

CHEMICAL Information BULLETIN



ACS
Chemistry for Life[®]

Summer 2014 — Vol. 66, No. 2

A Publication of the
Division of Chemical Information
of the ACS

ISSN: 0364-1910



Chemical Information Bulletin

A Publication of the Division of Chemical Information of the ACS

Summer 2014 — Vol. 66, No. 2

Svetlana Korolev, Editor,
University of Wisconsin, Milwaukee
skorolev@uwm.edu

Message from the Chair	2
CINF Webmaster Needed - You Can Help!	3
Letter from the Editor	4
Awards and Scholarships	5
2014 Lucille Wert Scholarship Announced	5
2014 CINF Scholarship for Scientific Excellence Presented	6
Applications Invited for CSA Trust Grants for 2015	7
Technical Program	8
Meet Your New Program Chair: An Interview with Erin Bolstad	8
Translational Cancer Bioinformatics	12
Neglected and Rare Disease Drug Discovery Needs Open Data	14
Ethical Considerations in Digital Scientific Communication and Publishing	15
Cloud Computing in Cheminformatics	18
Editors' Corner	20
Book Reviews	22
Energy for Future Presidents: The Science Behind the Headlines	22
Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications	23
Committee Reports	24
CINF Education Committee	24
ACS Committee on Ethics: An Overview	25
ACS Council	27
Joint Board-Council Committee on CAS	33
Joint Board-Council Committee on Publications	34
CINF Social Networking Events	38
Sponsor Announcements	39
InfoChem News	39
RSC: How Do You Solve a Problem Like Open Access?	40
ACS <i>Central Science</i> : A New Multidisciplinary Journal Coming in 2014	42
PerkinElmer Launches Cloud-based Platform	43
CINF Officers	44
Contributors to this Issue	45

ISSN: 0364-1910

Chemical Information Bulletin, © Copyright 2014 by the Division of Chemical Information of the American Chemical Society

Message from the Chair

Greetings from sunny Philadelphia!



It was wonderful to see many of you at the ACS National Meeting in Dallas. Hopefully, those who attended were able to enjoy many riveting talks, as well as take opportunities to network, discuss research, and simply hang out with friends. For those who did not attend, many presenters have graciously allowed us to post their slides online; visit <http://bulletin.acscinf.org/node/557> to browse the program and see those slides that are available. If you are a presenter and you have not supplied a copy of your slides, please consider doing so!

At the Saturday Executive Committee meeting, we discussed several topics that may be of broad interest. This spring, we will be reviewing our bylaws to ensure that our current practices are in compliance with our codified procedures; one of the changes that we hope to propose is a lessening of the restrictions on committee membership. Our current bylaws state that a committee appointment is for a single year, and that an individual may serve no more than three one-year terms on a committee. This is much more restrictive than the term limits on ACS National Committees, which allow members to serve three terms of three years each, and we propose to relax this restriction. To encourage more CINF members to become aware of and take part in the good work that our committees do, we will be hosting a “Committee Dinner” on Saturday evening at the Fall ACS National Meeting in San Francisco. Any CINF member is welcome to attend, talk to representatives from the various CINF committees, and then sit down to dinner with the committee of his or her choice to do some one-time committee work or (hopefully) begin a longer-term involvement!

The Executive Committee also discussed ACS Innovative Project Grants (<http://www.acs.org/content/acs/en/funding-and-awards/grants/acsccommunity/tdinnovativegrant.html>), which are awarded twice annually to technical divisions. These grants, of up to \$7,500 per project or \$12,500 per division per year, are given for new projects, activities, or initiatives proposed by the division. Projects may be proposed by any division member, but they must be accompanied by a letter of support from the chair. CINF has been particularly successful in securing IPGs for many of our initiatives, including recording national meeting presentations, producing career vignettes, and, most recently, a collaboration with the Division of Chemical Health and Safety (CHAS) to build a “Web platform and information management process to support a laboratory chemical risk assessment tool.” Many of the recent IPGs that CINF has put forward have been funded, but we are always looking for new ideas; if you have an idea for an innovative project, please contact the CINF Secretary, Leah McEwen (lrn1@cornell.edu).

CINF is actively seeking opportunities to partner with other scholarly societies and ACS technical divisions, local sections, and regions. We are a co-organizer of the International Conference on Chemical Structures (ICCS), which will take place from June 1 - 4, 2014, in Noordwijkerhout, The Netherlands (<http://www.int-conf-chem-structures.org/home.html>), and we will be organizing a symposium on open chemistry at the 2015 Pacificchem conference. We are also collaborating with the

Special Libraries Association's Chemistry Division (DCHE) to plan the next Bi-Society Symposium, which DCHE hopes to host at the 2015 SLA Annual Conference in Boston. The theme of that program will be chemical information in support of health and safety. Please stay tuned for more information on both the Pacifichem and Bi-Society programs! However, in addition to programming on a national level, we would like to become more involved with regional and local section programs. If you have an upcoming regional meeting in your area, please let us know, and consider volunteering to organize a symposium, session, or short-course surrounding an appropriate topic in chemical information!

Finally, following up on the long-range planning dinner that Tony Williams organized at the New Orleans National Meeting, the CINF Membership Committee will be embarking upon a number of projects, which include distributing a broad-reaching member survey and creating some more detailed member profiles. More information will be broadcast in the coming months; I hope that you will consider taking part in both projects, letting us know what you do and why you love it, why you value your CINF membership, and what CINF can do for you both now and in the future!

With best wishes for a healthy and productive spring,

Judith Currano, Chair, ACS Division of Chemical Information

CINF Webmaster Needed - You Can Help!

Danielle Dennie, our CINF Webmaster, has moved from the Chemistry Library to Webster Library as a Computer Science, Electrical/Computer Engineering and Math subject librarian at Concordia University. As a result, she will be stepping down as our Webmaster. We are grateful for her efforts in migrating the CINF website into a Drupal environment as well as ongoing maintenance of the site. We wish Danielle well in her new endeavors.

This means, though, that we now have an opening for a new Webmaster. If you have been thinking about ways to get involved, or to get more involved, with CINF, this is an excellent way to do so. Responsibilities include interacting with a variety of CINF members and Committees to upload new content on the site, including such things as the Chemical Information Bulletin, presentations from National Meetings, announcements and news, etc. You wouldn't need to generate the content yourself. Familiarity with Drupal would be helpful, but not required. Also, we have an Assistant Webmaster, so you wouldn't be on your own.

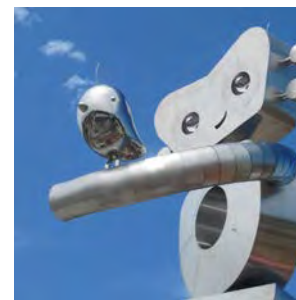
If interested, please contact me at d_martinsen@acs.org.

Thanks for your consideration, and thanks again to Danielle!

David Martinsen, Chair, Communications and Publications Committee

Letter from the Editor

As a salute to the attendees of the Spring 2014 ACS National Meeting I selected a photo of the “Travelling Man” sculpture (designed by artists Brad Oldham and Brandon Oldenburg, and put in 2009 in Dallas) for the cover page of this issue. Besides the image quality (by Dave Hensley), the “Travelling Man: Walking Tall” spirit speaks well to the ACS meetings conveying “the heights of possible achievements” dream and reaffirming a message about the importance of conferences: “Whether it’s the classic artist or the artful businessman, travel is an essential component of success.” ([The story](#)).



Based on the experiences of Spring conference attendees this issue provides well-rounded coverage of CINF happenings in Dallas. Starting with “Greetings” from Division Chair Judith Currano you will find out about activities planned and opportunities to get involved in CINF in the upcoming months. Congratulate Katrin Stierand and Ellen Strobel on their being selected as scholarship winners. Meet your new Program Chair Erin Bolstad to learn about her perspectives for the CINF technical program in the coming years. Erin’s response continues a sequence of “behind the stage” interviews with the past Program Chairs, [Rachelle Bienstock](#), [Rajarshi Guha](#), and [Leah McEwen](#) (then Solla). Jeremy Garritano served a short term in 2013 and shared some of his “know-how” in this issue too.

Read four CINF symposium write-ups, namely: *Translational Cancer Bioinformatics: Data, Methods and Applications* by Rachelle Bienstock and Shuxing Zhang, *Neglected and Rare Disease Drug Discovery Needs Open Data* by Sean Ekins, *Ethical Considerations in Digital Scientific Communication and Publishing* by Leah McEwen, and *Cloud Computing in Cheminformatics* by Phil McHale, as well as five committee reports: CINF Education Committee, and Joint Board-Council Committee on CAS, both chaired by Grace Baysinger, an overview of the ACS Committee on Ethics chaired by Gregory Ferrence (associated with a CINF symposium on “Ethical Considerations”), ACS Council, and highlights (with presentation slides by Brian Crawford) from the Joint Board-Council Committee on Publications. An attentive reader may notice that a few CINF members are actively engaged in organizing and chairing multiple symposia and committee meetings so that their writing numerous articles for this *Bulletin* was almost impossible. In this context, I would like to call for “roving reporters” of the CINF sessions. If you are planning to attend the next meeting in San Francisco and interested in writing for the *Bulletin*, please contact me at skorolev@uwm.edu. We all appreciate reading symposium-related articles, and it would be quite interesting to hear the perspective of the technical program from attendees.

Next, welcome David Shobe and Philip Heller! David, Assistant Editor of summer and winter issues of CIB, compiled a concise bibliography of crystallographic databases as a nod to the 2014 International Year of Crystallography for his new column, *Editors’ Corner*. Philip, Fundraising Chair, provided a list of enticing social events from Dallas and for San Francisco, and collected news from our sponsors for this issue. I would like to thank Max Espley for contributing a success story of the “Gold for Gold” pilot, which, coincidentally, fit nicely with a commentary of the upcoming new journal *ACS Central Science* provided by Sara Rouhi.

In conclusion, I would like to thank all writers for submitting their articles to this issue. Special thanks to Danielle Dennie for her fast-paced work as CINF webmaster, especially with uploading the Bulletins into Drupal overnight, and I wish her well in the future!

Svetlana Korolev, Editor, Chemical Information Bulletin

Awards and Scholarships

2014 Lucille M. Wert Scholarship Announced



Ellen Strobel (photo at left) has been selected as the 2014 recipient of the Lucille M. Wert Student Scholarship. She holds a B.S. in Biochemistry from the University of North Carolina Asheville and an M.S. in Physical Chemistry from the University of Tennessee Knoxville where she is currently pursuing an M.S. in Information Science.

Ellen is interested in a career as a university librarian with responsibilities over chemical information resources as well as in education and learning. 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.”

Andrea Twiss-Brooks, Chair, CINF Awards Committee

2014 CINF Scholarship for Scientific Excellence Presented

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) is designed to reward graduate students and post-graduate fellows in chemical information and related sciences for scientific excellence and to foster their involvement in CINF. Since 2005, the program has awarded scholarships at each of the ACS National Meetings and has awarded 50 scholarships in total.

The award at the Spring 2014 National Meeting in Dallas was jointly-sponsored by Springer and InfoChem. Applicants presented their posters at the CINF Welcoming Reception and the Sci-Mix session. Dr. Steffen Pauly of Springer (photo at right) presented the scholarship valued at \$1,000 to Katrin Stierand at the CINF Luncheon during the same meeting.

Katrin Stierand is a postdoctoral fellow at the Center for Bioinformatics (ZBH) at the University of Hamburg, Germany. Her excellent poster, co-authored by Matthias Rarey, was entitled “PoseView: visualization of protein-ligand interactions in two dimensions.”



The next scholarships are sponsored by the Royal Society of Chemistry and will be awarded at the ACS National Meeting in San Francisco, CA, in the fall of 2014.

Guenter Grethe, Coordinator, CINF Scholarship for Scientific Excellence



Chemical Structure Association Trust Grant: Applications Invited for 2015

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 now inviting the submission of grant applications for 2015.

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. One or more Grants will be awarded annually up to a total combined maximum 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; for example, 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 for the 2015 Grant is March 13, 2015. Successful applicants will be notified no later than May 2 of the relevant year.

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 chescot@aol.com prior to submission so that she can contact you if the e-mail does not arrive.

Recent Grant Awardees:

2013

Dr. Johannes Hachmann: Department of Chemistry and Chemical Biology at Harvard University, Cambridge, MA. He was awarded the Grant for travel to speak on “Structure-property relationships of molecular precursors to organic electronics” at a workshop sponsored by the Centre Européen de Calcul Atomique et Moléculaire (CECAM) that will take place October 22 – 25, 2013 in Lausanne, Switzerland.

Dr. Robert S. Paton: University of Oxford, UK. He was awarded the Grant to speak at the Sixth Asian Pacific Conference of Theoretical and Computational Chemistry in Korea on July 11, 2013. Receiving the invitation for this meeting has provided Dr. Paton with an opportunity to further his career as a Principal Investigator.

Dr. Aaron Thornton: Material Science and Engineering at CSIRO in Victoria, Australia. He was awarded the Grant to attend the 2014 International Conference on Molecular and Materials Informatics at Iowa State University with the objective of expanding his knowledge of web semantics, chemical mark-up language, resource description frameworks and other on-line sharing tools. He will also visit Dr. Maciej Haranczyk, a prior CSA Trust Grant recipient, who is one of the world leaders in virtual screening.

2012

Tu C Le: CSIRO Division of Materials Science & Engineering, Clayton, VIV, Australia. Tu 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.

