design of an IgG antibody with enhanced pH selective binding to improve its serum half life.

Woody Sherman (Schrödinger, United States) followed with a discussion of "Advanced structural modeling of biologics with BioLuminate." Bioluminate is Schrödinger's new product that provides for computational protein-protein docking (Piper), antibody modeling, long loop predictions and protein mutational studies. Dr. Sherman presented examples illustrating prediction of thermal stability and mutational effects on protein-protein binding energy with the barnase/barstar complex; thermal stability of SH3 domain mutants; and CDR antibody modeling predictions and de novo approaches to H3 loop modeling.

Enrico Purisima (National Research Council of Canada) rounded out the session with a presentation on using computational methods of directed evolution to enhance affinity maturation. Dr. Purisima's lab has used a combination of three in silico methods (SIE, FoldX and Rosetta) to redesign antibodies to enhance their interactions and affinities to VEGF-A and HER2. The designed antibodies were then tested with experimental screening methods using surface plasmon resonance, which resulted in redesign of the binding interface.

The symposium demonstrated the usefulness and potential contribution of computational methodologies to modeling, predicting, and redesigning protein-protein interactions with applications to the design of biologics (antibodies).

Rachelle Bienstock, Symposium Organizer

Multidisciplinary Program Planning Group (MPPG)

By all accounts, the 245th ACS National Meeting in New Orleans, April 7 – 11, 2013, was a great success with an attendance of over 15,000, including about 5,000 students. Unquestionably, part of the success was due to the location, but an excellent program with the theme “Chemistry of Energy and Food,” selected fittingly for New Orleans by MPPG, certainly played an important role. Organized by Professor Emeritus James N. Seiber, Environmental Toxicology at UC Davis, sixteen divisions presented twenty eight symposia associated with the theme including CINF with a symposium “Foodinformatics: Applications of Chemical Information to Food Chemistry” organized by Jose Medina-Franco and Karina Martinez Mayorga. The thematic symposium provided a small monetary reward in addition to the wide visibility of CINF listed on the eye-catching flyer symbolizing the meeting’s theme. Richard Love from ACS did an enormous job of bringing everything together.



MPPG was also involved in the selection of the speakers for “The Kavli Foundation Innovation in Chemistry Lecture” and the new “The Kavli Foundation Emerging Leader in Chemistry Lecture.” Both outstanding lectures were presented to a full house with the majority being young chemists. **Daniel G. Nocera**, Patterson Rockwood Professor of Energy, Harvard University, talked about “*The artificial leaf*” and **Christy L Haynes**, University of Minnesota, described her research on “Biological and ecological toxicity of engineered nanomaterials.” The Kavli Foundation agreed to continue the “Emerging Leader in Chemistry Lecture” for researchers under the age of 40 through 2016. Divisions will soon be solicited to send speaker nominations for the “Emerging Leader Lecture” series for the Dallas meeting to MPPG. Each Division can nominate two candidates and any nominations from CINF certainly will help the Division’s visibility.

The plenary session organized by Jim Seiber, presented again to a very large audience, consisted of four presentations by eminent scientists addressing both aspects of the theme: **Peter Schieberle**, Technical University of München, “The chemistry of food flavors: Simply pleasure or beyond?” **John Floros**, Kansas State University, “Feeding the world through science and technology: A look into our future food system,” **Harrison Dillon**, Solazyme, Inc., “Renewable oil technologies platform for bio-based products,” and **Cesar Vega**, Mars Botanical, “The kitchen as laboratory: Building bridges between science and the non-scientist.” If you did not have the chance to attend the plenary session, you certainly missed something.

At the General Meeting of MPPG in New Orleans, Professor Robert Weiss, University of Akron, theme organizer for the Indianapolis meeting in September 2013, outlined the thematic program and announced the slate of plenary and Kavli Lecture speakers. Based on this information we can look forward to a very interesting program. I might mention that the Indianapolis race track will be part of it. Don’t miss the program announcements in *C&EN*.

The future of thematic programming at ACS meetings looks bright. More and more technical divisions organize symposia related to the theme of a meeting, often cosponsored by other divisions indicating the interdisciplinary nature of chemistry. We definitely have seen a strong upwards trend

in the last few meetings. As per charter, themes for the next three years have been approved and organizers are in place for 2014 and 2015. The Program Committee of CINF should look closely at the themes and available synopses, and work together with the thematic program chairs and to organize companion symposia. Any symposium within a given theme will provide valuable publicity to the Division.

Here are the themes for future meetings:

S2014 Dallas, TX: *Chemistry and Materials for Energy*, thematic program chairs Michelle Buchanan, Oak Ridge National Lab, buchananmv@ornl.gov and Nitash Balsara, UC Berkeley, nbalsara@berkeley.edu

F2014 San Francisco, CA: *Chemistry and Global*, thematic program chair Robin Rogers, University of Alabama, rdrogers@as.ua.edu

S2015 Denver, CO: *Chemical Resources: Extraction, Refining and Conservation*, thematic program chair TBD

F2015 Boston, MA: *A History of Innovations: From Discovery to Application*, thematic program chair TBD

S2016 San Diego, CA: *Computers in Chemistry* (tentative), thematic program chair TBD

F2016 Philadelphia, PA: *Chemistry and Education* (tentative), thematic program chair TBD

S2017 San Francisco, CA: *Water and Chemistry* (proposed), thematic program chair TBD

F2017 Washington, DC: *Chemistry and Globalization* (proposed), thematic program chair TBD.

