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Chemical Information Bulletin

Message from the Chair

The San Diego meeting included a novel initiative for CINF: the Multi-Day Data Summit Symposium: Chemistry, Data and the Semantic Web and its related reception (both of which may become a recurring event). It took a great deal of effort to pull together this successful symposium and I specifically want to thank Erin Bolstad, Evan Bolton, Stuart Chalk, and Leah McEwen for all their work in making it so successful. Thanks also go to Graham Douglas for his help with fundraising and coordinating the reception venue with Erin.

A very successful, multiyear, combined CINF (Leah McEwen and Stuart Chalk) and CHED (Robert Belford) effort also came to fruition at this meeting, with the CHED symposium (cosponsored by CINF) on the Intercollegiate Cheminformatics Course. This course was the result of an Innovative Project Grant and has led to the development of a valuable online educational resource in the area of chemical information and cheminformatics. The online cheminformatics OLCC found at http://olcc.ccce.divched.org/Fall2015OLCC was offered at four universities in the fall of 2015 and features a series of superb teaching modules with contributions from many CINF members. Topics covered include chemical identifiers; comparing and searching chemical entities; 2D similarity methods; tutorials on advanced searching in PubChem using chemistry APIs, including the ChemSpider InChI API; and using chemical databases. At the San Diego meeting, it was great to see all of the students involved in the program, and I would like to see CINFs continued involvement with CHED in providing educational materials and direction in curriculum development in cheminformatics, chemical information, and methods for data analysis, all of which are becoming increasingly important.

The CINF program also featured some outstanding symposia covering significant topics in chemical information, such as: Overcoming Incompatibilities in Scientific Data; Applying Structural Knowledge in Drug Discovery and Development; Global Initiatives in Research Data Management and Discovery; Data Mining for Searching Noncovalent Interactions in Chemical Databases; ELNs; Chemical Information for Small Businesses and Startups; Linking Big Data with Chemistry: Databases Connecting Genomics, Biological Pathways and Targets to Chemistry; Impact of Funders on the Research Data and Publications Landscape; and Reimagining Libraries.

We enjoyed a superb luncheon with delicious food (thanks to the capable organization of Michael Qiu) and a fascinating speaker, Dr. Christopher Tubbs of the Conservation Education Division at the San Diego Zoo Institute for Conservation Research, whose topic **"**Dietary Phytoestrogens and Reproduction in Southern White Rhinoceros," addressed the impact of diet on the reproductive health of the rhino.

For Philadelphia we are also looking forward to some outstanding programming, including a cosponsored symposium with MEDI, on "Effectively Harnessing the World's Literature to Inform Rational Compound Design," sponsored by Genentech and organized by Dan Ortwine; the 2016 Skolnik symposium, and a symposium which I am chairing with ANYL on "New Directions in Chemometrics: Making Sense of Big and Small Chemical Data Sets."

I want to thank some CINF members who are stepping down from responsibilities and some who are assuming new responsibilities. Thanks to Dave Martinsen, stepping down from chairing Communications and Publications; Leah McEwen, stepping down from the office of Secretary; Belinda Hurley and Carmen Nitsche, stepping down as Webinar chairs, and Graham Douglas for assuming the role of Communications and Publications chair. Thanks also to Michael Qiu and Erin Bolstand who will be now be assisting with Webinars, and welcome to our new Secretary, Tina Qin; David Evans, our new Awards chair; and Bonnie Lawlor, our new Procedures chair.

If you have any suggestions or recommendations on how CINF can provide more services and reach out to its members more effectively, please let me know. As only 25% of members ever attend a national meeting, CINF is anxious to find ways that it can provide resources and benefits to members who do not attend these meetings. If you have any comments please email me at rachelleb1@gmail.com, and if you are in Philadelphia, please introduce yourself.

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Letter from the Editor

Greetings from overcast Philadelphia.

I am delighted to be writing to you once again as editor of the *Chemical Information Bulletin*, a role that I particularly enjoyed last time I held it. I think that some of the best information sources available to chemists are other chemists, and I am proud to be able to help CINF members tell others about their activities and the activities of the division at large.