A complete list of the previous grant awardees is at: <http://bulletin.acscinf.org/node/457>

Bonnie Lawlor, Chair, CSA Trust Grant Committee

Technical Program

Meet Your New Program Chair: An Interview with Erin Bolstad

Erin Bolstad heads up the US-based consulting wing of ChemAxon, with focus on services and project management for life sciences and the drug discovery process. She has been with ChemAxon since October 2011. Prior to that Erin spent several years in a few various adventures: cheminformatics research associate with focus on connecting several CNS-based research units and extracting relevant chemistry/biology information, a senior scientist working on molecular biology-based antibiotic design, and a postdoc working on structure-based drug design. Erin received a PhD in computational organic chemistry from the University of Montana in 2006. She has published in several journals from her various collaborative and academic works, and holds a patent from her postdoc work on designing inhibitors for dihydrofolate reductase.



Svetlana Korolev:

Erin, congratulations on being the new CINF Program Chair! Please tell us a little bit about your career path and research interests. What brought you to the field of chemical information? How does CINF overall and its technical program specifically complement your professional ambitions? How does your organization, ChemAxon, perceive your volunteering for CINF?

Erin Bolstad:

Thanks Svetlana! My career path has always kind of circled around the “hand in many pots” syndrome, and finding a way to integrate those interests. As a college junior I realized I could not work on a studio art degree and research-based computational chemistry degree in parallel, so I decided to major in computational chemistry with art as a recreational “spare time” interest (it seemed like a more reliable career path than an art major with computational chemistry as a recreational past time). Computational chemistry/drug design was an obvious segue from my interests in art, biology, chemistry and computers. From there it rapidly lead to cheminformatics, to make sense of the incredible amounts of data available on both the biology and chemistry fronts. I’ve since fallen in love with the pursuit of solving complex questions via handling of large-scaled sets of data from the A to Z areas of drug design.

The consulting work in ChemAxon is perfectly in line with this from both a scientific and human perspective, as the large-scale project management and “cat herding” also appeals to my interests. This tied-in perfectly with the CINF Division and Program Chair position, as CINF is heavily geared towards new mechanisms of large data management and research, as well as looking at how these techniques lead to novel drug design. ChemAxon is a global company in cheminformatics services and toolkits, so volunteering for this position falls right in line with our own interests and research. ChemAxon were very supportive of this.

SK:

How did it happen that you became the CINF Program Chair? What major activities or goals do you have for your tenure in this position? Over the past decade the term of the Program Chair has been reducing gradually from as long as three years to one year in 2013. Are you planning on reversing this trend?

EB:

At the ACS Spring Meeting of 2013, I was asked by a colleague who had served on the Program Committee for some time if I would be interested in the Program Chair position. He knew of my interests and felt it would be a good fit. Despite having zero ACS committee experience at the time, I was excited by the opportunity! Due to the turn-over speed, the 2014 Fall Meeting is the first one I've actually organized, and it's been quite the learning curve.

With current research in the life sciences field relying on big data, cheminformatics becomes more and more of a critical component for research. One of my goals for CINF Program Chair is to reach out to other divisions and look at this interdependency and how to bring it to the forefront of both awareness and research fronts. CINF is not just for "chemical libraries" and "data repositories" specialists as I once naively believed. I'd also like to look at novel ways for approaching the new generations of researchers who rely on several divisions (not just one) and how they can contribute across the board.

Yes, my tentative plan for the Program Chair term is for two years. With only two programs a year, it seems like that would be the most effective way to make an impact. Otherwise, I learn the ropes just in time to train someone else and pass them on. With a two-year term there's actually time to let experience guide some progress.

SK:

Erin, how do you evaluate the spring meeting in Dallas? What was the most exciting part of it? One noticeable hallmark was a high level of collaboration: all CINF symposia except for two were listed with cosponsorships, including a new partnership with RSC CICAG (Chemical Information and Computer Applications Group), an established relationship with the CSA Trust, and a blend of connections with many other ACS Divisions (CHAL, CHED, COMP, MEDI, ORGN, PHYS) and Committees (ETHX, PROF, YCC). What are the involvements and benefits of such co-sponsorships? How do you establish alliances with other organizations?

EB:

The spring meeting in Dallas was really a transitional time. While it was organized by the previous Program Chair, it was when I really stepped in as leading the programming for future events. I have to tip my hat to Jeremy Garritano (photo at right) for the excellent Dallas program, and I am looking forward to seeing how these future plans play out!



The questions regarding cosponsorships should be referred to Jeremy, who kindly shared his experience as follows: collaborations can be as simple as listing another ACS Division or Committee as a cosponsor. This gets a symposium cross-listed in the cosponsor's program as well. Other collaborations can occur where one of CINF's members helps to organize a session in another Division. In Dallas we had a great example of this where Tony Williams co-organized a symposium with Harry Pence on "Mobile Devices, Augmented Reality, and The Mobile Chemistry Classroom." This session took place in the CHED program, but CINF was a co-sponsor. Most of the time cosponsorship does not involve any financial commitment, so it is a way to cross-promote our program to other ACS Divisions or Committees. Another example is how the ACS Committee on Ethics and the Younger Chemists Committee (among others) agreed to be cosponsors for our session on "Ethical Considerations in Digital Scientific Communication and Publishing." Often it is as simple as asking the corresponding Program Chair if we can list the other Division or Committee as a cosponsor. Sometimes we will even ask for suggestions of potential speakers in order to draw interest from cosponsor members.

SK:

The thematic programming at ACS meetings has gained a strong upwards trend recently. The themes are being proposed for future meetings up to Fall 2017 (<http://bulletin.acscinf.org/node/539>). How far in advance do you plan the Division's technical program and how does the ACS thematic programming impact it overall? What kind of support does CINF have from the Multidisciplinary Program Planning Group (MPPG)? Which of the upcoming themes are easier (or harder) for our Division to tackle?

EB:

During our meetings we put heavy focus on actual symposia topics for one to two years ahead and keep our eye on thematic programming for as far in advance as four years. We had a few sessions that we were all a titter about organizing promptly, but they were shifted to a later year in order to match with the program overall. At the same time we keep an eye on the geographical location. For the upcoming Spring 2015 Denver meeting getting involved in some of the environmental-based symposia is a key objective we've been excited about.

We have been lucky to have Guenter Grethe on board as a proactive contributor to the CINF Program Committee meetings. Guenter is a well-experienced member of the MPPG Executive Committee, who has been involved in thematic planning over many years, including his being MPPG Chair in 2009.

Some of the upcoming themes are a little more challenging for CINF simply due to their vague nature such as "Innovation from Discovery to Application," while others have us falling out of our chairs with excitement like "Computers in Chemistry": hello! CINF has both the blessing and the curse of being applicable to almost any theme, as just about everything relies on chemical information. Trying to decide when to go all out on thematic programming is a delightful "burden of choice" type exercise for CINF.

SK:

Erin, we have seen questions at CHMINF-L about the availability of CINF presentation slides and/or recordings (audio synchronized with slides). ACS has been offering "Presentations on Demand" in the past few years and, moreover, as a member benefit since last year. Unfortunately, only a very small portion of the presentations (from two or three CINF symposia) become available online after the meeting. As CINF Program Chair do you have an influence on the selection of the symposia for "Presentations on Demand"?

EB:

The "Presentations on Demand" is a pretty complex issue. There are a lot of technical intricacies involved, that limit the number of recordings ACS can make. Beyond that, once a symposium has been selected, is the matter of the speaker giving permission to ACS for being recorded at oral sessions and then posting the audio and slides on the Internet. Thus, this makes for several steps in the process. Some members may recall that CINF was at the frontline for symposium recordings and did some experimental audio recordings (MP3) of technical sessions in 2006-2008 as a pilot funded by an ACS Innovative Projects Grant, and this turned out to be too labor-intensive and time-consuming to be continued by a division volunteer. We would certainly like to see more CINF talks available online. In the meantime, the Division can suggest which presentations we'd like to have recorded (hot topics, thematic relevance, awards symposia, etc.), but ACS has the final say. We've also had a renewed push to make presentation slides (with the speaker's permission) available immediately after ACS Meetings. Dallas was a renewal of this initiative and we ended up having most of the slides available within a week of the Spring 2014 ACS Meeting closing. We'll be trying to make this happen even faster with the upcoming meeting in San Francisco.

SK:

Erin, let me ask you a personal question about your "dream" conference program. What is the ideal conference for Erin Bolstad? Which venue (city) would you pick for such occasion? Is it going to be long or short program considering a number of days? What theme would you organize it for?

EB:

There's a lot of human dynamics to work around for a "dream" program. A geographical destination that everyone wants to go to, but attendees can afford to attend (Hawaii is thus right out, alas). San Francisco is pretty close to an ideal geographical location, with San Diego trailing a close second. I'm biased being a local, but Seattle would be also super fun.

I think a lot of people burn out over the course of four long, intense days; so a high-quality shorter program might keep people's interest till the very end. Put in an open forum in the middle, followed by a lightning round of up and coming software and methods from researchers and commercial developers as a general "state of the field" update, then settling down for an afternoon of deeper analysis with more talks. Also, there should be an open coffee bar and settle down an infinite number of freshly-baked cookies because it helps with scientific inquiry.

I like diversity and part of an ongoing personal initiative for me is CINF outreach, so I'd want to attract people from other realms of research to present their work from an informatics perspective: both academic and industrial. Informatics is **everywhere!** Come and see!

SK:

We've seen many interesting calls for papers for the upcoming ACS National Meeting in San Francisco, August 10-14, 2014. Please share with us some highlights of the CINF technical program planned for the Fall Meeting.

EB:

The next meeting is where we're starting to ramp up some broad perspective and then with spring of 2015 looking at some experimental programming (stay tuned!). For the Fall 2014 ACS National Meeting we have several nifty symposia: an entire day around the theme of global challenges and communication in scientific research, several symposia with a biological tilt (biosimilars, natural products, epigenetic drug discovery), and sessions on how new technologies are playing into cheminformatic research (like Google Glass, the Maker movement, and 3D printing). Start planning now for San Francisco!

SK:

Erin, thank you so much for your time and the privilege of introducing you to the readers of this Bulletin. Best wishes for you as Program Chair leading the CINF Division into the future.

CINF slides or links to the speaker presentations given at
the Spring 2014 ACS National Meeting are at: <http://bulletin.acscinf.org/node/557>

Translational Cancer Bioinformatics: Data, Methods and Applications

The rise in use of “-omics” techniques to develop effective cancer therapies, in particular the Cancer Genome Atlas project (TCGA, <http://cancergenome.nih.gov/>), has demonstrated the significant role of computational and informational science in the study and treatment of cancer. It is with the tremendous significance of such topics in mind that this symposium was organized. Four speakers, Drs. Carlos J. Camacho (Computational and Systems Biology, University of Pittsburgh), Wenyuan Li (Molecular and Computational Biology, University of Southern California), Iwona Weidlich (CODDES LLC, Rockville, MD), and Shuxing Zhang (Department of Experimental Therapeutics, MD Anderson Cancer Center), delivered excellent presentations covering diverse aspects of ongoing research topics in this area.

Dr. Carlos Camacho (University of Pittsburgh) discussed “New chemistry and powerful interactive technologies to discover PPI antagonists,” focusing on his group’s development of computational tools for rational design of protein-protein inhibitors of critical cancer targets. He also discussed implementation and use of Pocket Query (<http://pocketquery.csb.pitt.edu/>), a web-based tool for identification of hot spots and binding pockets defined by clusters of residues at the interface of protein-protein interactions. This method can be used for virtual screening and computational design of protein-protein interaction inhibitors. The methodology has been extended to the development of Anchor Query (<http://anchorquery.csb.pitt.edu/>), an interactive tool for rational design of protein-protein interaction inhibitors through the use of defined pharmacophores and conformational searching. This methodology has been applied to the MDM2/p53 system and other cancer targets.

Dr. Wenyuan Li (University of Southern California, Los Angeles) presented his work in Dr. Jasmin Zhou’s group (<http://www.cmb.usc.edu/people/xjzhou/zhou.htm>), “Integrative analysis of multidimensional cancer genomics data,” focusing on the development of software tools and analytical methods to analyze the multi-dimensional ovarian cancer data from the TCGA project, including the copy number variation, DNA methylation, gene expression, and microRNA expression data. Using their methodology, termed Sparse Multi-Block PLS regression, they have successfully identified pathways and associations that would have been overlooked with only a single type of data. Their software is useful for recognizing hidden patterns and biological implications in multi-dimensional “-omics” data.

Dr. Iwona Weidlich (CODDES), with a title of “New application to estimate the diversity of molecular databases,” discussed Diversity Genie (www.diversitygenie.com), a set of computational tools useful for analysis of small organic molecule datasets to understand and characterize the diversity in the chemical space. The package can also be employed to sort, merge, and handle large sets of small organic molecules, including conversion between different data formats (e.g., SMILES, InChI, SDF, etc.) and filtering based on chemical and structural properties along with visualization.

Dr. Shuxing Zhang (MD Anderson Cancer Center) completed the symposium with “Computational analysis of pleckstrin homology (PH) domains for cancer drug development,” (<http://www.imdlab.org/>), a very specific example of rationally designing inhibitors for targeted cancer therapies using integrated cheminformatics, bioinformatics, and systems biology approaches.

The pleckstrin homology (PH) domain is critical in more than 250 families of proteins involved in intracellular signaling and molecular recognitions. For instance, the PH domain plays a critical role in recruiting oncogene proteins (e.g., Akt) to the membranes for their activation contributing to cancer cell growth. As the 3D folds of PH domains are highly conserved and individual PH domains possess different affinities and specificities for a variety of phosphoinositides, genomics and bioinformatics

analyses, along with structure-based methods, and can play a significant role in the rational design of selective inhibitors of these crucial cancer signaling proteins. The integrated approaches developed by this group have been rigorously cross-validated with a large set of PH domain structures, and it was successfully applied to the prediction of several PH domain proteins, followed by discovery of potent PH domain inhibitors (<http://www.phusistherapeutics.com/index.html>).