The CINF Program Chair will be notified about the details of these themes as soon as they become available.

Guenter Grethe, CINF representative to Multidisciplinary Program Planning Group

Join Us Again in Indianapolis



Image credit: <http://portal.acs.org/portal/PublicWebSite/meetings/fall-2013/index.htm>

Registration & Housing will open May 29, 2013

Book Reviews

Continuing a trend begun in the previous issue of *Chemical Information Bulletin*, books on more alternative information aspects of chemistry are reviewed. After all, when some of us entered the chemical information profession, our resources were titled “chemical literature.”



First to be reviewed is a book of two plays by Carl Djerassi, *Chemistry in Theatre; Insufficiency, Phallacy, or Both*. Imperial College Press, London, 2012, 112 pp. ISBN 978-84816-938-8 (paper) \$24.⁵

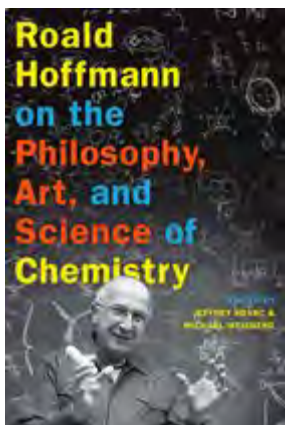
Djerassi, in addition to a multitude of scientific articles and five monographs, is also the author of several works of chemistry oriented nonfiction including eight plays. The most notable of the latter includes *Oxygen*, a play co-authored with Nobelist Roald Hoffmann. In this ninth book of plays, Djerassi makes a strong case in the introduction for writing plays to be read and not necessarily produced on stage. He posits that in general even famous plays are often read by more people, especially by students, than actually see the plays on stage. He describes the stages in play crafting, writing the play as literature aimed at the reader, writing for a reading (on stage or radio), and finally writing for performance. *Oxygen* was the latter although it appeared in print before it was performed (a video of a performance exists, University of Wisconsin, 2003). Other plays with chemical subjects are also discussed, all too few in the opinion of the author.

The two plays in this volume were written to be read. The first, *Insufficiency*, concerns the battles of an immigrant chemistry professor to obtain tenure at a “second-rate” American university. His research topic is bubbles, specifically in champagne and beer, which is deemed by his department to be trivial which results in the tenure battle. The play is in nine scenes and is cast with eight characters and involves romance, intrigue, academic politics, and a pretty fair portion of authentic physical chemistry.

The second (pun intended) play, *Phallacy*, is in 27 relatively brief scenes and is cast for eight characters. Set in the world of art in Vienna, there’s another battle going on, this one between the director of museum antiquities and a professor of chemistry who’s also head of the art conservation department of a technical institution. The subject is the authenticity of a bronze statue, described in her lifework by the art historian as Roman, but discredited by the chemist, using trace metal analysis, as being a Renaissance “fake.” Both of the protagonists’ assistants are also roped into the battle which, since they are romantically involved with each other, makes for more intrigue and humor. A series of historical flashback intermezzi contributes to the eventual resolution of the dispute.

The two plays make enjoyable reading even if the reader is not a chemist nor in academia. I also recommend them to schools for classes in literature and drama as well as in science and chemistry. My family has scientists, actors, and teachers and I intend to bring this book to their attention.

⁵ Previously reviewed by G. B. Kauffman in *J. Chem. Education*, **2013**, *90*, 147-148. DOI: 10.1021/ed300869q



Second to be reviewed is a book, *Roald Hoffmann on the Philosophy, Art, and Science of Chemistry*, edited by Jeffrey Kovac and Michael Wessberg. Oxford University Press, New York, 2012. 390 pp. ISBN 978-0-19-975590-5 (hardback). £22.50.

The title is an abstract. The editors have assembled a collection of essays by Nobelist Roald Hoffmann, several of which have appeared in *American Scientist*. Hoffmann, a self-described theoretical chemist, also considers that chemical synthesis is at the core of chemistry as a creative human activity. (This reviewer heartily agrees because his all-too-short lab career involved chemical synthesis, about the only way that this otherwise non-artistic person could feel creative.)

Hoffmann's writing style is excellent and versatile, mirroring his writing as a polymath in the sciences, poetry, and drama. Items on the history of chemistry are salted throughout the text. Consistent with the scientific style, the text is heavily footnoted, which can lead to a whole new library for reading.