This is the first time that I have edited a post-meeting issue of the *CIB*, and my experience differed greatly from editing a pre-meeting issue. Rather than worrying about the formatting of information from the technical program (and praying that the ACS systems used to obtain this information had supplied us with the correct room numbers, times, and session organizers), I was free to read and contemplate interesting and informative reports from many of these self-same technical sessions. I have always loved this aspect of the post-meeting *CIB* because ACS meetings have gotten so busy that it is impossible to attend every single talk that sounds interesting. I extend my gratitude to the many session organizers who, although they had already worked extremely hard to organize symposia on cutting-edge topics in our discipline, were still willing to expend extra time and effort to prepare reports and summaries of the happenings at their symposia.

We certainly live in an "interesting time" in the field of chemical information, and I am not sure whether this is a blessing or a curse. Many of the symposium topics centered on acquiring, using, and reusing research data in ways that are in keeping with funders' mandates for the sharing of data and publications. These topics reflect the establishment and growth of many new avenues for chemical information research and practice. The danger, as always, lies in the fact that many of us must simultaneously maintain traditional services and research practices while expanding into new areas. It is the job of our community to meld the old with the new, developing systems and workflows that will merge the traditional with the innovative. Based on the six symposium reports encapsulated in this issue, we are definitely up to the challenge!

In addition to the symposium reports, I am pleased to present two feature articles: an interview with Stuart Chalk by Svetlana Korolev and a retrospective on the SPARC *Organic Letters* experiment by David Shobe. Both are extremely interesting reading, and I hope you will find them inspiring and thought-provoking, respectively. While you are reading, be sure to take note of the activities of our committees and our sponsors, and, if you have a hankering for more reading in our discipline, check out the book reviews so thoughtfully provided by Bob Buntrock.

Before concluding, I must apologize for the tardiness of this issue, which came due at the busiest time of the semester, and acknowledge the support and assistance of the many people who worked on short notice to make it as interesting and error-free as possible! My heartfelt thanks go to the production team, Stuart Chalk, Bonnie Lawlor, David Shobe, and Wendy Warr for the hours that they put in copyediting and preparing the digital version of the *CIB*, which would not exist without their efforts.

Although we do live in "interesting times," I, for one, would definitely be bored if it were otherwise!

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Awards and Scholarships

Val Metanomski Meritorious Service Award

The CINF Awards committee unanimously approved the nomination of Leah Rae McEwen for the 2016 Val Metanomski Meritorious Service Award. Leah is cited in the nominating letter "for her outstanding contributions to the division" including six years as Secretary, also serving as Program Chair, and Education Chair. Leah has been tireless in her work on division and society committees, organizing symposia, supporting colleagues, and building bridges between the various communities within our division. This may best be described as it was in one supporting letter; she is "not happy unless she [is] working to make CINF the best division that it could be". The award will be presented during the CINF luncheon at the ACS National Meeting in Philadelphia in August 2016.

David Evans, Chair, CINF Awards Committee

Lucile M. Wert Student Scholarship

Allison Langham has been selected as the 2016 recipient of the Lucille M. Wert Student Scholarship. The award is for $1500 to “help persons with an interest in the fields of chemistry and information to pursue graduate study in library, information, or computer science.”

Allison holds a B.S. in Chemical Engineering from Rose-Hulman Institute of Technology, and a PhD from the University of Minnesota. She is currently pursuing a MA in Library and Information Studies at the University of Wisconsin-Madison.

Allison enjoyed a nearly six-year career at the Center for Naval Research as a research scientist before realizing her true path lay in chemical information. She is currently applying skills and knowledge from her background exploring the sustainability of data archives. She is interested in ensuring the availability of scientific data beyond the primary investigator group that created it.

David Evans, Chair, CINF Awards Committee

Applications Invited for CSA Trust Grant for 2017

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 2017.

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). Grantees have the option of payments being made in U.S. dollars or in British Pounds equivalent to the U.S. dollar amount. 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 (including the presentation of an already-accepted research paper), to gain access to special computational facilities, or to acquire unique research techniques in support of one's research. Grants will not be awarded for activities completed prior to the grant award date.