In summary, the symposium covered diverse topics from development of useful software for identifying genomic mutations in cancer pathways, to analysis and manipulation of small organic molecules, and to the rational design of promising therapeutics for targeted cancer therapies.

Rachelle Bienstock and Shuxing Zhang, Symposium Organizers



Oral presentations captured at the ACS Spring National Meeting in Dallas will be available to ACS Members after April 28, 2014 at www.presentations.acs.org

The following presentation was recorded at the “Translational Cancer Bioinformatics Data, Methods and Applications” symposium:

CINF23 New application to estimate the diversity of molecular databases. Iwona Weidlich.

CINF series of free webinars is archived at: <http://acscinf.org/content/webinars>

Please stay tuned for announcements of the upcoming CINF webinars at CHMINF-L

Neglected and Rare Disease Drug Discovery Needs Open Data

This short symposium consisting of four presentations was organized by Sean Ekins, Antony Williams and Joel Freundlich. The following three presentations (and one no show) were brought to the spring meeting attendees on Sunday afternoon, March 16, 2014 in Dallas.

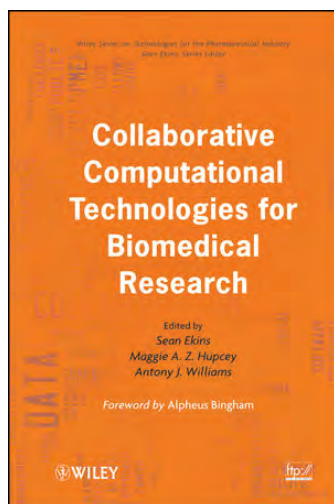
The first talk was given by Sean Ekins (Collaborative Drug Discovery) entitled “Looking back at mycobacterium tuberculosis mouse efficacy testing to move new drugs forward.” Sean Ekins described the collaborative efforts with co-authors, including co-chairs of this session, Antony Williams (Royal Society of Chemistry) and Joel Freundlich (Rutgers University), to curate and analyze a dataset of mouse *in vivo* information for tuberculosis research. He described various machine learning models based on 773 molecules, and presented external testing and molecular descriptor analyses. In addition, Sean highlighted the development of open source fingerprints used in the new version of TB Mobile and to build models that could be shared openly.

The second talk by Antony Williams described “Royal Society of Chemistry developments to support open drug discovery.” In particular, Tony discussed their cheminformatics support of [the Indian Open Source Drug Discovery](#) effort working on tuberculosis. In addition, he highlighted their involvement with [PharmaSea](#) to help to identify the classes of antibiotics by searching the oceans. Finally, Tony reviewed the acquisition by RSC of [MarinLit](#), a database of marine natural products research. This complements their natural product portfolio which includes Natural Product Reports and Natural Product Updates, and represents over 27,000 molecules to be added to ChemSpider.

The final talk by Evan Bolton (NIH) explored “How can PubChem be leveraged for neglected and rare disease drug discovery?” Evan listed NIH resources for rare diseases like the National Center for Advancing Translational Sciences (NCATS), the Therapeutics for Rare and Neglected Diseases (TRND), Genetic and Rare Diseases Information Center (GARD) and other programs. He pointed out that it is not easy to get disease information in PubChem and that they are considering how to improve it. Evan proposed that scientists working on open source rare and neglected disease research could upload their data in PubChem.

This session may be one that could be expanded in future to track the developments in data and tools for rare and neglected diseases.

Sean Ekins, Symposium Co-Organizer



[Collaborative Computational Technologies for Biomedical Research](#):
Technologies for the Pharmaceutical Industry Series
Editors: Sean Ekins, Maggie A. Z. Hupcey, Anthony J. Williams.
Hardcover ISBN: 9780470638033
July 2011, 576 pages, \$146, Wiley.

Ethical Considerations in Digital Scientific Communication and Publishing

Poor editing, sloppy bookkeeping, fudgy analysis, falsification? Misunderstanding, variable technical practice, outright fraud? Sightings in the published scientific literature of apparent data manipulation raise eyebrows and many such questions. A community blog discussion on a controversy around inconsistently-reported elemental analyses last summer suggests that several layers of action by multiple parties might be involved in such issues, some intentional, some perhaps not, and very few publically disclosed (<http://blog.chembark.com/2013/08/09/the-om-paper-vs-drinkels-phd-thesis/#comment-52402>). There is very little understanding through the copies of record of this research to indicate to the reading public what the process might have been regarding the review that the articles underwent and how both the editors and authors approached any confusion over data representation and adjustment.

One way or another, it appears that the community is becoming more aware of potential concerns with the responsible reporting of data and other ethical issues with the scientific publication process. How much of this awareness might be arising from more transparent community discussion via blog and twitter-spheres, less transparency of handling data from measurement through analysis and eventually as publication quality figures, and/or greater pressures on the research and publication systems globally is complicated to sort out. Engaging the chemistry research community in conversations is certainly an important part of the process. To members of the American Chemical Society (ACS) Ethics Committee (ETHX) and Division of Chemical Information (CINF) it seemed timely to organize a symposium on the ethical challenges that arise in the course of preparing for presentation.

ETHX and CINF teamed up with the ACS Divisions of Chemistry and the Law (CHAL), Professional Affairs (PROF), and Publications to bring together a diverse group of editorial professionals at the recent ACS National Meeting in Dallas, TX to discuss a range of challenges, old and new, and strategies to re-enforce responsible conduct in the publication process. The international speaker set included senior staff and science editors from several core chemistry publishers including the ACS, the Royal Society of Chemistry (RSC) based in the UK, and Wiley-VCH based in Germany and publishing the journals of the Gesellschaft Deutscher Chemiker (the German Chemical Society, GDCh). Also represented were several other publishing and supporting organizations concerned with ethical issues, some with particular focus on data representation, including the Cambridge Crystallographic Data Centre (CCDC), and the American Physiological Society (APS), the Committee on Publication Ethics (COPE), and CrossRef. Abstracts and some slides are available on the CINF site at: <http://bulletin.acscinf.org/node/557>. Following are my own reflections from my notes; any omissions or misrepresentations are my error.

Considering the above case, curation of data is an important concern in the publication process, including best practices for representation, processes for checking and validation, and communicating with authors on subsequent corrective action. Some data types such as crystallographic data are regularly deposited with articles as part of the review process and subsequently curated in databases. The CCDC receives and curates standardized files of coordinates from a variety of publishers, validates the structures in-house and sends back identified errors to authors for correction. The accumulated database is searchable with software that enables further analysis, visualization, curation, and system development that are sustained through distinct subscription streams. Another example is the representation of visual types of data in figures, such as protein separation gels used in physiological research. The APS has found that figure manipulation accounts for a large majority of problems that raise ethical flags in the course of article submission, including general presentation issues: splicing images, adjusting contrast or dropping backgrounds, and poor resolution. An in-house

discipline-trained scientist has been assigned to analyze the types of problems and detection scenarios, develop a communication process with authors, and publication guidelines including a policy of transparency concerning image rearrangement as well as a list of “don’ts” to curb misplaced efforts up front. These organizations are focused on engaging authors and the research community through community curation scenarios and graduate education outreach.

Data manipulation and similar ethical concerns have accompanied the exchange of scientific information for centuries. An article on fraud in science in a Wiley journal quotes 19th century British scientist Charles Babbage of the Royal Statistical Society classifying misconduct: “hoaxing, forging, trimming, and cooking,” (DOI: 10.1111/j.1740-9713.2007.00215.x pg 24). The most common types of ethical concerns brought forward by the journal editors presenting in this session included questions of authorship, prior publication and self-plagiarism. Apparently, not all authors are always aware that their names have been included on submitted manuscripts, and the ACS Publications Division now issues letters to all authors listed on manuscripts to verify submission and that all are aware. Prior publication can be particularly confusing as it is acceptable in some situations such as theses, earlier communication articles and in some fields, preprint repositories. Specific policies concerning prior publication often lie with the editorial offices of specific journals to contend with the shifting research priorities appropriate to the subject coverage and it is important for both the editors and authors to be in communication and up front about handling prior publication of research results. Other concerns include duplicate submission, almost impossible to detect before publication; self-plagiarism, particularly problematic in review articles intended to build across the art of a research area; and “dry-labbing,” reporting of procedures not actually performed that becomes evident with reporting of unrealistic reaction conditions or inappropriate results.

Many organizations are interested in the questions of ethics arising in the course of scholarly publication. A memo from the Office of Science and Technology Policy (OSTP) in 2010 directed US funding agencies to “establish principles for conveying scientific and technological information to the public” (<http://www.whitehouse.gov/administration/eop/ostp/library/scientificintegrity>). In Europe, promotion of responsible conduct is discussed by the European Association for Chemical and Molecular Sciences (EuCheMS, <http://www.euchems.eu/divisions/ethics-in-chemistry.html>). The ACS Committee on Ethics serves as an educational resource and clearinghouse on ethical considerations and coordinates communication and programming activities (see the committee overview in this issue of *CIB*). Publishers take their editorial role in these concerns very seriously. They associate through various professional organizations to streamline and network best practices and collectively support the process of addressing challenges. Various tools are available to support the work of editors, reviewers and the overall publication process, including the CrossCheck screening tool developed by CrossRef to flag overlapping text against a growing corpus of full text scholarly literature for further review and implemented by publishers as part of the editorial workflow (<http://www.crossref.org/crosscheck.html>). It is not a plagiarism detector or a comprehensive sweep of all published literature, missing most supplemental information and interpretation of image data, including equations. Collaboratively-sourced tools for developing clear and consistent guidelines and process flowcharts are also available from the publisher member-based COPE (<http://publicationethics.org/about>). Community-based discussions of specific example cases are collated and anonymized into a knowledge bank of lessons learned available for the broader public. A recent analysis of the cases suggests a shift in focus towards more discussion of conflict of interest, correction of the literature, data, misconduct or questionable behavior, and peer review.

It is increasingly important to support clear and consistent processes for all parties involved in review, handling identified concerns, reaching resolution and developing understanding of the broader issues and responsibilities. RSC has assigned a dedicated staff position to follow the overview of cases and address consistency, with a goal of striving for agreement among all parties, including in cases of

retraction, where authors sign retraction notices before they are posted. The ACS also supports authors through a suite of educational materials related to issues of ethics, including episodes of the Publishing Your Research 101 video series on ethical considerations, copyright and the review process (<http://pubs.acs.org/page/publish-research/index.html>).

Representation issues are all around us in the irrepressibly malleable digital environment. How much manipulation is inadvertent? How much of this activity is concerned with attempting to look professional, how much is involved in striving for the right story, how much wrapped up in building reputation, how much is simply confusion over proper procedure? Creativity in research that builds usefully on the scientific corpus is inherently a juggling act between consistency and aberration. Researchers are entrusted with due diligence in their experimental design, analysis and documentation. Feeding back into the corpus involves additional juggling of representation and expression of data and rationale. The importance of the moment of publication in defining a line of inquiry and the critical role of trust in upholding the integrity of the scientific record speaks to the long-standing oversight of the editorial process in scientific publication. As the acceleration of research output outpaces traditional publication outlets and the digital environment opens new opportunities for data sharing and communication, both curated and wild, the supportive processes of ensuring responsible conduct in research and publication are put to the test. The questions of what is involved in the editorial process in the era of digital scientific publishing and what are the ethical considerations that arise continue to evolve with the practices of both science and publishing.

The author would like to thank the presenters, the co-sponsors of the symposium, with particular acknowledgement of the organizing efforts of Heather Tierney, for bringing this endeavor to successful fruition. Supporting sources are referred in-line.

Leah McEwen, Symposium Co-Organizer



Oral presentations captured at the ACS Spring National Meeting in Dallas will be available to ACS Members after April 28, 2014 at www.presentations.acs.org

The following four presentations were recorded at the “Ethical Considerations in Digital Scientific Communication and Publishing” symposium:

CINF52 Tools for identifying potential misconduct: The CrossCheck service from CrossRef.
Rachael Lammey

CINF53 Mapping the terrain of publication ethics. Charon Pierson

CINF55 Ethics in scientific publication: Observations of an editor and recommended best practices for authors. Kirk Schanze

CINF57 Role of the journal editor in maintaining ethical standards in the changing publishing environment. Jamie Humphrey.

Cloud Computing in Cheminformatics

This symposium was ably organized by Rudy Potenzzone, who put together an excellent roster of speakers covering many aspects of cloud computing. Rudy was unable to attend the event as he had to attend to family business, so I stepped in to chair the session.

Six papers were presented (and one was withdrawn) by a range of speakers: one was about to celebrate ten year's operating in the cloud; some were already in the cloud when it used to be called "online," and others were just beginning to provide tools and solutions for delocalized organizations that want to take advantage of the speed of implementation and scalability of cloud-based solutions.

Barry Bunin of Collaborative Drug Discovery (CDD) opened the session talking about "Ten Years of Collaborative Drug Discovery in the Cloud." CDD provides a fully-fledged solution for drug discovery, providing all the capabilities expected in an in-house system (chemical registration, assay data management, SAR analysis, collaboration), yet delivered in a secure, auditable and hosted cloud-based system. Barry described several collaborative drug discovery programs hosted at CDD, including various permutations of academia, government agencies, CROs and big and small pharma companies. One of CDD's success factors has been its ability to integrate private with external data in a secure yet collaborative environment which is scalable and which fosters synergies between complementary techniques.