The book is organized into five sections: chemical reasoning and explanation, writing and communicating, art and science, chemical education, and ethics in science. In the first, explanation does not always lead to reasoning. Ockham's Razor is discussed in detail including strengths and weaknesses and why it is often misused. Communication covers the debate on third person, passive scientific writing. Hoffmann makes the case for a more human approach. He also stresses the need for scientists to communicate with the public in an approachable style.

In the section on art and science, Hoffmann confesses that he once considered a career in art history. His track record as a poet and playwright is excellent. The section also covers science and crafts as well as the beauty of molecules. In education, the expectations of the teacher and the students do not necessarily match and a merger of the expectations and results should be the goal. He advocates that students should take lecture notes by hand and then transcribe or rework them after class. (Again, this reviewer agrees since this was method he used more than 50 years ago.) In the section on ethics, Hoffmann posits that science is not ethically neutral. The environment and green chemistry are discussed in detail.

Drawings, chemical structures, artwork, cartoons, and reproductions of classic articles are prominent in the text.

Overall, an excellent read on a number levels. Highly recommended for students, teachers, and practitioners of chemistry as well as the technically oriented public.

Robert E. Buntrock
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COMMITTEE REPORTS

CINF Education Committee

The Education Committee met at the ACS Spring 2013 National Meeting in New Orleans on Saturday, April 6, 2013, from 2-4 PM in Room 229, Ernest N. Morial Convention Center.

Attendees: Grace Baysinger (Chair), Chuck Huber, Marion Peters, Terri Vogel, Donna Wrublewski. *Visitors:* Judith Currano, Jeremy Garritano, Adrienne Kozlowski. *Absent:* Christina Keil, Yi Li. *Resigned:* Olivia Sparks.

Chemical Information Literacy webpage

Catalyzed by a reference from the ACS Committee on Professional Training Supplement on Chemical Information Skills (<http://www.acscinf.org/content/chemical-information-literacy>) to consult CINF's website for more detailed information on the development of chemical information literacy, Marion Peters compiled content for a new Chemical Information Literacy webpage. Many thanks to Dave Martinsen for approving this addition and to Danielle Dennie for putting this information up on the CINF website. It is listed on the top level on CINF's website and the URL is: <http://www.acscinf.org/content/chemical-information-literacy>.

Explore Chemical Information Teaching Resources (XCITR)

FIZ CHEMIE Berlin has been very generous to developing and hosting the XCITR website, but due to changing circumstances is no longer able to do so. The Royal Society of Chemistry (RSC) has graciously agreed to host XCITR for the coming year. At the end of the year, RSC and the XCITR Board will evaluate future support needed for XCITR. The URL has stayed the same: <http://www.xcitr.org>. There are approximately 50 items in the XCITR collection now. The current goal is to encourage more submissions from busy colleagues so that content they have already created can be used by other librarians and by chemistry instructors who are teaching chemical information skills. Strategies on how the CINF Education Committee might help increase the number of submissions were discussed.

The ACS Committee on Professional Training Guidelines – Proposed Revisions for 2014

The ACS Committee on Professional Training (CPT) issues guidelines for accrediting Bachelor Degree programs in Chemistry. Last issued in 2008, the Guidelines include a supplement on Chemical Information Skills. CPT is developing the next revision of the Guidelines, which will be adopted in 2014. In the Fall 2012 Report to ACS Council and in the Fall 2012 issue of the CPT Newsletter, CPT provided information about the need to revise the Guidelines.

In January 2013, CPT suspended the requirement in the 2008 ACS Guidelines for access to *Chemical Abstracts*. "This change will take effect immediately for all new periodic reports and applications and for those currently under review. CPT anticipates a shift in focus from access to specific resources to the development of student skills in the searching, retrieval, and use of the chemical literature."

At the 2013 ACS Spring National Meeting in New Orleans, there was a CPT Open Meeting that was attended by Marion Peters and a CPT's Symposium on the "Evolution of the ACS Approval Process: Moving Beyond the 2008 Guidelines" that was attended by Grace Baysinger and Marion Peters. As a follow-up, the Education Committee plans to send comments to CPT about proposed changes to the Chemical Information Searching part of the Guidelines. The Education Committee also plans to review the Chemical Information Literacy Competencies for Undergraduate Chemistry Students to see if any revisions are needed. CPT will hold an open meeting at the 246th ACS National Meeting in Indianapolis on Sunday, September 8, 2013.

For more details, please see:

ACS Committee on Professional Training

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

Background Documents

[ACS Guidelines for Bachelor's Degree Programs](#), Spring 2008

[Supplement on Chemical Information Skills](#)

[CPT Newsletter](#), Fall 2012

[Committee on Professional Training – Report to Council](#) (August 2012)

Recent and Proposed Changes to CPT Guidelines

[CPT approves change in requirement for access to Chemical Abstracts](#)

[Proposed Changes to the ACS Guidelines and Evaluation Procedures for Bachelor Degree Programs](#), Prepared January 2013

Chemical Information Competencies

Information Competencies for Chemistry Undergraduates. Issued jointly by Special Libraries Association, Chemistry Division, and American Chemical Society, Division of Chemical Information. Updated on Wikibooks. May 2011

http://en.wikibooks.org/wiki/Information_Competencies_for_Chemistry_Undergraduates

Information Skills for Graduate Students – Draft Document for Discussion

Spearheaded by Judith Currano, a draft document on information skills needed for successful graduate students was shared with the Committee. There was not enough time to review it during the meeting so Education Committee members were encouraged to review it afterwards and post comments on the ACS Network site for the committee.