Application Requirements:

Applications must include the following documentation:

- 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;
- 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);
- A brief biographical sketch, including a statement of academic qualifications and a recent photograph;
- 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. A copy of the completed application document must be supplied for distribution to the Grants Committee and can be submitted via regular mail or e-mail to the Committee Chair (see contact information below).

Deadline for Applications:

The application deadline for the 2017 Grant is March 31, 2017. Successful applicants will be notified no later than May 9, 2017.

Address for Submission of Applications:

The application documentation can be mailed via post or emailed 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.

Past Grant Recipients

2016

Thomas Coudrat: *Monash University, Australia*, was awarded a Grant to cover travel to present his work at three meetings in the United States: the Open Eye Scientific CUP XVI, The American Chemical Society Spring Meeting, and the Molsoft ICM User Group Meeting. His work is in ligand directed modeling.

Clarisse Pean: *Chimie Paris Tech, France*, was awarded a Grant to cover travel to give an invited presentation at the 2016 Pacific Rim Meeting on Electrochemical and Solid State Science later this year.

Qian Peng: *University of Oxford, England*, was awarded a Grant to attend the 23rd IUPAC Conference on Physical Organic Chemistry. His research is in the development of new ligands for asymmetric catalysis.

Petteri Vainikka: *University of Turku, Finland*, was awarded a Grant to spend the summer developing and testing new methods for modelling organic solvents in organic solutions with Dr. David Palmer and his group at the University of Strathclyde, Glasgow, Scotland.

Qi Zhang: *Fudan University, China*, was awarded a Grant to attend a Gordon Conference on Enzymes, coenzymes and metabolic pathways. His research is in enzymatic reactions.

2015

Dr. Marta Encisco: *Molecular Modeling Group, Department of Chemistry, La Trobe Institute for Molecular Science, La Trobe University, Australia* was awarded a Grant to cover travel costs to visit collaborators at universities in Spain and Germany and to present her work at the European Biophysical Societies Association Conference in Dresden, Germany in July 2015.

Jack Evans: *School of Physical Science, University of Adelaide, Australia* was awarded a grant to spend two weeks collaborating with the research group of Dr. Francois-Xavaier Coudert (CNRS, Chimie Paris Tech).

Dr. Oxelandr Isayev: *Division of Chemical Biology and Medicinal Chemistry, UNC Eshelman School of Pharmaacy, University of North Carolina at Chapel Hill*, was awarded a Grant to attend summer classes at the Deep Learning Summer School 2015 (University of Montreal) to expand his knowledge of machine learning to include Deep Learning (DL). His goal is to apply DL to chemical systems to improve predictive models of chemical bioactivity.

Aleix Gimeno Vives: *Cheminformatics and Nutrition Research Group, Biochemistry and Biotechnology Dept., Universitat Rovira I Virgili* was awarded a Grant to attend the Cresset European User Group Meeting in June 2015 in order to improve his knowledge of the software that he is using to determine what makes an inhibitor selective for PTP1B.

2014

Dr. Adam Madarasz: *Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences.* He was awarded a Grant for travel to study at the University of Oxford with Dr. Robert S. Paton, a 2013 CSA Trust Grant winner, in order to increase his experience in the development of computational methodology which is able to accurately model realistic and flexible transition states in chemical and biochemical reactions.

Maria José Ojeda Montes: *Department of Biochemistry and Biotechnology, University Rovira i Virgili, Spain*. She was awarded a Grant for travel expenses to study for four months at the Freie University of Berlin to enhance her experience and knowledge regarding virtual screening workflows for predicting therapeutic uses of natural molecules in the field of functional food design.

Dr. David Palmer: *Department of Chemistry, University of Strathclyde, Scotland*. He was awarded a Grant to present a paper at the fall 2014 meeting of the American Chemical Society on a new approach to representing molecular structures in computers based upon on ideas from the integral equation theory of molecular liquids.