Alex Clark of Molecular Materials Informatics discussed "Cloud-hosted APIs for Cheminformatics Designed for Real Time User Interfaces." The growth in the use of the cloud has been paralleled by the increasing ubiquity of chemically intelligent, yet underpowered, mobile devices. While these can provide a pleasing user experience, the only way they can interact with large volumes of data, or kick off compute-intensive calculations is to outsource the data storage and calculations to the cloud and to access them via some type of web API. The challenge for the developer is to select the best partitioning between what should be accomplished locally on the mobile device and those that need to be sent to the powerful external server. Alex illustrated this with a very nice SAR table app for groups of compounds and data that provides clustering, scaffold analysis and assignment, and allows plotting of R-groups against each other with properties of the compounds color-coded for quick visual analysis.

There was lively discussion during the lengthened intermission, and I used the time to practice saying the next speaker's name, and then Valery Tkachenko of the Royal Society of Chemistry (RSC) described "Application of Cloud Computing to Royal Society of Chemistry Data Platforms." The focus of the talk was ChemSpider, and how the RSC has moved it to the cloud. The ChemSpider database now contains over 30 million compounds and provides data to 50 thousand visitors (from 40 thousand unique connections) each day, for 100 – 400 concurrent users at any time, so the compute power and scalability of the cloud are essential to an operation of this scale. As more properties are added to the database or calculated from structures, big data challenges arise in areas such as indexing, navigation, visualization, and Valery described techniques for addressing these. The eventual aim is for ChemSpider to become a chemistry validation and standardization platform.

Evan Bolton of the National Center for Biotechnology Information (but informally known as Mr. PubChem) spoke next on "PubChem in the Cloud." PubChem as a data repository for chemical structures and their associated properties is a self-confessed online database, so effectively pre-dates the cloud, and yet it continues to evolve to take advantage of new technologies and methods of access. With 140,000 users every day, PubChem has added a JSON-based API for uploading data, a REST-style version of its Power User Gateway, and JavaScript-based PubChem widgets that provide a rapid way to display some commonly requested PubChem data views. There is also a new

PubChemRDF, which can help researchers work with PubChem data on local computing resources using semantic web technologies.

Next up was Sharang Phatak of Dotmatics, who discussed “Your Data in the Cloud: Facts and Fears.” The talk started with a high-level overview of the increasingly delocalized and dispersed nature of current R&D, and highlighted the major concerns that are often expressed by researchers, CIOs and Intellectual Property lawyers when going to the cloud is raised. These are: is the data comprehensive; are the system and data structure flexible and scalable; is there control; can data be shared collaboratively; and is there secure access via preferred devices, including mobile? Sharang then illustrated how these fears can be dispelled by using a number of Dotmatics’ web-based tools included in the Dotmatics Platform on the Cloud to address common R&D data capture and analysis tasks.

The final speaker in the session was Nic Encina of PerkinElmer who talked about “Moving Mainstream Chemical Research to the Cloud.” While in-house installed electronic laboratory notebooks have become well accepted and widely deployed across much of the biopharma industry, and to a lesser extent in academia, the increasing acceptance of the cloud as a viable platform for collaborative research has led to the demand for easier to deploy yet powerful systems that facilitate user-driven data capture and organization, coupled with social aspects such as annotation and team-based collaboration. Nic described a new cloud-based collaborative scientific platform called Elements which allows researchers to assemble just the tools they need and to organize them how they want in an open, collaborative environment. Individuals can work in the way they prefer, while sharing project and related data through a common infrastructure.

All the speakers are to be thanked for presenting a fascinating series of talks that highlighted both the challenges and the promise of the cloud for cheminformatics; and the audience is to be commended for staying until 5:30pm.

Phil McHale, Symposium President



As well as being a world-renowned scientific publisher, the Royal Society of Chemistry (RSC) has an established presence in the field of cheminformatics hosting various resources of value to the chemistry community. Our multi-award winning [ChemSpider](#) database now contains over 30 million chemicals and provides data to many tens of thousands of scientists every day. Our micropublishing platform, [ChemSpider SyntheticPages](#), provides the most up-to-date method for chemists to deposit their synthetic procedures and share them with the community, thereby building reputation and exposure for their work. We encourage the community to take benefit from these resources.

RSC is happy to support the CINF Division with our sponsorship and to encourage further exposure to the riches that chemical information and cheminformatics can deliver.

Antony Williams, CINF Immediate Past Chair 2014, Royal Society of Chemistry

Editors' Corner



The year 2014 has been designated the International Year of Crystallography by the United Nations General Assembly, to commemorate the 100th anniversary of the discovery of X-ray diffraction and the 400th anniversary of the observation of the symmetry of ice crystals. In accordance with this, we thought it would be appropriate to describe some of the crystallographic databases that may be of interest to the chemical information professional.

The **Biological Macromolecule Crystallization Database**, available at <http://xpdb.nist.gov:8060/BMCD4/index.faces>, contains data on 43,000 proteins, nucleic acids, and viruses. It is provided as a free service by the National Institute of Standards and Technology. Each entry includes identifying data such as protein function and the species it is derived from, as well as space group and unit cell data. It does not contain a complete crystallographic structure, but a bibliographic reference to primary literature is provided.

The **Cambridge Structural Database** (CSD), found at <http://www.ccdc.cam.ac.uk/Solutions/CSDSystem/Pages/CSD.aspx>, is provided by the Cambridge Crystallographic Data Centre. The CCDC was originally part of the Department of Chemistry at the University of Cambridge, but is now a separate entity. The CSD contains crystal structures of nearly 700,000 organic, organometallic, and boron-containing compounds; over 40,000 new structures are added per year. One has to pay to access the database, but submission of new structures is free.

CRYSTMET, available at <http://www.tothcanada.com/databases.htm>, is provided by Toth Information Systems. The database provides crystallographic and supporting bibliographic information on inorganic systems, with a focus on metals, alloys, intermetallic compounds, and minerals. Three-dimensional structures can be displayed, with a variety of plot options. One has to pay for CRYSTMET; there is a demo version, but that requires Materials Toolkit, which is not free.

The **Database of Zeolite Structures**, available at <http://www.iza-structure.org/databases>, is provided by the International Zeolite Association, free of charge. It contains structural information, bibliographic references, and powder diffraction data for zeolites. The database is designed to be searched by three-letter structural code (e.g. FAU for faujasite).

The **Inorganic Crystal Structure Database** (ICSD), which can be found at <http://www.fiz-karlsruhe.de/icsd.html>, is provided by FIZ Karlsruhe. It contains about 166,000 crystal structures for elements and inorganic compounds. The term "inorganic" is used strictly here: organometallic structures are not included. The ICSD is not free, although there is a 30-day demo version. It is available on STN, or at a dedicated, password-protected website.

MINCRYST, found at <http://database.iem.ac.ru/mincryst/index.php>, is provided by the Institute of Experimental Mineralogy Russian Academy of Sciences. As the name implies, this is a mineralogical crystallographic database. MINCRYST includes 8557 entries (some minerals have more than one entry), containing space group, unit cell parameters, atomic positions, and other data. It is provided free of charge.

NIST Crystal Data Standard Reference Database, described at <http://www.nist.gov/srd/nist3.cfm>, is provided by the National Institute for Standards and Technology. One has to pay for this database, but it appears to be fairly inexpensive (\$490 and that's not a per-year charge) as these things go. The NIST Crystal Data Standard Reference Database contains data on "more than 237,671" organic and inorganic systems, including minerals, drugs and pesticides.

The **Nucleic Acid Database**, available at <http://ndbserver.rutgers.edu>, is a free service provided by researchers at Rutgers University. It contains three-dimensional structures of about 7000 DNA and RNA species, and their complexes with drugs and proteins. Structures from solution NMR are included, as well as those derived from X-ray diffraction. The site includes a rotatable 3D viewer.

The **Pauling File**, described at <http://paulingfile.com>, is provided by Japan Science and Technology Corporation (JST) and Material Phases Data System (MPDS). The Pauling file contains phase diagrams, crystal structures, and physical properties of elements and inorganic compounds. It includes 271,710 crystal structures. The Pauling File is commercially available from several vendors in various formats, including from ASM, Materials Design, and Springer Materials, although some of these are subsets of the complete Pauling File.

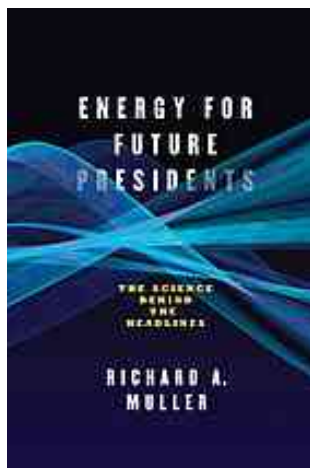
The **Powder Diffraction File**, found at <http://www.icdd.com/products/pdf4.htm>, is provided by the International Centre for Diffraction Data. An annual subscription is required. The inorganic database contains 340,653 structures; the organic database, sold separately, contains 479,278 structures. A minerals-only database is also available, for less than the full inorganic database.

The **Protein Data Bank** (PDB), available at <http://www.rcsb.org/pdb/home/home.do>, is provided by the Research Collaboratory for Structural Bioinformatics. It contains structures of just under 100,000 proteins and nucleic acids. The PDB is available for free, and the site includes a rotatable 3D viewer. A "detailed view" gives such information as the space group, the primary structure (amino acid or base sequence), the resolution of the structure, and a citation to the primary literature.

Thus, several crystallographic databases are available to the information professional, either online or via shippable media. Some are free of charge; others require either a one-time fee or an annual subscription. Most specialize in some broad region of chemical space, such as biomolecules or inorganics. On that last note, the ACS Division of Inorganic Chemistry hosted "A Celebration of Crystallography in Solid-State and Materials Chemistry: Complex Problems and New Solutions in Inorganic Small-Molecule Crystallography" at the Spring 2014 ACS Meeting, indicating that research in this useful technique continues to be performed.

David Shobe, Assistant Editor, Chemical Information Bulletin

Book Reviews



Muller, Richard A. *Energy for Future Presidents: the Science Behind the Headlines*, W. W. Norton & Co., New York, NY, 2012: pp. 350 + xvii, ISBN 978-0-393-34510-0 (softcover), \$16.95.

Q&A. Q: Why review this book here?

A: The title could relate to the “Chemistry and Materials for Energy” theme of the Dallas Meeting and the subtitle could suggest: “A Reference for the Rest of Us” like it is for every volume of the ubiquitous “for Dummies” series.

Q: Why here since it’s written by a physicist and deals with technology, economics, politics, and just a little chemistry?

A: All of these topics are important and at least related to chemistry.

Q: Why in the *CIB*?

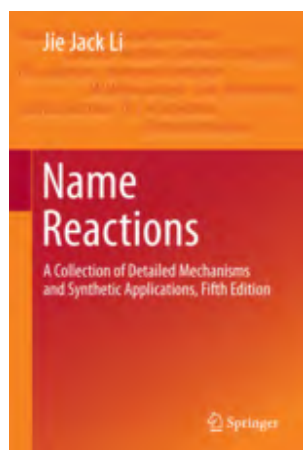
A: It contains a lot of valuable information as well as well-thought out policy recommendations, important not only to librarians and information specialists, but students, teachers, and scientists, as well as J. Q. Public.

In the Preface, the author posits 15 results of energy analysis, sans politics, to be discussed in depth in the remainder of the book. They include several contentious and controversial conclusions including energy catastrophes, nuclear energy, biofuels, automotive design, and solutions to increased carbon dioxide production. Remedies proposed for seven of the conclusions involve natural gas. He also champions nuclear energy. The catastrophes include the Fukushima disaster, the 2010 Gulf oil spill, and global warming and climate change. The first two are discussed in the context of other disasters in their industries. Muller describes himself as a climate change skeptic, but after much analysis seems convinced that it is real, with reservations. He presents his list of six categories on the political spectrum of those reacting to and commenting on climate change ranging from the extremes of Alarmist to Denier. Both classes of extremists are said to “pay little attention to the science” and deal in exaggeration to further their stances.

The remainder of the book is organized into a section on the energy landscape, including sources, and a section on alternative energy sources and utilization. The book concludes with a section on advice to a President, as if one were a presidential science and technology advisor. Included are aspects of energy technology policy, key considerations including foreign policy, and five topics to beware of. Even if one has no intentions of being a Presidential advisor, these topics are food for thought if providing advice to other government officials, colleagues and friends, or the public in general.

Muller is no stranger to controversy. In fact, he tends to generate even more than may already exist. You may disagree with some to many of his findings. Environmentalists and activists may disagree with the values and productive effects he places on recycling or environmental effects of nuclear energy. Politicians may disagree that many of their policy decisions are based on political rather than sci/tech considerations. However, Muller provides enough analysis and calculations that critics must expend the same amount of energy to debate his findings. Recommended for libraries, students, teachers, and the general public.

Bob Buntrock, Member, CINF Communications and Publications Committee



Li, Jie Jack. *Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications*, 5th ed. Springer, Heidelberg, New York, NY. 2014. pp. 681 + xxii, ISBN 978-3-319-03979-4 (hardcover), \$119.

This latest edition of the author's series on named organic chemical reactions appears five years after the 4th edition. Twenty-seven reactions have been added and references to all reactions have been updated where appropriate. The references concentrate on reviews when available and the first reference listed also gives a brief biography of the inventor. Nobel Awardees are also noted. In addition to the classic reactions named for their inventor(s) (e.g., Diels-Alder), reactions are also named by type as subsections after the parent reaction (e.g. Hetero-Diels-Alder) and are so indexed. The index also lists reactions by type and category (e.g., oxidation, rearrangement, microwave-facilitated reactions). Reagents are also indexed including named reagents. The tradition of illustrating international stamps honoring Chemistry Nobelists has been continued.