Symposia and Conferences

- CINF Programs in New Orleans (Spring 2013): Library Cafes, Intellectual Commons and Virtual Services, Oh My! Charting New Routes for Users into Research Libraries (Sunday), Scholarly Communication: New Models, New Media, New Metrics (Monday), Food Informatics: Applications of Chemical Information to Food Chemistry (Monday PM), Public Databases Serving the Chemistry Community (Tuesday & Wednesday AM).
- CINF Programs in Indianapolis (Fall 2013): Graduate Student Research Symposium in Cheminformatics, Information Science, and Library Science; Before and After Lab: Instructing Students in 'Non-chemical' Research Skills; Print Resources in a Digital World: Publishing, Acquiring, Using, Managing, and Preserving Chemistry Library Collections.
- Biennial Conference on Chemical Education: Grand Valley State University, Allendale, MI, August 3-7, 2014 (<http://www.bcce2014.org>).
University of Northern Colorado, Greeley, CO, July 31-August 4, 2016.
- ConfChem online conferences by the ACS Division of Chemical Education Committee on Computers in Chemical Education (<http://www.ccce.divched.org/OLCC>)
Teaching and Learning Chemistry with Moodle, May and June 2013

Housekeeping

The Education Committee needs to recruit two (or three) faculty to the Committee membership.

The CINF Education Committee webpage (<http://www.acscinf.org/content/education>) needs to be revised. There is a list of previous meetings that should be deleted and old workshop materials that need to be put into an Archive section.

All committee members need to join the CINF Education Committee private group on the ACS Network (<https://communities.acs.org/groups/cinf-education-committee-members>).

Communicating virtually between meetings to keep the momentum going is desired.

Grace Baysinger, Chair, CINF Education Committee

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It is with great pleasure that Bio-Rad Laboratories, a long-time sponsor of CINF, invites your school to participate in a free 30-day evaluation trial of **KnowItAll U** - the world's largest collection of spectral data (NMR, IR, Raman, MS, UV-Vis). This resource has been used successfully in the teaching curriculum, academic research in chemistry, biology, and other applied science disciplines, as well as in a library setting. For more information, please visit <http://www.knowitallu.com>, view a recording of our "Introduction to KnowItAll U" webinar (presented by Farrel Borden) at http://www.knowitall.com/webex_archives, or contact Farrel Borden at 267-322-6938, or register online at <http://www.knowitallu.com/trial>. It's that easy!

Report from the ACS Council Meeting

The Council of the American Chemical Society met in New Orleans, LA on Wednesday, April 10, 2013 from 8:00am until approximately 12:00pm in the Grand Ballroom A-C of the Hilton New Orleans Riverside Hotel. The meeting opened with recognition of deceased Councilors and a moment of silence in their honor. The minutes of the prior Council meeting held in Philadelphia, PA were approved as was an interim action of the Council Policy Committee who had elected Carolyn Ribes as Vice-Chair. Below are highlights of the meeting as well as the results of actions that were taken during the meeting.

Nominations and Elections

President-Elect: The Committee on Nominations & Elections (N&E) identified four nominees for the office of 2014 ACS President-Elect. They were as follows: G. Bryan Balazs, Charles E. Kolb, Jr., Carolyn Ribes, and Diane Grob Schmidt. The four nominees answered questions at the Town Hall meeting that was held on Sunday, April 7th, and each gave a three minute presentation at the Council meeting. By electronic ballot, the Council selected G. Bryan Balazs and Charles E. Kolb, Jr. as candidates for 2014 President-Elect. These two candidates, along with any candidates selected via petitions, will stand for election in the Fall National Election.

Other Elections

The Committee on Nominations and Elections announced the results of the election to select *candidates* from the list of *nominees* to serve as Directors from District II and District IV on the Board of Directors for the term 2014-2016. Nominees for District II included George M. Bodner, Jed F. Fisher, Alan A. Hazari, and Robert A. Pribush. Nominees for District IV included John P. Fackler, Jr., Rigoberto Hernandez, Larry K. Krannich, and John A. Whittle. By mail ballot, the Councilors from these districts selected George M. Bodner and Alan A. Hazari as District II candidates; and Rigoberto Hernandez and Larry K. Krannich as District IV candidates. Ballots will be mailed on or before October 10 to all ACS members in District II and District IV 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 2014-2016 term: Susan B. Butts, Thom H. Dunning, Jr., Dorothy J. Phillips, and Kathleen M. Schulz. 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, 2013.