Sona B. Warrier: *Departments of Pharmaceutical Chemistry, Pharmaceutical Biotechnology, and Pharmaceutical Analysis, NMIMS University, Mumbai*. She was awarded a Grant to attend the International Conference on Pure and Applied Chemistry to present a poster on her research on inverse virtual screening in drug repositioning.

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 took 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*. She 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-Knappat of the Freie University of Berlin and Professor Jean-Phillipe Vert of the Paris MinesTech to continue his work on the development of atomic partial charge kernels.

2010

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

2009

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

2008

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

2007

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

2006

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

2005

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

2004

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

2003

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

2001

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

Meeting a New CINF Volunteer Extraordinaire

An Interview with Stuart Chalk

After engaging for six years as an editor of the *Chemical Information Bulletin* I wanted to continue the "Meet your new CINF functionary" interview series (http://www.acscinf.org/content/interviews). For this issue I asked Professor Stuart Chalk to talk about his growing involvement in the Division of Chemical Information. In 2016, Stuart became a new coordinator of the CINF Scholarship for Scientific Excellence program, an assistant Webmaster (and now Webmaster); a co-organizer of the first CINF Data Summit (http://www.acscinf.org/content/cinf-2016-data-summit-251st-acs-meeting-san-diego); a co-author of the Fall 2015 InterCollegiate Cheminformatics Course (http://olcc.ccce.divched.org/Fall2015OLCC), with a follow-up symposium about this course in the Division of Chemical Education program (https://ep70.eventpilotadmin.com/web/page.php?page=Session&project=ACS16spring&id=208333, https://ep70.eventpilotadmin.com/web/page.php?page=Session&project=ACS16spring&id=216599); and a co-author of ten presentations at the spring ACS national meeting in San Diego. In December 2015, he participated in multiple symposia at PacifiChem. Antony Williams, Erin Davis, and Stuart Chalk have formed a task force spearheading outreach activities for CINF.

Stuart Chalk is an associate professor of chemistry at the University of North Florida. He earned a B.S. degree from Loughborough University (U.K.) and a Ph.D. degree from the University of Massachusetts at Amherst (U.S.A.). Dr. Chalk is trained as an analytical chemist with expertise in flow analysis methodology and instrumentation. Over the last fifteen years he has morphed into a cheminformatician working on research projects to develop data standards (the Analytical Information Markup Language: AnIML; Common Standard for eXchange: CSX; Experiment Markup Language: ExptML); electronic laboratory notebooks (the Eureka Research Workbench); scientific ontologies (the Chemical Analysis Ontology: CAO); and scientific data representation.

***Svetlana Korolev**: Stuart, let's start at the beginning of your career path. Please take us back to the time when you realized you wanted to be a scientist. Can you name people who influenced your career? How did you become interested in cheminformatics next?*

Stuart Chalk: Coming out of high school (in the United Kingdom) I knew I wanted to do something technical. I really liked math and logic, but I did not want to be math teacher (the only job I thought you could do with math at the time), and I was not interested in a career in physics. I chose chemistry because it was something I liked and, although it was not my best subject, I could see myself working in a lab. This was heavily influenced by my high school chemistry teacher, Mr. Hunt. He let me be the stockroom prep assistant for his classes, and it gave me a great deal of pride.

I picked an undergrad degree in Chemistry with Analytical Science and graduated in 1984, having done an internship as part of the degree that made me realize I was absolutely in the right area. I started getting into computers and started using a Mac in my senior year, which really turned me on to computing. The research advisor I worked for, Julian Tyson, helped me see how research fit in with the grand picture of chemistry, and I was excited when I graduated and got my first job at The Wellcome Foundation (as it was then) in Dartford, Kent.

It wasn't long, though, before I was starting to think about graduate school, and, after a few months, I went back to see Prof. Tyson to talk about doing a Ph.D. He emigrated to the United States and I followed to do my Ph.D. During my Ph.D., I found I like collecting citations and ended up doing lots of scanning of references and optical character recognition (OCR). Then I organized them into this new software called EndNote. From then on I was hooked on informatics as a hobby … at least until recently.