Along with many organic synthesis chemists, my lab career involved name reactions from the beginning. The Diels-Alder reaction is still my favorite and was involved in a third of my thesis. Li has moved from industry (Pfizer) to academia (University of San Francisco) and has aimed this edition as a teaching tool for undergraduates. Highly recommended for chemistry students, both undergraduate and graduate and their supporting libraries as well as for chemistry professionals. Also available in an e-edition.

Bob Buntrock, Member, CINF Communications and Publications Committee

ACS Symposium SERIES

Special Issues in Data Management

Editors: Norah Xiao, Leah Rae McEwen

Volume 1110

Sponsoring Division: ACS Division of Chemical Information

Publication Date (Web): November 15, 2012

Hardcover 22 March 2013, 184 Pages, \$150 [Oxford University Press](#)

This book originated from the American Chemical Society (ACS) National Meeting Chemical Information Division (CINF) Symposium entitled "Data Archiving, E-Science and Primary Data" in Anaheim, California on March 28, 2011. It was organized to "explore the challenges and opportunities of supporting e-science research and data management in research libraries" with particular interest in "current applications and practices and preparation opportunities for information professionals." Only one author from the original symposium was able to contribute. With this interesting twist, the book now brings new and refreshing perspectives to the topic by authors from different sectors with diverse background and experience; researchers in science, information science and data management, librarians, and publishers.

Committee Reports

CINF Education Committee

The CINF Education Committee met on Saturday, March 15, 2014, from 1-3 PM in the Omni Dallas Hotel, Arts District 4.

Attended: Grace Baysinger (Chair, Stanford University), Chuck Huber (University of California Santa Barbara), Ye Li (University of Michigan), Donna Wrublewski (Caltech), Susanne Redalje* (University of Washington), Jeremy Garritano* (Purdue University), Adrienne Kozlowski* (Central Connecticut State University, Emerita). [* committee consultant]

Excused: Christina Keil (Pfizer), Marion Peters (University of California Los Angeles, Emerita), Teri Vogel (University of California San Diego).

Draft Goals for 2014: to provide benchmarks and a framework for the committee's activities, the following goals were drafted and briefly discussed at the meeting:

- Have the Chair spend more time on Committee work (ongoing)
- Organize symposium on MOOCs for the Fall 2014 Meeting (March 2014)
- Secure an Assistant Chair for the Committee (April 2014)
- Find a member who is willing to organize symposia for the Committee (April 2014)
- Update [Committee webpage](#), maintain [ACS Network page](#) [private] (May 2014)
- Improve communication by having virtual meetings between ACS Meetings (May, July, November, January)
- Finish reviewing draft of Graduate Student Competencies (July 2014)
- Review procedures manual for Education Committee (July 2014)
- Review Undergraduate Competencies and update after the ACS Committee on Professional Training (CPT) changes are finalized (December 2014)
- Solicit, cajole, and entice colleagues to submit content to [XCITR](#) (Send email monthly).

As BCCE (Biennial Conference on Chemical Education) 2014 is being held right before the Fall ACS National Meeting, no one from the CINF Education Committee will be participating in it. We do plan to send copies of the XCITR flyer to BCCE to let attendees know about this resource.

Action item:

- [Chemical Information Literacy](#) page needs to add Currano, Judith N., and Dana Roth. *Chemical Information for Chemists: A Primer*. Cambridge : RSC Publishing, 2014. ISBN 9781849735513. DOI: <http://dx.doi.org/10.1039/9781782620655>

Round Robin: relevant news and activities were shared among Education Committee members.

Additional action items:

- Reach out to the ACS Committee on Professional Training about information resources listed on the CPT survey.
- Recruit new members for the CINF Education Committee.

Grace Baysinger, Chair, CINF Education Committee

ACS Committee on Ethics: An Overview

The ACS Committee on Ethics (ETHX) is an “other” committee of the Council and is currently chaired by Dr. Gregory M. Ferrence. Appointments are made by the ACS President, with the advice of the Committee on Committees. ETHX is a relatively new committee, having been established in 2006 during ACS President Anne Nalley’s progression. The Committee is charged with coordinating the ethics-related activities of the Society and serving as an educational resource and clearinghouse. It is specifically a *non-adjudicating* body. The Committee is also charged with developing and overseeing “such other ethics-related activities as will serve ACS members and promote the Society’s standards of ethical conduct within the profession of chemistry and its related disciplines.” Its membership comprises Councilors and non-Councilors who have an interest in ethics, particularly in ethics education, professionalism, and responsible conduct of research. To meet the charge, the Committee subdivides its efforts into three main areas: communications and awareness; education and materials; and programming and screening. The Committee closely aligns its strategic plan with the broader ACS Strategic Plan. The Committee on Ethics has the vision that “ethics will permeate the culture of chemistry.” The Committee has adopted four well-defined goals, stated and contextualized below. The goals are considered equally important. The perhaps esoteric choice to tag them with element symbols is meant to allow the goals to be listed in no particular order, yet each goal may be easily referenced.

Goal Hf of the ETHX Strategic Plan is to promote and increase **ethics awareness** in the community of chemistry and related disciplines. One approach is to contact units within ACS and organizations connected to ACS to make them aware of ethics-related activities and to identify their needs for these activities. The Committee works with these stakeholders to promote ethics through the development of symposia, workshops and other programs and activities. For example, at the recent ACS National Meeting in Dallas, an important and well-attended *Ethical Considerations in Digital Scientific Communication and Publishing* symposium and panel discussion was cosponsored by the Chemical Information Division (CINF), the Division of Professional Relations (PROF), the Division of Chemical Education (CHED), the Younger Chemists Committee (YCC), the Division of Chemistry & the Law (CHAL), and ETHX. The speakers and cosponsors made this an exceptional and positive event. We invite all ACS Divisions and Committees to contact us regarding opportunities for cosponsoring symposia. We are enthusiastic to promote **YOUR** ethics related programming. In the future, the Committee would like to develop an awards program to recognize individuals and/or ACS units and other organizations that have demonstrated support of high standards of ethical conduct in the sciences.

Goal Rf of the ETHX Strategic Plan is to support the ethics initiatives of ACS Committees, Divisions, Local Sections and other units. The committee aims to do this through proactive communication within ACS and external organizations, such as the Association for Practical and Professional Ethics (APPE; <http://appe.indiana.edu>), the Committee on Publication Ethics (COPE; <http://publicationethics.org>), and the National Center for Professional and Research Ethics (NCPRE; <http://ethicscenter.csl.illinois.edu>). Key leaders from each of these organizations have attended ETHX executive sessions and engaged the Committee in dialogue regarding the current ethics landscape to identify and act upon opportunities to enhance ethics related initiatives. For example, ETHX provided input to the ACS Board of Directors during the development of the *Volunteer/National Meeting*

Attendee Conduct Policy adopted in December, 2013. The Committee also uses materials from ACS and other sources to support embedded programming at all levels. Like goal Hf, goal Rf is in part, realized by working with stakeholders to develop and deliver relevant programs and activities such as symposia and workshops. Watch for symposia cosponsored by ETHX at upcoming National Meetings.

Goal Ti of the ETHX Strategic Plan is to catalyze **ethics education** within the scientific communities. The Committee collaborates with other units in the ACS, such as CHED, PROF, the Committee on Chemical Safety (CCS), the Committee on Patents and Related Matters (CPRM), and the Committee on Economic and Professional Affairs (CEPA) to incorporate ethics education throughout the society. ETHX is participating in CCS' newly-formed Task Force for Safety Education Guidelines (TFSEG) to "develop guidelines for laboratory safety education for primary, secondary, undergraduate, and graduate education." The Committee seeks funding to support the development of high quality education materials and consistently update items with currency in technology. For example, Susan Schelble will lead the Innovative Project Grants for Divisional Enhancement funded project *Developing Short Video Ethics Scenarios for Ethics Education in Chemistry*. The award is to PROF and Sue is both a PROF officer and a Committee on Ethics member. ETHX also develops portable workshops and symposia for international (e.g. Pacificchem), national, regional and local ACS meetings. Recently I was invited to present on the topic of Ethics to the Wabash Valley ACS Local Section. I delivered *Generating Enthusiasm for Dialogue (Information Flow) About Ethical Conduct and Integrity in the Community of Chemistry and Related Disciplines* as an interactive "clicker" enhanced presentation. It was well-received and members of the Wabash section suggested it should be added to the ACS Online Speaker Directory.

Goal Zr of the ETHX Strategic Plan is to identify and aggregate relevant **resources** and disseminate them to the community of chemistry and related disciplines. The Committee has been posting resources and links to resources in several key locations. General information about ETHX may be found on the ACS website (www.acs.org/ethics), and the committee maintains a webpage (<https://www.acs.org/content/acs/en/careers/profdev/ethics.html>) with a consolidated list of links to the ACS's major Ethical and Professional Guidelines and to the committees and divisions offering guidance on ethics-related matters. The committee has posted additional information within the ACS Network (<https://communities.acs.org>); see the group called *ACS Ethics Committee*, and at the NCPRE's *Ethics CORE* website (<https://nationalethicscenter.org>). In particular, a series of ethics-related case studies has been prepared and vetted by ETHX members. Case studies include material regarding chemical health and safety, interpersonal dynamics, collecting and managing data, safety and comportment, cheating, dishonesty, and plagiarism.

The Committee welcomes liaisons from committees and divisions. Learn more about ETHX online at www.acs.org/ethics, and by all means, if you have questions for, comments for, or interest in the Committee, please reach out to Greg Ferrence, ferrence@ilstu.edu, or the Committee's staff liaison, Eric Slater, e_slater@acs.org.

Gregory Ferrence, Chair, Committee on Ethics

ACS Council Meeting

The Council of the American Chemical Society met in Dallas, TX on Wednesday, March 19, 2014 from 8:00am until approximately 11:30am in the Dallas Ballroom A-C of the Sheraton Dallas Hotel. There were several items for Council Action and they are summarized below.

Nominations and Elections

President-Elect: The Committee on Nominations & Elections (N&E) identified four nominees for the office of 2015 ACS President-Elect. They are as follows: Peter K. Dorhout, William A. Lester, Jr., Christopher K. Ober, and Henry F. Schaefer, III. The four nominees answered questions at the Town Hall meeting that was held on Sunday, March 16th, at 4:45pm in the Sheraton Dallas Hotel. Council voted to select Peter Dourhout and William Lester as the final two candidates whose names will appear on the fall ballot.

Other Elections

The Committee on Nominations and Elections announced the list of nominees to represent District III and District VI on the Board of Directors for the term 2015-2017. Nominees for District III include Dee Ann Casteel, Pat N. Confalone, Anne S. DeMasi, and Kathryn E. Urich. Nominees for District VI are Allison A. Campbell, Paul W. Jagodzinski, Lee H. Latimer, and Eleanor D. Siebert. By mail ballot, the Councilors from these districts selected Pat N. Confalone and Anne S. DeMasi as District III candidates; and Paul W. Jagodzinski and Lee H. Latimer as District VI candidates. Ballots will be mailed on or before October 10, 2014 to all ACS members in District III and District VI 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 2015 - 2017: Dawn A. Brooks, William F. Carroll, Jr., Barbara A. Sawrey, and Ellen B. Stechel. 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, 2014

Continuation of Committees

Having completed their five-year review, the Committee on Committees was given unanimous approval by Council for the continuation of the following committees: Chemical Safety, Chemistry and Public Affairs, and Minority Affairs.

ACS Dues for 2015

Council voted to approve the recommendation from the Committee on Budget and Finance with regard to the 2015 membership dues (an increase of \$4.00 from \$154 to \$158). 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 2014:	\$154.00
Change in the Consumer Price Index, Urban Wage Earners, Services Category:	
December 2013 CPI-W (Services):	\$274.948
December 2012 CPI-W Services:	268.661
Change in CPI-W Index:	2.34%
2015 Dues, fully escalated:	$\$154.00 \times 1.0234 = \157.60
2015 Dues, Rounded:	\$158.00

Dues Allocations to Divisions

Every three years at a spring national meeting the Committee on Divisional Activities (DAC) is required to bring to Council a formula for allocation of dues funds to Divisions. The one presented in Dallas was a slightly modified version of the current formula. There are four general buckets from which Divisions earn allocation funds. Base Allotment, the Per Member Allotment, the Innovative Projects Allotment, and Total Programming Allotment (the latter reflects a division's activity at national meetings).

Two changes to the existing formula were proposed. One slightly increases the percentage of the Base Allotment that all divisions receive from 12.5% to 15%. The other calls for a slight decrease in the funds allocated to divisions for their Total Programming Allotment from 65% to 62.5%. The intent of the change is to provide small divisions (those with less than 2,000 members such as CINF) with a modest increase in funds in order to enhance their opportunity for success. The large divisions (those with more than 3,500 members) will lose no more than 2.5% of their funding.

After voting to postpone its implementation by one year, the Council voted to approve the revised formula. It will be effective with allocations for 2015 division performance.

Change in Local Section Territory

Council approved the Committee on Local Section recommendation to expand the territory of the North Jersey Local Section to include the former Monmouth County Local Section territory. The latter section dissolved on 12/31/13 due to inactivity and is currently an unassigned territory.

Petitions for Vote

Petition to Charter an International Chemical Sciences Chapters

On recommendation of the Committee on International Activities and subject to the concurrence of the Board of Directors, the Council voted to approve petitions to charter the South Korea International Chemical Sciences Chapter and the Malaysia International Chemical Sciences Chapter.