Two vacancies on the Committee on Committees were created by the election of Ingrid Montes to the ACS Board of Directors and the appointment of H.N. Cheng as chair of the Committee on International Activities. Prior to the New Orleans meeting, the Committee on Nominations and Elections presented to the Council the following slate of candidates for membership on the Committee on Committees beginning 2013: Christopher J. Bannochie, Arindam Bose, David Lohse and Jason Ritchie. Christopher J. Bannochie and Jason Ritchie were selected to fill three-year and one-year terms, respectively.

ACS Dues for 2014

Council voted to accept the recommendation from the Committee on Budget and Finance with regard to the 2014 membership dues (an increase of \$3.00 - from \$151 to \$154). The increases to ACS dues are based upon an escalator defined in the ACS Bylaws (Bylaw XIII, 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 2013: \$151.00

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

December 2012 CPI-W Services:	268.661
December 2010 CPI-W Services:	262.954
Change in CPI-W Index:	2.17%

2014 Dues, fully escalated: $\$151.00 \times 1.0217 = \154.28

2014 Dues, Rounded: \$154.00

Change in Committees

The Committee on Committees (ConC) put forth a recommendation for the continuation of the committees that have been reviewed as required by the Committee Sunset Laws. The committees reviewed were the Committees on Chemical Abstracts Service, Environmental Improvement, and Younger Chemists. Council VOTED unanimously to continue these committees until their next evaluation. Continuation of these three committees requires Board concurrence.

Petitions for Vote

Petition to Amend National Election Procedures

After some discussion, a vote to approve the Petition to Amend National Election Procedures FAILED (85% against, 15% in favor). The petition sought to shorten the campaign period for candidates for President-Elect and to charge the Committee on Nominations and Elections (N&E) with proposing two candidates for President-Elect. Currently, N&E proposes four *nominees* from which Council selects two *candidates*. Other nominees, as now, would be put forth by members by petition, and procedures for preferential balloting would remain unchanged. All candidates would then be invited to a public forum, such as a Town Hall meeting, at the fall national meeting, and would appear on the ballot. This process would shorten the campaign period, allow all candidates to be seen by Council and other members, and ease the burden on N&E. However, under this petition, Council would no longer vote on a list of nominees. In collaboration with the Committee on Nominations and Elections, the Council Policy Committee authorized a joint task force on election timelines and procedures. This task force will examine the entire election system.

It should be noted that this change was not put forth by and was opposed by the Committee on Nominations and Elections.

Revision to Charter Bylaws for the International Chemical Sciences Chapters

The Committee on Constitution and Bylaws (C&B), in cooperation with the Committee on International Activities, asked Council to approve changes in the Charter Bylaws for the International Chemical Sciences Chapters. These changes are primarily in the Amendments section, for C&B to review bylaw changes before proposed changes are approved by the membership of the chapter. Other changes are editorial. The Council VOTED to approve changes to the Charter Bylaws for New International Chemical Sciences Chapters.

Petition to Charter One new International Chemical Sciences Chapter

One legal application had been received for the formation of the Romanian International Chemical Sciences Chapter. It consists of the Territory of Romania which is not part of any other Local Section or Chapter of the Society. The application was signed by members in good standing of the Society who reside in the Territory. It met all of the requirements and included a proposed budget for the Chapter's operations (which includes no funding from the Society). The ACS Board has authorized this action and was seeking Council approval, after which (if given) the Chapter could begin operation. The Council VOTED, in concurrence with the Board of Directors, to approve the petition to charter the Romanian International Chemical Sciences Chapter, consisting of the Territory of Romania.

Approval of Academic Professional Guidelines

The Committee on Economic and Professional Affairs (CEPA) submitted for Council approval a revision of the Academic and Professional Guidelines. It contained updates to the current version which was last revised in 2008. This was a minor revision. A more extensive revision is underway and will be presented for Council consideration in 2014. This draft was presented for Council consideration in Philadelphia and has been approved by ACS legal Counsel. The Council VOTED to approve the Academic Professional Guidelines as submitted by the Committee on Economic and Professional Affairs. These guidelines apply to those members of the academic community whose job function impacts directly or indirectly on scientists practicing the profession of chemistry.

Proposed Formula to Distribute the Local Section Allocation

The Committee on Local Section Activities (LSAC) proposed a new formula for the distribution of the Local Section Allocation beginning in 2014. The proposed formula replaces an existing formula that is not tied to the Local Section Allocation, but is instead expressed in dollar amounts that is adjusted upwards each year. The present formula is being replaced because distributions may soon exceed the Local Section Allocation. The new formula will use percentages. The total base allotment of 49% of the total local Section Allocation will be shared equally among all Local Sections. The per member allotment of 43% of the total Local Section Allotment will be divided by the total number of Local Section members and distributed based upon the number of members in a Local Section. The LSAC program funds of 8% of the total Local Section Allocation will be used to support

Society initiatives, strategic planning, and Board directives. The Council VOTED to approve a new formula for the distribution of allocations to individual Local Sections beginning in 2014.