SK: *You relocated from the United Kingdom to the United States of America in 1989. Could you walk us through what it was like? Please share your viewpoints of the academic systems in two countries. Are there any noticeable distinctions in the ways how students study, conduct research, or seek for scientific information?*

SC: Retrospectively it was a courageous thing to do on my own, but at the time it was an adventure and I had nothing to lose. Certainly, the two academic systems are different, with the United Kingdom being much more prescribed in terms of the classes. There was no "picking a major" when you get to college. I picked my undergraduate course when I was in the last year of high school. The levels of educational advancement were also different. Students in graduate school were not as far along in the United States, and this helped me do well my first year as I repeated some classes I had done in the United Kingdom. As for doing research, there was not much difference in the approaches between the two systems, with the exception that it was generally easier to get inter-library loans in the US.

SK: *At "The Growing Impact of Openness in Chemistry: a Symposium in Honor of J.C. Bradley" during the fall 2015 ACS meeting you introduced the beta version of the Open Spectral Database (OSDB, http://osdb.info), and next talked about this project as well as the NIST- IUPAC Solubility Data Series (https://sds.coas.unf.edu/) and the Flow Analysis Database (FAD, http://www.fia.unf.edu) during PacifiChem in December 2015. Please tell us a little bit more about your current research projects. Why do you work on them? How does your research fit in the larger scheme of the field? Do you have collaborations through CINF?*

SC: My initial foray into informatics was based on an interest in my research field. The OCR work I mentioned before turned into a Web site of citations on the general area of flow analysis. The scope of this spans the areas of flow injection analysis (FIA), sequential injection analysis (SIA), zone fluidics (ZF), and post-column derivatization for HPLC. The Web site (https://www.fia.unf.edu/) is still available, although these days it looks terribly dated. I am working on a new version (currently at https://chalk.coas.unf.edu/fad) that will replace the old site over the summer and uses all the current technology and provides an application programming interface (API).

The initial work on the FAD server was done using an Apple Server, Lasso, and FileMaker. This first Web site got me into a grant from the NSF NSDL (National STEM Education Distributed Learning, 2001) program to develop the first Analytical Sciences Digital Library Web site (ASDL, http://asdlib.org). In doing that I learned how to use Apache, PHP, and MySQL, which I liked much better as a development system (and it fits my budget: it was free). This also got me into Dublin Core and implementing an OAI-PMH (Open Archives Initiative Protocol for Metadata Harvesting) interface to allow the main NSDL site to harvest the collection from the ASDL.

My current motivation is grounded in the firm belief that although it takes time and effort there are a lot of research data out there that are high-quality and deserve to be picked out of the research literature haystack and made available, searchable, and re-usable. This is why I am working on projects with SpringerMaterials extracting property data from the Landolt-Börnstein database, and NIST to "semanticize" (if that's a word) the existing IUPAC Solubility Database Series volumes that were originally digitized twenty years ago. These are quality data sets and, in today's environment, difficult to use, as they are electronic (PDF) but not useable in an informatics sense. Yes, there is a lot of tedious work to accurately capture the property data and annotate its context well enough to make it useful, but it's worth it. Good data are worth it; they are a valuable commodity in today's big data marketplace, and scientists need them for many different applications.

As for CINF collaborations I don't yet have any formal ones, as I am new to the community. However, CINF has been a revelation for me. By that, I mean for years I have attended Pittcon (Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy), presenting papers and posters on the informatics work I was doing. No real interest. Then, Bob Lancashire of the Joint Committee on Atomic and Molecular Physical Data (JCAMP) fame invited me to give a talk at the ACS meeting in Indianapolis in fall of 2013. Wow! There was a group of people that liked the things I was doing, and they were doing really cool stuff. It was a career moment; I had found a real home. Since then it has been a race to catch up with the community and now I am hitting my stride. Of course, I have also been encouraged by the most charismatic of CINF members, Tony Williams, to work on cool projects. The OSDB (Open Spectral Database) is one of those: instigated over a beer in Denver. Tony said: "We need open spectra, period." I said: "OK," and went away to build the Web site in a few months. It is all about

making data accessible and usable; why else would we put it on a Web site? I am also interested in molecular structure representation, scientific units, ontologies for chemistry, electronic lab notebooks, bibliometrics… too many interesting things…