Committee Oral Reports

Budget and Finance (B&F)

In 2013, ACS generated a Net from Operations of \$15.1 million, which was \$2.0 million favorable to the budget. This represents the Society's tenth consecutive year of positive operating results. Total revenue was \$490.5 million, which was \$8.8 million (or 1.8%) lower than budget, and essentially flat when compared with 2012. Expenses totaled 475.4 million which was \$10.8million (2.2%) favorable.

This result was largely attributable to cost-containment measures throughout the ACS. Unrestricted Net Assets rebounded in 2013, rising to \$207 million, and more than doubling from the 2012 level.

Education (SOCED)

SOCED approved a pilot program to form ACS International Student Chapters.

Standing Committees

Membership Affairs (MAC)

For 2014, MAC authorized an individual member test for India to allow for a \$52 full Member dues rate. At this meeting, MAC extended the test to include new and renewing members in India for three years.

Economic and Professional Affairs (CEPA)

Findings from the ACS 2013 New Graduate Survey have been compiled and reveal troubling news: overall unemployment among new graduates rose from 12.6% in 2012 to 14.9% in 2013. This is primarily due to the high unemployment among recent Bachelors degree chemists. New graduates must be at the top of the Committee's priority list for employment assistance in 2014. Median salary has also dropped from \$40,000 to \$39,560.

Meetings and Expositions (M&E)

As of the morning of March 19, 2014, the ACS spring national meeting had attracted 13,680 registrants, including 6,853 regular attendees, 5,140 students, 304 guests, 954 exhibitors, and 429 exposition-only registrants. The meeting had 10,050 papers presented.

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 27th)
2013: New Orleans, LA:	15,596 (as of Wednesday morning, April 10th)
2014: Dallas, TX:	13,680 (as of Wednesday morning, March 19th)

The new ACS Mobile Application had over 6,000 downloads by meeting attendees.

M&E voted to eliminate the author index in the hard program meeting program book beginning with the spring 2015 meeting. The searchable author index is now available via the mobile application and other electronic means. M&E reported that the Spring 2023 meeting will be held in Indianapolis, IN.

Divisional Activities (DAC)

Operating as a DAC subcommittee, the Multidisciplinary Planning Group is proposing the following 2017 national meeting themes to the divisions for their consideration:

Spring, San Francisco: Advanced Materials, Technologies, Systems and Processes

Fall, Washington, DC: Chemistry's Impact on the Global Economy

Local Section Activities (LSAC)

LSAC will initiate the process to dissolve the Ocean County (New Jersey) Section as a result of the group's failure to meet the criteria to remain an active section. The committee also announced special Local Section anniversaries: Maryland (100th), South Plains (50th), and the 75th anniversary for Sioux Valley, Penn-York, Memphis, Baton Rouge, Green Mountain and Illinois Heartland.

Constitution and Bylaws (C&B)

In Fall 2013, C&B announced a new optional process for expedited bylaw reviews, offering limited customization but faster than the current three month turnaround. C&B has now created a new, easier way for local sections and divisions to prepare bylaw revisions for C&B review. They are not as restrictive as those permitted through the expedited process. After a unit indicates its willingness to update its bylaws, C&B would then offer to create a first draft of proposed bylaws changes for consideration by the unit. Alternatively, the unit may still propose its own draft changes for C&B review. There are currently no petitions for action at the 2015 Spring ACS meeting.

Other Committees

Chemical Safety (CCS)

CCS has published its first-ever Safety Alert concerning the Rainbow Demonstration, in *Chemical and Engineering News*, March 17, 2014. Copies were distributed to Councilors.

Chemists with Disabilities (CWD)

The committee has updated and digitized its publication "Teaching Chemistry to Students with Disabilities." It will be available in April 2014 and linked to the CWD website.

Community Activities (CCA)

Copies of the publication *Celebrating Chemistry*, a product of the ACS Department of Volunteer Support in conjunction with CCA, were distributed to Councilors. Local Sections can order up to 750 copies of this publication for Chemists Celebrate Earth Day.

Minority Affairs (CMA)

The committee reminded Councilors that the ACS Scholars Program is celebrating its twentieth anniversary in 2015. The program has enabled 1,400 students to achieve university degrees in the chemical sciences. CMA will highlight accomplishments and successes of the Scholars Program throughout 2015.

Special Discussion Item

A special discussion item was put on the Council agenda for this meeting. ACS President Tom Barton presented and moderated a discussion on “What can ACS do to increase the quality of science education in grades K-12? Following the presentation, 39 Councilors engaged in a robust discussion on the factors impacting the quality of K-12 science education in the United States.

ACTIONS OF THE BOARD OF DIRECTORS

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

The Board’s Committees and Working Groups

The Board of Directors received reports from its Committees on Grants and Awards (G&A), and Executive Compensation.

On the recommendation of the Committee on Grants and Awards, the Board voted to approve a Society nomination for the National Medal of Science, which is bestowed by the President of the United States to individuals in science and engineering who have made important contributions to the advancement of knowledge in the fields of behavioral and social sciences, biology, chemistry, engineering, mathematics and physics.

The Board received an extensive briefing and approved several recommendations from its Committee on Executive Compensation. The compensation of the Society’s executive staff receives regular review from the Board.

The working group on Society Program Portfolio Management briefed the Board on its activities. The working group was charged with delivering a process for portfolio management of Society programs in the divisions of Membership and Scientific Advancement, Education, and the Office of the Secretary and General Counsel (Office of Public Affairs).

The Board held a discussion on operational issues relating to virtual versus face-to-face committee meetings, the appropriate detail and format of information presented to the Board and committee members, and the proper length of committee meetings.

The Executive Director/CEO Report

The Executive Director/CEO and her direct reports updated the Board on the following: ACS financial trends and near term outlook; the launch of the recently approved American Association of Chemistry Teachers, which will support K-12 teachers of chemistry by providing them with a professional home that addresses and is responsive to their needs; and the activities and plans of CAS (Chemical Abstracts Service) and the ACS Publications Division. As a follow-up to the Publications report, the Board voted to approve three journal editor re-appointments. The Board also VOTED to approve one appointment to the ACS Green Chemistry Institute Governing Board and one reappointment to the ACS Governing Board for Publishing.

Other Society Business

The Board also:

Expressed its gratitude and thanks to Madeleine Jacobs, Executive Director and Chief Executive Officer, who on March 6 announced her plan to retire at the end of the year. The Board then began a discussion of the process and logistics of identifying and hiring her successor.

Received reports from the Presidential Succession on their current and planned activities for the remainder of 2014 and 2015.

Approved a resolution congratulating Robert Massie on his retirement at the end of this month for twenty-one years of successful leadership of the Chemical Abstracts Service (CAS).

The Board's Open Session

The Board held a lively, well-attended open session which featured a special forum focused on the question: "What is the one thing you like that ACS does, and why?" Members attending the session also received a brief review of the questions posed at the spring 2013 Board Open Session in New Orleans and the follow-ups undertaken by governance and staff. Board members continue to be pleased by the new format, turnout and quality of the discussions.

ADDITIONAL INFORMATION

The following is a list of the email addresses and URLs presented on slides at the Council meeting.

d.schmidt@acs.org, president@acs.org email address for ACS President-Elect Diane Grob Schmidt

m.wu@acs.org email address for ACS Immediate Past President Marinda Wu

nomelect@acs.org email address for the Committee on Nominations and Elections and to submit questions to Town Hall Meetings

<http://www.yellowbook.acs.org> ACS Directory (member number required)

<http://www.acs.org> Society's audited finances and IRS Form 990 filings (click on "About Us" and scroll down to "ACS Financial Information")

<http://www.acs.org/bulletin5> ACS governing documents including petitions and certified bylaws

<http://www.acs.org/content/acs/en/about/governance/committees/cwd/publications.html>
Teaching Chemistry to Students with Disabilities digitized version will be published in April 2014

<http://www.acs.org/chemistry-over-coffee> Conversations with Celebrated Chemists

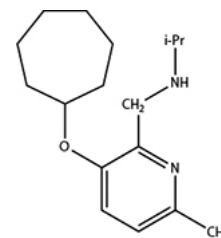
www.acs.org/getinvolved Information for local sections and divisions, community outreach

Andrea Twiss-Brooks and Bonnie Lawlor, CINF Councilors

Joint Board-Council Committee on CAS

The Committee (CCAS) met in Executive Session on March 14, 2014 where CAS President Manuel Guzman shared his vision for CAS, and management reported on highlights from 2013.

The CAS databases reached record growth for indexed articles, patents and reactions. In [November](#), CAS registered the 75th millionth small molecule in the CAS REGISTRY from a substance published in a chemical catalog, highlighting one example of the variety of sources of disclosed chemical information CAS covers.



[SciFinder](#) was enhanced strengthening its value to researchers with workflow improvements including quick links to patent PDFs, structure drawing options, and API capabilities.

Customers are embracing multi-year SciFinder agreements, and the [ACS Member SciFinder Benefit](#) has been overwhelmingly popular.

[CAS and PerkinElmer](#) announced a collaborative effort that will allow ChemBioDraw users to launch a SciFinder search from the ChemBioDraw interface. Committee members were also pleased to learn that the new non-Java CAS structure editor is now available in SciFinder.

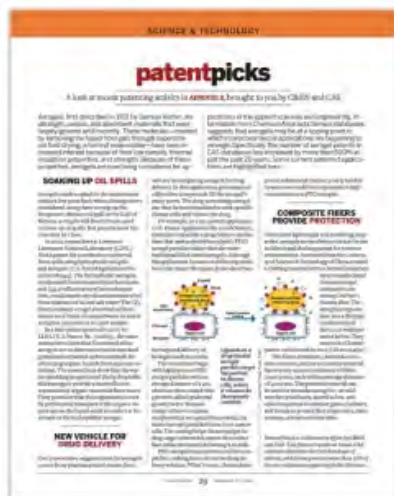
New [STN Version Two](#) was released, featuring full text patent content and integrated patent family content for a complete view of an invention.

CAS announced an exciting collaboration with *C&EN* to publish Patent Picks, a monthly feature highlighting hot topics found in the patent literature from the CAS databases.

CAS is also producing an informative video series to give visitors to [cas.org](#) an inside look into how CAS builds its databases.

CCAS continues its role as a conduit of information between Society members (and users of CAS services), the ACS Governing Board for Publishing and CAS management.

Grace Baysinger, Chair, Joint Board-Council Committee on CAS



Patent Picks feature debuted in the January 27, 2014 issue of *C&EN*. Look for it in the last issue of each month. Patent Picks will look at trends in patents about [aerogels](#) (January), [biofuels](#) (February), [Chinese drug Industry](#) (March), graphene, lithium-ion batteries, and more.

Joint Board-Council Committee on Publications

The open session of the Joint Board-Council Committee on Publications (JBCCP) was held on March 14, 2014 in Dallas, TX. The President of the ACS Publications Division, Brian Crawford, provided an overview and highlights of 2013 accomplishments of the Division. His [presentation slides](#) and the following summary were kindly provided by Debra Davis, ACS Staff Secretary of the Committee.

Advanced the Society's mission with the publication of new journals

During 2013, the Division completed the successful first full calendar year of publication of ACS *Sustainable Chemistry & Engineering* and embarked upon the early editorial and marketing introduction of two new journals prior to their scheduled commercial availability in 2014: ACS *Photonics* and *Environmental Science & Technology Letters*.

Strengthened key journals through editorial succession

Five leading scientists were selected by separate Editor Search committees convened in accordance of the bylaws, appointed by the Board of Directors and contracted by ACS Publications management, commencing respective editorial tenures effective January 2014:

- Dr. Jillian Buriak (University of Alberta) *Chemistry of Materials*
- Dr. Cynthia J. Burrows (University of Utah) *Accounts of Chemical Research*
- Dr. Kenneth M. Merz, Jr. (Michigan State University) *Journal of Chemical Information and Modeling*
- Dr. Vincent M. Rotello (University of Massachusetts-Amherst) *Bioconjugate Chemistry*
- Dr. Phillip E. Savage (University of Michigan) *Industrial & Engineering Chemistry Research*

Sustained editorial excellence across the ACS journals portfolio

The 2012 Thomson Reuters *Journal Citation Reports* (JCR) demonstrated strong performance for the ACS peer-reviewed journals portfolio, with ACS journals receiving more than 2.2 million total citations and posting a #1 ranking in either Impact Factor and/or Total Citations across 15 subject categories. A total of 22 ACS journals increased their Impact Factors and 18 had an Impact Factor of 5 or greater. (See <http://pubs.acs.org/page/jcr/index.html> for details.) Notable individual journal achievements include:

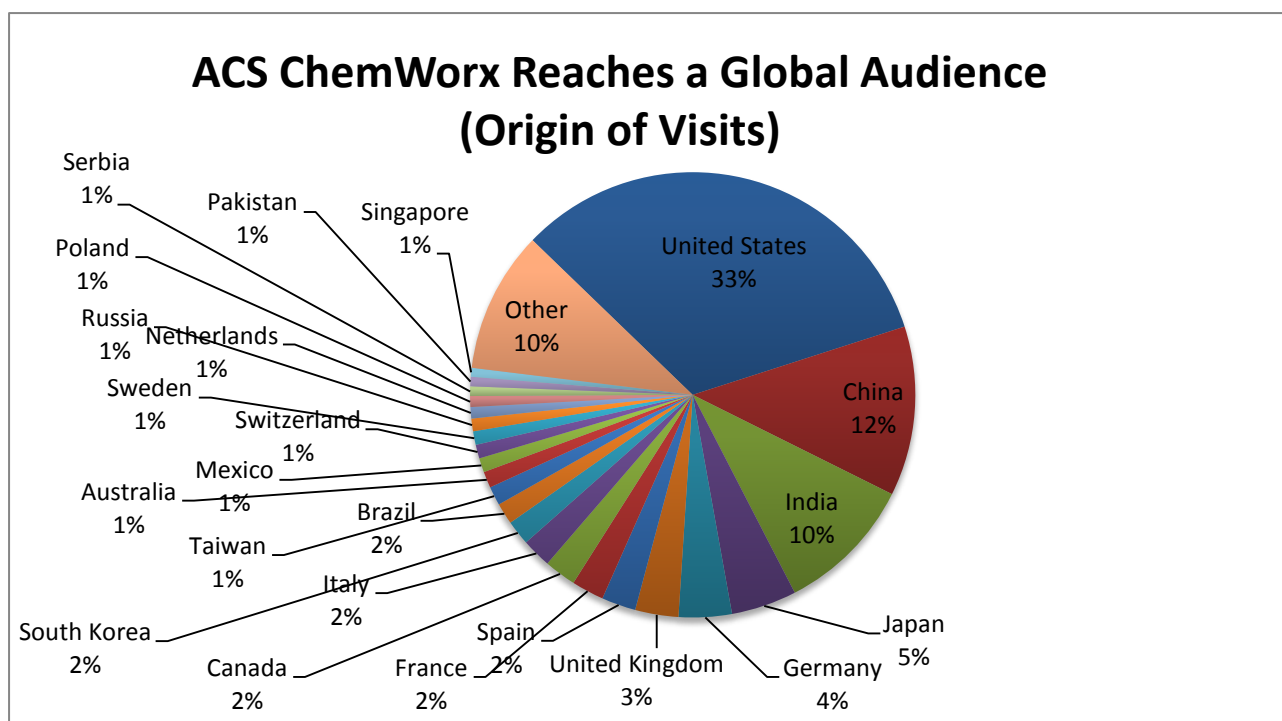
- *The Journal of the American Chemical Society* increased its Impact Factor to 10.677, a new record for the journal, and continued to be the most cited ACS journal with more than 430,000 citations.
- *Chemical Reviews* increased its Impact Factor to 41.298, a new record for the journal, and remains the ACS journal with the highest Impact Factor.
- *Nano Letters* had the highest non-review journal Impact Factor among all ACS journals at 13.025.

Innovated with evolving technologies in the development of ACS ChemWorx

In March of 2013, ACS Publications introduced ACS *ChemWorx* as a novel, new, free service for research management that combines reference discovery and management, professional networking, group and task management, and manuscript preparation in a single interface, accessible from anywhere. The collaboration software is powered by ACS Publications' development partner, colwiz, Ltd. ACS *ChemWorx* includes a Publishing Center developed and hosted by ACS, and is integrated with the ACS Web Editions Platform for journal content delivery, by virtue of a new document viewer,

ACS ActiveView PDF, that has proven to be very popular with end users. The ActiveView PDF display format for ACS articles provides a means for interacting with Reference Quick View, for annotation of the article, and for storage in a user's *ACS ChemWorx* library.

Two iterative releases built upon the original software were made in Q3 and Q4. These releases provided additional apps for users in the Publishing Center, including the ability to track the geographic distribution of readers of ACS articles, author/reviewer appreciation certificates for download, and a user guide. Beginning in December, all authors returning galley proofs of articles were directed to the *ACS ChemWorx* Publishing Center, which is anticipated to drive further uptake and usage. Developed as a new author service under the *ACS ChemWorx* umbrella, this application replaces the previous author galley site provided through our journal delivery platform, Literatum. A notable feature of the new site is a prompt to sign into *ACS ChemWorx* as part of the proof review process, positioning ACS to offer expanded author services.



Continued to enhance efficiencies of editorial operations

ACS Editorial Office Operations oversaw the addition of 69 new editors, including 3 Editors-in-Chief, for ACS journals, for a net increase of 38 editors under contract, through December 2013. These editor appointments are reflective of the global nature of the chemical research enterprise, with 33% of the new appointees residing outside North America. The addition of these editorial decision-making resources expands the division's capacity to oversee the peer review of the now more than 100,000 manuscript submissions received annually, reflecting growth of nearly 8% in author demand year over year.

Extended efficiencies of journal production and expanded web usage

Journal Production and Manufacturing Operations (JPMO) in Columbus published a total of 39,151 articles in issues across the ACS journals portfolio, exceeding the annual published output of 2012 by

2.5%. Total web-based article requests were up 3.0% versus prior year, and exceeded 83 million article downloads in 2013, for an all-time high.

Continued collaborations with CAS on product enhancements and workflows

Collaboration between CAS Editorial Operations and ACS Publications successfully implemented three projects:

- **Tagging of patent citations:** improved the XML tagging for patent citations in the ACS Publications journals during the production process for ingestion into the CAS editorial workflow. This production enhancement reduced the amount of manual intervention required by CAS editorial staff.
- **Improved author affiliation tagging:** more granular XML tagging of the institutional information for which an author is affiliated beyond just the institution in the ACS Publications journals during the production process, e.g., department, division, city, etc. This production enhancement reduced the amount of manual intervention required by the CAS editorial staff.
- **Author's original document:** capture the original content files submitted by the ACS journal authors and make the content available to CAS Editorial Operations for analysis. Completion of this project enabled CAS to obtain and store highly-enriched electronic information supplied by authors early in the ACS Publications journal production process.

Announced a major new commitment to support Open Access

In November, ACS Publications announced a multi-pronged strategy to position ACS as an open access publisher. The program consists of four components: 1) *ACS Central Science*, a new journal that will be free to both readers and authors; 2) *ACS Editors' Choice*, designed to provide free public access to new research of importance to the global research community; 3) *ACS Author Rewards*, a loyalty program intended to encourage ACS authors to choose open access, via \$60 million in open access publishing credits redeemable over the period 2015-2016; and 4) *ACS AuthorChoice*, expanded in 2014 to include new and affordable licensing options to help authors meet open access requirements. The "ACS is Open" initiative is being promoted widely during 2013-2014; details are available at a dedicated website (www.acsopenaccess.org).

Celebrated C&EN 90th anniversary throughout 2013

In 2013, *Chemical & Engineering News* celebrated 90 years of continuous publication since 1923. *C&EN* used the opportunity of the anniversary to promote the content of *C&EN Archives*. Each week *C&EN* posted riveting images and memorable quotations from *C&EN Archives* in a Tumblr blog called The Watch Glass. This feature was a finalist, along with *Glamour* and *Entertainment Weekly*, in the 2013 Folio Awards for Best Use of Social Media, Tumblr Category. Each month *C&EN* devoted one editor's page to a reexamination of past coverage, as gleaned from *C&EN Archives*. The special issue, published on Sept. 9, highlighted nine ways that chemistry changed the world. The nine topics were chemical bonding, plastics, antibiotics, nanotechnology, catalysis, molecular biology, analytical instrumentation, computational chemistry, and environmental awareness. A bonus poster accompanying the special issue illustrated highlights of nine decades of chemistry discoveries. Celebrations reached a climax with two live events at the ACS National Meeting in Indianapolis. One was a webinar on the topic of food fraud. The other was a sold-out performance by celebrity chef and award-winning author Alton Brown, which was followed by a highly-attended and especially festive reception.

Expanded ACS on Campus globally

During 2013, ACS Publications led and participated in 30 ACS on Campus events held both in the US and around the globe. These cross-divisional events, coordinated with Membership and Scientific Advancement, CAS, Education, and Petroleum Research Fund, provide important venues to showcase the Society's diverse offerings of programs and services, and serve as an important outreach method in strengthening our relationships with librarians, chemistry faculty and students, and in building ties with current and prospective authors and ACS members. A list of the 2013 ACS on Campus events is appended herewith for reference.

Date(s)	University	Location
March 12	University of Oxford	Oxford, UK
March 13	The University of Manchester	Manchester, UK
April 12	Seoul National University	Seoul, Korea
April 15	KAIST	Daejeon, South Korea
April 15-16	University of Rochester	Rochester, NY
April 18	The University of Tokyo	Tokyo, Japan
April 19	National Institute for Materials Science	Tsukuba, Japan
April 19-20	Binghamton, University	Binghamton, NY
April 22	Kyoto University	Kyoto, Japan
July 5	University of KwaZulu-Natal	Durban, South Africa
July 8	Wits University	Johannesburg, South Africa
Sept. 8	SciFinder Future Leaders in Chemistry program	Indianapolis, IN
Sept. 23-24	University at Buffalo	Buffalo, NY
Sept 25-26	RWTH Aachen	Aachen, Germany
Oct. 4-5	Missouri State University	Springfield, MO
Oct. 4	University of Utrecht	Utrecht, Netherlands
Oct. 7	LMU Munich	Munich, Germany
Oct. 17	ACS MWRM - Midwest Regional Meeting	Springfield, MO
Oct. 16	National Tsing Hua University	Hsinchu, Taiwan
Oct. 17	National Taiwan University	Taipei, Taiwan
Oct. 21	Nanjing University	Nanjing, China
Oct. 22-23	Arizona State University	Tempe, Arizona
Oct.22	Zhejiang University	Hangzhou, China
Oct. 24-25	University of Arizona	Tucson, Arizona
Oct. 29-30	University of Wisconsin - Madison	Madison, WI
Nov. 4	University of Maryland College Park	College Park, MD
Nov. 7	Georgia State University	Atlanta, GA
Nov. 20	Pierre and Marie Curie University - Paris 6	Paris, France
Nov. 25	IIT Kharagpur	Kharagpur, India
Nov. 27	IIT Madras	Madras, India
Nov. 29	NIIST/IISER	Thiruvananthapuram, India

Debra Davis, Staff Secretary, Joint Board-Council Committee on Publications

CINF Social Networking Events

Thanks to our sponsors the Division of Chemical Information was able to host a number of excellent social networking events during the ACS Meeting in Dallas last month. CINF members and friends got to enjoy these social occasions due to the generosity of many organizations. On behalf of the Fundraising Committee I cannot express enough how much we appreciate their patronage. Without the support of our sponsors these events would not be possible.



Starting at the CINF Welcoming Reception the meeting attendees had a pleasure to discuss and judge Scholarship for Scientific Excellence [posters](#) on Sunday. Katrin Stierand was selected to be the award recipient. The Scholarship for Scientific Excellence was sponsored by [InfoChem](#). The Welcoming Reception was co-sponsored by [InfoChem](#), [Journal of Cheminformatics](#), [PerkinElmer](#), and [RSC Publishing](#).

Following a Division tradition since the early 1960's CINF members once again enjoyed chatting to old acquaintances and making new friends at Harry's Party set up in a suite at the Sheraton Dallas on Monday. Harry's Party was sponsored exclusively by [ACS Publications](#). (See an [article](#) about Harry's Party in the *Chemical Information Bulletin* and a [page](#) on the CINF website).

Next, in our well-established schedule for a CINF Luncheon on Tuesday, Andrew Yeung of Texas A&M was our guest speaker in Dallas. Dr. Yeung shared his views on "Chemistry in Wikipedia: A Personal Perspective." The Luncheon was sponsored exclusively by [RSC Publishing](#).

For the San Francisco Meeting we have ever-expanding numbers of the social networking events planned for Division members. These include:

- Saturday Dinner – this will give you an opportunity to meet committee chairs and help you decide how you may want to get involved in CINF
- CINF Welcoming Reception & Scholarship for Scientific Excellence Posters on Sunday
- Harry's Party on Monday
- CINF Luncheon on Tuesday
- Herman Skolnik Award Reception honoring Engelbert Zass on Tuesday.

If you plan on coming to San Francisco please come to as many of the CINF events as you can. These gatherings are a great chance to discuss and relax with your colleagues. If you are interested in sponsoring or co-sponsoring an event please contact me at philip.heller@thieme.com.

In closing I would also like to extend a note of thanks to my predecessor, Graham Douglas, for all of his efforts during this transition. He has and continues to be a wealth of information and support.

Philip Heller, Chair, CINF Fundraising Committee

CINF photos from the Spring 2014 ACS National Meeting are at:
<https://www.flickr.com/photos/cinf/sets/>
Photos by Grace Baysinger and Wendy Warr

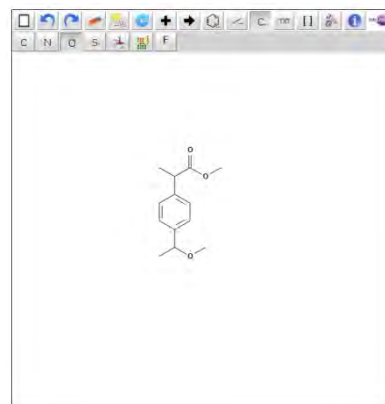
Sponsor Announcements



InfoChem News

New ICEDIT version released

InfoChem is pleased to announce the release of ICEDIT version 3.0. This new version of InfoChem's drawing and depicting tool offers scaling and adjusting the standard bond length in sketches. Improved display options such as transparent background and layout format definition for OLE objects have also been integrated. In addition, template structures with super-atoms and brackets are now allowed.



Click here for more information about [ICEDIT](#) and to test the JavaScript version.

Name Reaction search to be included in SPRESImobile App



InfoChem is pleased to announce a new release of SPRESImobile in March 2014. The free App for iPhone and iPad is developed to perform structure and reaction searches on mobile devices and offers access to more than 500,000 reactions: a subset of the SPRESI reaction data ([ChemReact](#)). Additionally, SPRESI subscribers have access to the entire SPRESI reaction content.