Re-alignment of Electoral Districts

At the 2012 fall meeting, Councilors called for a broader and long-lasting solution to requirements that Board electoral districts have parity in member populations. At this meeting, the Committee on Nominations and Elections reported on their discussions of a revised redistricting proposal which brings all six election districts within 400-1,000 members of the mid-point of the permissible range. This proposed action is designed to eliminate the need for frequent small changes for some time to come. The proposal will be up for vote at the fall Council meeting in Indianapolis.

Society Finances

The Committee on Budget and Finance reported on the current status of ACS' finances. Despite the sluggish economy, ACS generated favorable operating results in 2012. Total revenue was \$490.7 million, which was \$6.1 million or 1.3% greater than the approved budget, and 3.9% higher (\$18.6M) than 2011. The Net from Operations was \$20.2 million, or \$4.3 million favorable to budget. This was largely attributable to better-than-expected performance by ACS Publications and CAS, and represents the Society's 9th consecutive year of positive operating results. While operating performance was favorable, Unrestricted Net Assets declined \$1.4 million to \$100.6 million:

Net from Operations:	\$20.2M
Investment Gains:	\$28.2M
Leadscope Expense:	(\$22.6M)
<u>Pension costs:</u>	<u>(\$27.2M)</u>
	(\$1.4M)

Finally, ACS ended the year in compliance with four of the five Board-established financial guidelines.

Member Statistics

Society membership at the end of 2012 was 163,322 - 893 lower than the total for year-end 2011 despite recruiting 24,943 new members. The net loss occurred primarily in the Regular, full member category. There was continued growth in both the Student Member undergraduate and international categories, which helped mitigate the overall decline in membership. The Membership Affairs Committee approved five pilot market data tests to increase membership.

Divisional Activities Name Change Request

The Divisional Activities Committee (DAC) received a request from the Division of Colloid and Surface Chemistry to change its name to the Division of Colloids, Surfaces and Nanomaterials. Six divisions have registered opposition to the proposed name, largely due to the use of the term 'nanomaterials.' DAC will ask Council to vote on the new name in Indianapolis, with a recommendation to approve.

Attendance Report

As of the morning of Council, the spring national meeting had a total of 15,596 attendees as follows:

Regular:	8,105
Guests:	347
Students:	5,793
Exhibitors:	946
Exhibit-only:	395

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)
2013: New Orleans, LA:	15,596 (as of Wednesday morning, April 10 th)

11,232 papers in total were presented.

Special Discussion Item

A special discussion item was put on the Council agenda for this meeting. ACS President Marinda Li Wu presented and moderated a discussion on “What else should ACS do to help members to thrive in the global chemistry enterprise?” ACS has established a strategic goal to “Empower an inclusive community of members with networks, opportunities, resources, and skills to thrive in the global economy.” In support of this goal, President Wu commissioned a task force entitled, “Vision 2025: Helping ACS Members Thrive in the Global Chemistry Enterprise,” to identify globalization opportunities and engage members in advocacy for improving the business and job climate. Following the presentation, 29 Councilors engaged in a robust discussion on what the Society currently offers or could offer to help members thrive in the global chemistry community.

Actions of the Board of Directors

The Board’s Committees and Working Groups

The Board of Directors received reports from its committees on Grants and Awards (G&A), Executive Compensation, Professional & Member Relations (PM&R), Planning, and the oversight group on Society Program Portfolio Management.

The Committee on Grants and Awards presented the Board with screened lists of nominees for the 2014 Priestley Medal 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 two awards at 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.

On the recommendation of the Committee on Professional & Member Relations, the Board VOTED to approve an alliance with the Latin American Federation of Chemical Associations (FLAQ) and to renew an alliance with the Chinese Chemical Society. The signing ceremony for alliances with the Chinese Chemical Society and the South African Chemical Institute (which was previously approved) took place prior to the open meeting of the Board of Directors. The signing ceremony for FLAQ will take place at the fall national meeting.

The Committee on Planning led a discussion based on its initial findings from the ACS Environmental Scan/Strategic Context Research; and the oversight group on Society Program Portfolio Management briefed the Board on its current activities, including plans for the remainder of 2013. In 2012, the oversight group outlined a process to effectively and efficiently enable the Society to routinely manage, prioritize and rebalance its portfolio of diverse Society programs. Currently, the oversight group is developing the necessary processes, tools, and documentation related to the initiative to put a process in place for 2014.

The Executive Director/CEO Report

The Executive Director/CEO and her direct reports updated the Board on the following: highlights of accomplishments from 2012; the major challenges and projects facing the Society in 2013; and the activities of CAS (Chemical Abstracts Service), the ACS Publications Division, and the Society's General Counsel. As part of the Publications report, the Board VOTED to approve journal editor re-appointments and an appointment to the ACS Governing Board for Publishing.

Other Society Business

The Board ratified several of its interim actions, including an appointment to the Committee on Executive Compensation.

The Board also received reports from the Presidential Succession on their current activities and plans for the remainder of 2013 and the beginning of 2014; a briefing from the new director of the ACS Green Chemistry Institute; and a report on the newly instituted ACS Career Pathways Workshops.