SK: *At the University of North Florida (UNF) you teach a Senior Seminar and courses on Modern Analytical Chemistry, Quantitative Analytical Chemistry, Structure Elucidation, General Chemistry, and Chemical Informatics. In 2004 you were recognized by receiving a UNF Outstanding Undergraduate Teaching Award. Your students posted some fascinating "rate my professors" comments about you, for example: "He has a wonderful sense of humor and an extraordinary grasp of his subjects! He is overly competent and truly prepares his students for their majors… if you like sci-fi and British humor, he is definitely the professor for you." Could you share with us some of your brightest teaching moments that make students praise you so highly at UNF? Also, please talk about the Fall 2015 InterCollegiate Cheminformatics Course.*

SC: I have been lucky to be a very different type of person in the Department of Chemistry at UNF (this is my 20th year). By that I mean, I am really not a hard-core chemist, not naturally good at chemistry. This means I have always had to work at learning and understanding chemistry, and I think it's that background that helps me relate to students. I try and bring professionalism and organization to the classroom, with high expectations, but I also realize that to communicate chemistry effectively you have to be engaging, honest and real. In addition to having a wry sense of humor and a British accent (a common joke I make in class is "I don't have an accent – y'all have an accent!"), I regularly do strange things in class or make weird analogies when I see students eyes glaze over. If you create a 'memorable' moment, students remember that. At some point I might actually do step aerobics in class to talk about energy transformations, but I'm not quite courageous enough yet!

I am lucky to have had many meaningful teaching moments in my career so far, especially all those of my research students that have gone on to graduate/professional school, and others coming well after the fact. One example is a chemistry major that, a few years after graduating, contacted me and wanted to let me know that he really appreciated what I did for him. In particular, at the end of our senior level Instrumental Analysis course, I gave the student an A-. He remembered asking "Why didn't I get an A?", to which I replied: "Because your work wasn't A quality." It made him really think about what quality meant and used it to great advantage in getting a job at Anheuser-Busch. He has risen through the ranks and is now a Global Senior Quality Assurance Manager there.

More recently, last month in fact, out of the blue I got the following email from a student who was at UNF for only one year.

> *"It's been awhile. I can guarantee that you won't remember me, but you were my general chemistry professor in the fall of 2011. I am writing you today because I want to thank you. On May 7th, I will be graduating with a degree in chemical engineering from the University of South Florida and I owe it all to you... I sat in your class the first day of the fall semester completely hating the fact that I had to take general chemistry. My high school teacher ruined the subject for me. After taking your course, I learned to love chemistry in a new way, which I attribute that [sic] to your teaching style. It was in that classroom that I first learned of chemical engineering as an option. I decided to leave UNF and change my major from finance to chemical engineering…Anyway, I wanted to thank you for changing my life's path to something I would have completely disregarded without your course.*"

As you might expect it is this kind of feedback that makes teaching so rewarding, and makes it easy to continue even though you've been doing it a long time.

But doing new things is also good. For me that has been teaching Chemical Information Science as a class to juniors and seniors. I've done this for a while but the class has morphed in terms of content, which goes along with there not really being a good definition of what the topic area is exactly. Luckily, I got to meet Dr. Bob Belford who has been running the OLCC (OnLine Chemistry Course) funded by NSF for a while. He put together a group of faculty to develop different modules for the course, and we taught it as a "flipped" style class. Students

at four campuses participated and each one of them got a lot out of the experience (and many presented at the ACS meeting in San Diego this last March). Likely, this will end up as course material on the ChemWiki, and we will teach it again in the next couple of years.

SK: *How do you satisfy your own chemical information needs? Which databases, search engines, or current awareness tools do you use the most?*

SC: I use the common ones like PubChem, ChemSpider, Chemical Identity Resolver, and CrossRef. I also like to build Web sites to serve up data and for that I use Apache, MySQL, and PHP. I also use JavaScript and Bootstrap for the GUI (graphical user interface). I am very interested in using JSON-LD (JavaScript Object Notation for Linked Data) for storing and semantically representing chemical data.