Name Reaction searching has been integrated in the new App version. After registration users see a new button for name reaction searches in the reaction search form. Furthermore, all users (including those not registered) will see a new hyperlink with the Name Reaction in the reaction hit list, when named reactions are hits for a reaction search. This hyperlink allows users to retrieve all reactions assigned to the specific mechanism.

For more information about SPRESImobile please click [here](#).

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

Valentina Eigner-Pitto, InfoChem



How Do You Solve a Problem Like Open Access (OA)?

Impactful initiative from the Royal Society of Chemistry

Born out of the recognition that researchers are often asked to publish OA, but do not necessarily have the funding to do so, the Royal Society of Chemistry came up with Gold for Gold.

Initially piloted in the United Kingdom in the summer of 2012, this initiative rewards all institutions who subscribe to RSC Gold (the Royal Society of Chemistry's premium online package, comprising 41 international journals, databases and magazines) with voucher codes to publish a selected number of accepted RSC articles Gold Open Access (OA), free of charge.

"With research budgets tight, ensuring that exciting results reach the widest possible audience is often difficult. Allowing open access to my PCCP paper via the Gold for Gold initiative provides an opportunity to promote this research and I am therefore delighted to be the first recommended for this scheme by my School...." Dr Ian Lane, Lecturer in Physical Chemistry, QUB, UK.

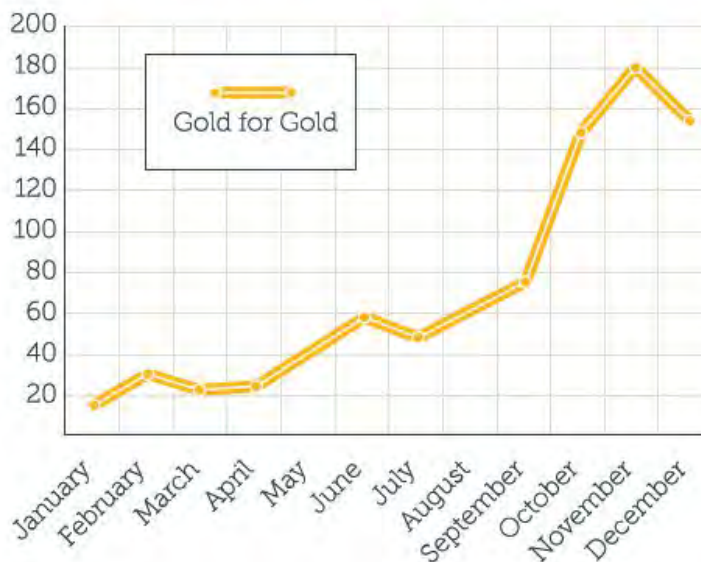
Strength to strength

At the beginning of 2013 Gold for Gold went global, and its popularity has soared. All of the world's top 30 academic institutions subscribe to RSC Gold, entitling them to Gold for Gold voucher codes. Those currently benefiting include: California Institute of Technology, United States; Stanford University, United States; University of Oxford, United Kingdom; University of Toronto, Canada; University of Tokyo, Japan.

A total of 878 Gold for Gold applications from 187 institutions in 26 different countries were made in 2013, with a monthly record number of 184 Gold for Gold applications made in November. Unsurprisingly, due to enhanced awareness, the United Kingdom led the way with 278 Gold for Gold articles, followed by the United S with 100. Other prominent users include Germany, Switzerland, the Netherlands, Japan and Australia.

ChemComm, the largest and fastest publisher of high quality communications within the general chemistry arena, had the highest number of applications in 2013 with 143, followed by *Physical Chemistry Chemical Physics* and *Dalton Transactions*.

Gold for Gold articles 2013



A thumbs up from researchers and librarians

Gold for Gold has been praised for its simplicity, flexibility and the lack of additional paperwork when it comes to licenses, saving researchers time.

“When my paper was accepted for publication, I contacted our librarian to request a complimentary Gold for Gold voucher; with that in hand the article was soon converted for publication under a Creative Commons OA license. It was that easy and quick to see that our work would be placed in a well-regarded journal, but not locked up behind a pay wall.” Professor Kit Cummins, MIT, United States and, Associate Editor of *Chemical Science*.

Librarians have also noted the opportunity this initiative provides to introduce an easy way for chemistry faculties to experiment with OA. Information specialists in the United States have been particularly proactive here; UCSF, UCLA and Stanford all have web pages dedicated to Gold for Gold.

And what about consortia?

Many institutions from countries throughout the world benefit from receiving Gold for Gold voucher codes as part of an existing consortium deal, but the DFG (German Research Foundation) - RSC Gold license agreement in Germany fulfilled a burning need amongst German researchers to publish Gold OA, representing a very real success story.

In Germany, 87 institutions plus all Max Planck and Fraunhofer Institutes, will profit from more than 900 Gold for Gold voucher codes in 2014. This is the first nationwide deal of its kind and will last for three years. It further reflects demand evidenced by a significant increase in submissions and published articles at the Royal Society of Chemistry in the past six years.

“The Alliance-RSC GOLD License agreement, negotiated with the Royal Society of Chemistry, is innovative. Not only does it offer our users easy access to all RSC journal content, but all participating institutions receive a certain quantity of Open Access (OA) vouchers with which their authors can publish OA free of charge in any RSC journal.” Uwe Rosemann, Director German National Library of Science and Technology and University Library Hannover (TIB/UB), Germany.

For more information on the Gold for Gold scheme, consult your Account Manager at the Royal Society of Chemistry. Alternatively e-mail goldforgold@rsc.org.

Max Espley, Royal Society of Chemistry



Home > What's New at the Library > Open Access Publishing Vouchers Available for RSC Journals

OPEN ACCESS PUBLISHING VOUCHERS AVAILABLE FOR RSC JOURNALS

June 28, 2013



Chemistry provides the fundamental connections across scientific disciplines – that’s why it’s known as the “central science.” To explore new perspectives on these links at the forefront of scientific research, ACS will launch a first-of-its-kind open access journal, *ACS Central Science*, later this year. “We are excited to launch the Society’s first fully open access journal, and the first highly selective, pure open access journal to cover the breadth of chemistry in relation to other sciences, medicine, computational science, and engineering,” said Kevin Davies, VP Business Development, American Chemical Society. “*ACS Central Science* will offer a unique viewpoint and complement the Society’s portfolio of subscription-based journals, for those authors who seek to publish in an open access forum of distinction.”

Under the leadership of a renowned scientist and an international editorial board, *ACS Central Science* will publish 100 - 200 peer reviewed articles each year. Active research scientists, representative of the journal’s planned disciplinary and geographic diversity, will oversee peer review. A more detailed statement of the journal’s scope will be announced once an Editor-in-Chief is selected and an Editorial Board is appointed.

ACS Excellence magazine asked Darla Henderson, Assistant Director, Open Access Programs, American Chemical Society, a few questions about the new journal:

ACS Excellence: Are there any author charges to publish in the journal?

Darla Henderson: No, but authors who want to publish under a Creative Commons license – or who are required to do so by their funding agency, may elect to do so as an additional fee-based option.

AE: Are there any subscription fees to access content?

DH: No. All articles will be freely-available immediately upon publication and will remain free to access. Once launched, the journal will be found on the ACS Publications website.

AE: How will peer review be handled for *ACS Central Science*?

DH: The journal will employ the same high standards of peer review, speedy publication times, and rigorous editorial processes as exemplified by the Society’s publishing program.

AE: When will *ACS Central Science* begin accepting papers and when will the journal begin publishing articles?

DH: We are currently establishing a small search committee of outstanding scientists, who will lead our effort to identify the founding Editor-in-Chief. We expect that the journal will be accepting submissions before the end of the year.

This article was originally published in the [spring 2014 issue of *ACS Excellence*](#) (page 20).

Sara Rouhi, ACS Publications

PerkinElmer Launches Innovative Cloud-Based Platform for Collaborative Academic Research



PerkinElmer, Inc., a global leader focused on the health and safety of people and the environment, announced the launch of the Elements platform, a cloud-based expandable scientific collaboration tool for students and researchers, at the 247th American Chemical Society National Meeting.

The Elements platform is a first-of-its-kind tool for academic scientists providing a cost-efficient solution for safe, secure record keeping that eliminates the need for investment in digital infrastructure. “Despite the wide range of technology offerings available in the marketplace today, a recent study we conducted revealed that more than 75 percent of research academics still use a paper notebook for recording lab notes,” said Michael Elliott, CEO and Chief Analyst, Atrium Research & Consulting. “Electronic lab notebooks (ELNs) are changing this practice in how labs at major universities embrace electronic data capture, cloud-based applications and collaborative tools to modernize their research environments.”

The Elements platform was created through PerkinElmer’s 20+ years of experience developing scientific computing tools combined with the cloud-based scientific collaboration platform that PerkinElmer obtained through its recent acquisition of Wingu, Inc., a Google Ventures backed software development firm. This unique blend of capabilities allows PerkinElmer to deliver a cloud-based collaboration solution to an increasingly distributed global research marketplace.

Features:

- **Expandable platform:** Sets the stage for a rapid pace of innovation by delivering an application framework for deep scientific support through modular apps that can be combined into sophisticated scientific experiments.
- **100 percent cloud-based:** Enables users to be up and running in minutes without the need for lengthy deployment and installation steps.
- **Electronic data capture:** Facilitates easy, effective data capture and electronic collaboration within an individual research group or among varying research groups.
- **ChemDraw integration:** Embeds PerkinElmer’s drawing tool so that chemical compounds and reactions can be easily drawn and captured in the Elements framework, in addition to creating publication-ready, scientifically intelligent drawings for use in databases and publications.

The new Elements platform expands upon PerkinElmer’s legacy in the ELN marketplace. The company created the [E-Notebook](#), one of the industry’s most widely deployed electronic laboratory notebooks.

More information is at: <http://t.co/P2NnMWCMhC>

Phil McHale, PerkinElmer

CINF Officers and Functionaries

Chair:

Ms. Judith Currano
University of Pennsylvania
currano@pobox.upenn.edu

Chair Elect:

Rachelle Bienstock
National Institute of Environmental
Health Sciences
rachelleb1@gmail.com

Past Chair/Nominating Chair:

Dr. Antony Williams
Royal Society of Chemistry
williamsa@rsc.org

Secretary:

Ms. Leah McEwen
Cornell University
lrn1@cornell.edu

Treasurer/Finance Committee Chair:

Dr. Rob McFarland
Washington University
mcfarland@wustl.edu

Councilor:

Ms. Bonnie Lawlor
National Federation of
Advanced Information Services
blawlor@nfais.org

Councilor:

Ms. Andrea Twiss-Brooks
University of Chicago
atbrooks@uchicago.edu

Alternate Councilor:

Mr. Charles Huber
University of California, Santa Barbara
huber@library.ucsb.edu

Alternate Councilor:

Dr. Guenter Grethe
Scientific Research Consultant
ggrethe@att.net

Program Committee Chair:

Dr. Erin Bolstad
ChemAxon
erinbolstad@gmail.com

Membership Committee Chair:

Dr. Gregory Banik
Bio-Rad Laboratories
gregory_banik@bio-rad.com

Archivist/Historian:

Ms. Bonnie Lawlor
National Federation of
Advanced Information Services
blawlor@nfais.org

Audit Committee Chair:

TBD

Awards Committee Chair:

Ms. Andrea Twiss-Brooks
University of Chicago
atbrooks@uchicago.edu

Careers Committee Co-Chairs:

Ms. Susan Cardinal
University of Rochester
scardinal@library.rochester.edu

Ms. Pamela Scott
Pfizer
pamela.j.scott@pfizer.com

Chemical Information Bulletin Editors:

Ms. Svetlana Korolev (summer & winter)
University of Wisconsin, Milwaukee
skorolev@uwm.edu

Dr. Vincent Scalfani (spring & fall)
University of Alabama
vfscalfani@ua.edu

Assistant Editors:

Dr. David Shobe (summer & winter)
Patent Information Agent
avidshobe@yahoo.com

Ms. Teri Vogel (spring & fall)
University of California, San Diego
tmvogel@ucsd.edu

**Communications and Publications
Committee Chair:**

Dr. David Martinsen
American Chemical Society
d_martinsen@acs.org

Constitution, Bylaws & Procedures:

Ms. Susanne Redalje
University of Washington
curie@u.washington.edu

Education Committee Chair:

Ms. Grace Baysinger
Stanford University
graceb@stanford.edu

Fundraising Committee Chair:

Mr. Philip Heller
Thieme Publishers
philip.heller@thieme.com

Tellers Committee Chair:

Ms. Susan Cardinal
University of Rochester
scardinal@library.rochester.edu

Webmaster:

Ms. Danielle Dennie
Concordia University
danielle.dennie@concordia.ca

**Contributors to this Issue of
*Chemical Information Bulletin*****Articles & special features**

Grace Baysinger
Rachelle Bienstock
Erin Bolstad
Bob Buntrock
Christine Casey
Judith Currano
Valentina Eigner-Pitto
Debra Davis
Sean Ekins
Max Espley
Gregory Ferrence
Philip Heller
Jeremy Garritano
Guenter Grethe
Svetlana Korolev
Bonnie Lawlor
Leah McEwen
David Martinsen
Phil McHale
Sara Rouhi
David Shobe
Andrea Twiss-Brooks
Antony Williams

Editing & production

Danielle Dennie
Svetlana Korolev
Bonnie Lawlor
David Shobe
Wendy Warr

A CINF directory including mail addresses, fax and phone numbers of the [Executive Committee](#), [Committee Chairs](#), [Divisional Representatives](#), and [other Functionaries](#) is at the [CINF website](#).