The Board's Open Session

The Board held a lively, well-attended open session which featured a special forum focused on two questions: 1) "What one thing would you like from ACS that you don't get now?" 2) "What one thing do you get from another organization that you wish you got from ACS?"

Members attending this standing-room only session received a brief overview of current Society offerings followed by an exchange of several ideas on future services and products.

Additional Information

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

m.wu@acs.org – contact information for ACS President Marinda Wu

www.acs.org/leadscopeqa - ACS vs. Leadscope questions and answers

www.acs.org/newmember - information on “Why should I join the ACS?”

nomelect@acs.org – email address for the Committee on Nominations and Elections

www.acs.org – then click on “About Us” and scroll down to ACS Financial Information for information on the Society’s finances

safety@acs.org – email address for comments and suggestions about chemical safety to the Committee on Chemical Safety

www.acs.org/bulletin5 - ACS governing documents including information on petitions and certified bylaws for all units

bylaws@acs.org – email to send petitions (deadline May 22)

www.acs.org/ei - information on the ACS Entrepreneurial Initiative

www.acs.org/sequester - location for completing the survey on sequestration

www.acs.org/supportfedscience - information on ACS materials related to federal S&T funding

www.acs.org/ethics - information on the ACS Committee on Ethics

<http://nationalethicscenter.org> – “Ethics CORE” web address and the chemistry landing page which links to chemistry related ethics content (click ‘resources by discipline’ then click ‘chemistry’)

Local Section Resources

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

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

speakers@acs.org – nominate speakers for Online Speaker Directory

[outreach@acs.org](http://www.acs.org/outreach) – information on “Celebrating Chemistry” for 4th – 6th graders

Bonnie Lawlor and Andrea Twiss-Brooks, CINF Councilors



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Highlights from the Joint Board Council Committee on Publications

The open session of the ACS Joint Board-Council Committee on Publications (JBCCP) is usually scheduled on Friday afternoon before each National Meeting and is open to any society members. The President of the ACS Publications Division, Brian Crawford, provides an update on the activities of the Division over the past 6 months to the Committee and the ACS membership. Highlights from the New Orleans presentation are posted [here](#). The following summary was provided by Leah McEwen, Committee Member and CINF Secretary. Questions regarding the Committee may be directed to the Committee Chair, Stephanie L. Brock, email: sbrock@chem.wayne.edu.

Highlights from the ACS Publications Division operations included the following:

- Two new journals, *ACS Macro Letters* and *ACS Synthetic Biology*, published full schedules in 2012. Forthcoming titles in 2013-2014 include *ACS Sustainable Chemistry & Engineering* and *ACS Photonics and Optoelectronics*. New Editors-in-Chief were announced for *Chemical Research in Toxicology* and *Inorganic Chemistry*.
- The ACS Member Benefit Program offers to members a variety of access options to the full publication suite, including a pre-determined number of complementary downloads. 20% of members have utilized the service since it launched in late 2011. More information is [here](#).
- The *ACS Style Guide*, 3rd Edition is now available as PDF with XML metadata files on the Publications platform (<http://pubs.acs.org/isbn/9780841239999>). The guide is accessible to institutional subscribers, users with ACS passwords, and through the new ChemWorx management tool.
- *C&EN* enjoyed several new enhancements to the website, mobile platform, syndicated content delivery, blog-space and other social media. In addition to providing for information venues to members, these avenues have encouraged connections with other journalists and news outlets. The *C&EN Mobile* app won an award from the American Association of Publishers and is now available through Apple's Newsstand.
- Several process and infrastructure enhancements significantly increased the quality of graphics, reduced publication time, and increased peer-review and editorial staff efficiency. The ACS Publications and CAS editorial production systems are now on a common platform. New platform features include: enhanced reference and author linking, digitization of legacy supplementary information, and soon PDF annotation.
- The international presence of the Publications Division continues to increase through editorial visits, participation in scientific meetings, the [ACS On Campus](#) program, and institutional subscriptions and usage.
- ChemWorx was launched in early 2013. It is a research management tool designed for researchers in the chemical and related sciences that combines reference discovery and management, professional networking, group and task management, and manuscript preparation in a single interface. The initial version is free to anyone with an ACS login ID. For more information, see <https://pc.acschemworx.acs.org>.

Continuing from 2012, the Publications Division is focusing on more library outreach, including the launch of several online resources: the online version of the *ACS Style Guide*, post-cancellation access to PDF and HTML formats instead of CDs, enhancements to ACS Mobile, new episodes of

the Publishing 101 series, the launch of the new information management system ChemWorx and expansion of the ACS On Campus program. A Summit Program is underway to further engage in dialogue to understand library priorities and concerns and demonstrate commitment to the library community. 2014 pricing will be value-based and focus on electronic subscriptions.