SK: Do you have plans to write a book? If so, what is its subject?

SC: I've had a plan to write a book for the last five years. It's called "XML, Metadata and Markup Languages for Chemists." I have had trouble writing it because there are so many interesting things to do, but if I were to start one right now it would be "Semantic Technologies for Chemists." Hopefully, someday I will get to do both of these.

SK: *Stuart, you are now actively contributing to the Division of Chemical Information technical program and various functionary activities. What was your first encounter with CINF? Are you a member of any other ACS divisions or professional societies? What do you enjoy most about your involvement in our division? Could you speak of some initiatives considered by a new outreach taskforce?*

SC: My first encounter with CINF was at the fall 2013 meeting in Indianapolis where I met Tony Williams. Tony has been a great mentor to me since then and I have learned a lot, especially what a "skunkworks" project is. I am a member of the Analytical Division of ACS, the Royal Society of Chemistry (RSC), and ASTM, and I hope to soon be involved with IUPAC. The CINF division has been very welcoming to me and it has been great to talk to people that I can really relate to. The best (and worst) part about this I can't seem to say "No" to projects that people propose. As for the outreach taskforce, that is still in its infancy, but we are definitely looking to identify members of CINF who can liaise with other divisions and we would like to organize symposia at meetings in other divisions to get the word out.

SK: *Would you like to talk about the CINF Scholarship for Scientific Excellence program? What made you volunteer for the position of its coordinator? Has everything worked out as planned for San Diego? Was it highly competitive for the applicants and a tough decision for the jury? Do you have long-term commitments from its sponsors (e.g. InfoChem/Springer for spring and RSC for fall), or do you have to find funds for the next year?*

SC: I thought that the CINF Scholarship for Scientific Excellence was a way that I could contribute to the CINF division without taking on a large burden. Thanks to Guenter Grethe's advice, everything went well and we had a great group of submissions. Picking the winners was not so easy because of the variety and quality of submissions, but I think we got it right. ACS Publications has kindly agreed to sponsor the Scholarship Program for the fall meeting in Philadelphia, and we are hopeful they will continue it further.

SK: *The Division of Chemical Information was featured in the ACS National Meeting highlights for its first Data Summit organized for five days in San Diego. Please share some highlights of your symposium "Chemistry, Data, and the Semantic Web: An Important Triple to Advance Science" organized in collaboration with Evan Bolton. If you were to give "The Best Presentation Award," would you name a special talk at the Data Summit?*

SC: Wow. That's a tough question. I would probably pick Michel Dumontier from Stanford, who gave a talk on semantic approaches for biochemical knowledge discovery. In his talk he clearly demonstrated the tools and approaches that chemists need to work toward in order to really make knowledge discovery. I particularly liked his question: "How can we automatically find the evidence that supports or disputes a scientific hypothesis using the latest data, tools and scientific knowledge?" This is the crux of what we in informatics are trying to do: encode meaning to information so that computers can infer relationships from large data repositories using semantic technology. All the infrastructure is there; we need to translate chemical knowledge across to the digital area using appropriate ontological representation. I believe we will have this in the next ten years *if* we make quality research data open and reusable to the community.

SK: *Which symposia and presentations are you planning for the Fall 2016 ACS National Meeting in Philadelphia?*

SC: Sadly, I won't be attending the fall ACS meeting this year. It is the first week of fall classes at UNF and thus bad timing for me.

SK: *You joined a small taskforce for investigating a new host for the CINF Web site last fall. Would you like to share any updates of your investigations? Are there any other challenging issues with the CINF Web site?*

SC: All I can say right now is that the current Web site is in dire need of a revision. I think those of us looking into this see a lot of opportunity to use a new Web site as a way to engage the community, reach new members, and provide tools for members to be able to show off aspects of their work and interests in a practical way. We also need to capture more data about our members, their interests, needs, skills, and that is an obvious way to give our members more for their membership.