Crawford discussed the Open Access publishing strategy for the Publications Division. He characterized a competitive landscape, including various hybrid strategies being pursued by the nearest competitors, as well as successful journals “born” OA such as *PLOS ONE* and new potentially “disruptive” models emerging such as PeerJ and eLife. He said that in 2011, 9% of the papers indexed in *Journal Citation Reports* were available via open access, with the balance of 91% available through subscriptions. Pressure for openly accessible federally funded research output is increasing through the Fair Access to Science and Technology Research Act ([FASTR](#)), and the recent memo from the Office of Science and Technology Policy (OSTP) in response to the “We the People” [petition](#), directing federal agencies with more than \$100 million in research and development expenditures to develop plans to support increased public access to the results of federally-funded research. The OSTP memo states that each agency “shall use a twelve-month post-publication embargo period as a guideline for making research papers publicly available; however, an agency may tailor its plan as necessary to address the objectives articulated in this memorandum, as well as the challenges and public interests that are unique to each field and mission combination.”

Meanwhile, the Research Councils in the UK (RCUK) have issued a new policy on OA publishing based on the previous Finch report and new funding mechanisms to cover article publishing charges ([revisions](#), 4/8/2013). The European Union is considering this issue as part of their [Horizon 2020](#) research program. Asia has not yet emerged on the OA stage, but represents a significant and growing portion of authors, revenue, and usage of the ACS Publications suite.

The ACS Publications Division policy currently supports both mandated Green OA and Gold OA through the [AuthorChoice Program](#), which includes discounts for members. Looking forward, the Publications Division will foster dialogue with editors and authors, push support for incentive programs for AuthorChoice, and consider interoperability. On the data access front, discussion is continuing with editors as reported at the last open meeting.

Comments from the floor: Thanks for the online availability to the *ACS Style Guide*.

Crawford: Considerations for more interactive features are underway.

Leah McEwen, Member, Joint Board Council Committee on Publications



The ACS Division of Chemical Information offers a series of free webinars.

The next webinar will be held on June 27, 2013, 11 am US EST

Using Wikipedia as a Source of Chemical Information

Martin A. Walker, SUNY Potsdam

Meeting Access: <http://acspubs2.adobeconnect.com/cinfwebinar-jun2013>

For more information (abstract, speaker bio) visit <http://www.acscinf.org/content/webinars>

CINF Social Networking Events

As fellow CINF members like to praise: “We know how to have fun!” The Spring Meeting in New Orleans was no exception. At this meeting we had a slight change in the pre-conference day schedule, arranging for a “Functionary Thank-You/Future Brainstorming Dinner” on Saturday evening instead of the usual long-range planning lunch. Our Chair Tony Williams, together with Secretary Leah McEwen and Chair-Elect Judith Currano, encouraged CINF members and those interested in CINF to get together over a delicious dinner and to share their views on why CINF is useful and what can be done better. The dinner held at Calcasieu private dining was fantastic: lovely ambiance and impressive cuisine. It was enjoyed by 32 attendees. Over dinner each table put together a series of notes led by a facilitator on what had made them join CINF and why they stayed on as well as which membership benefits might be missing. After a bit of discussion the notes from each table were gathered and categorized, and then led to an interesting set of themes that will be useful in charting CINF’s future.

On Sunday evening we gathered at the CINF Welcoming Reception supported by seven helpful sponsors: [ACS Publications](#), [Bio-Rad](#), [Chemistry Central](#), [InfoChem](#), [Optibrium](#), [Perkin Elmer](#) and [Thieme Chemistry](#). Despite a somewhat rocky start, the reception got back on track thanks to quick thinking on the part of the Convention Center staff. The Welcoming Reception was attended by over a hundred people including both CINF members and guests. It was good to see many well-known faces as well as quite a few new ones. During the reception we arranged an impromptu membership drive resulting in a number of new sign-ups. As before, the Welcoming Reception hosted the CINF Scholarship for Scientific Excellence poster session (sponsored by [Accelrys](#)) and this meeting saw four posters being presented.

The CINF Luncheon on Tuesday was our final social event at the Spring Meeting. Sponsored exclusively by the [Royal Society of Chemistry](#), the Luncheon gathered about 75 attendees for a delicious meal and an excellent talk by science comedian, Brian Malow, who regaled us with jokes and puns on science topics, and also discussed the issues around broadly communicating science to non-scientist audiences. During the Luncheon the CINF Scholarship for Excellence awards were presented to the winners, Julien Thibault (University of Utah) and Amir Seddik (University of Vienna). Congratulations to the recipients!

We gratefully appreciate and thank all our sponsors. Without their generous support the Division would not have been able to host these social networking events. We are also thankful to our CINF colleagues, Leah McEwen and Judith Currano, for taking on the herculean task of arranging venues, keeping track of paperwork, and ensuring that it all came together.

Due to various circumstances, we had to curtail some of our social events such as Harry’s Party, but we certainly made the best of what we had. I have no doubt that we will entertain a series of delectable social networking events at the next Fall Meeting, where I hope to see many of you again!

Rajarshi Guha, Chair, Fundraising Committee

Photos from the Spring 2013 ACS National Meeting are at
<http://www.flickr.com/photos/cinf/>

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