SK: *Stuart, let me finish our interview by asking a few personal questions. What are your favorite activities outside work? How would you spend your "dream" vacation? What kind of music do you like to listen? Is there anything else I did not ask that you want to add?*

SC: I'm a runner, which helps me unwind, and I love to play golf. As for a dream vacation: some place with beaches, golf courses, and plenty of good (dark) beer. Musically I am quite varied, all the way from electronic (Jean-Michel Jarre), to hard rock (Rush), to 80's (Abba). I love to sing and whistle along to tunes at work and my colleagues are very patient with me. I might try singing in a band at some point; who knows?

A parting comment would be this: *We need to show that informatics in chemistry is important. Not to ourselves, but to the real bench chemist. Once we get folks to realize that what we can do for the chemistry community will make them more efficient, more knowledgeable, and improve the quality of the work they do, we will really be able to move chemistry into the digital era.*

SK: *Thank you for sharing your expertise with the Division of Chemical Information. Best wishes for all your endeavors.*

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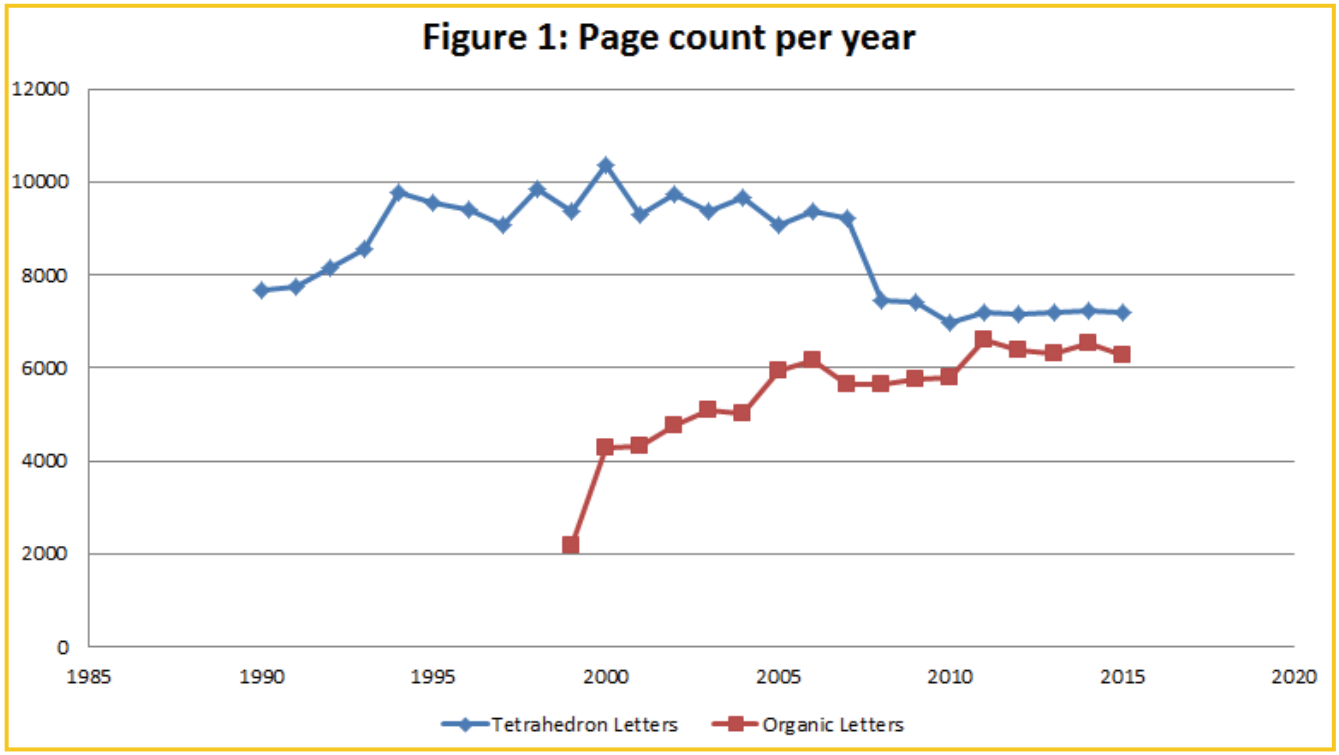
Editors' Corner

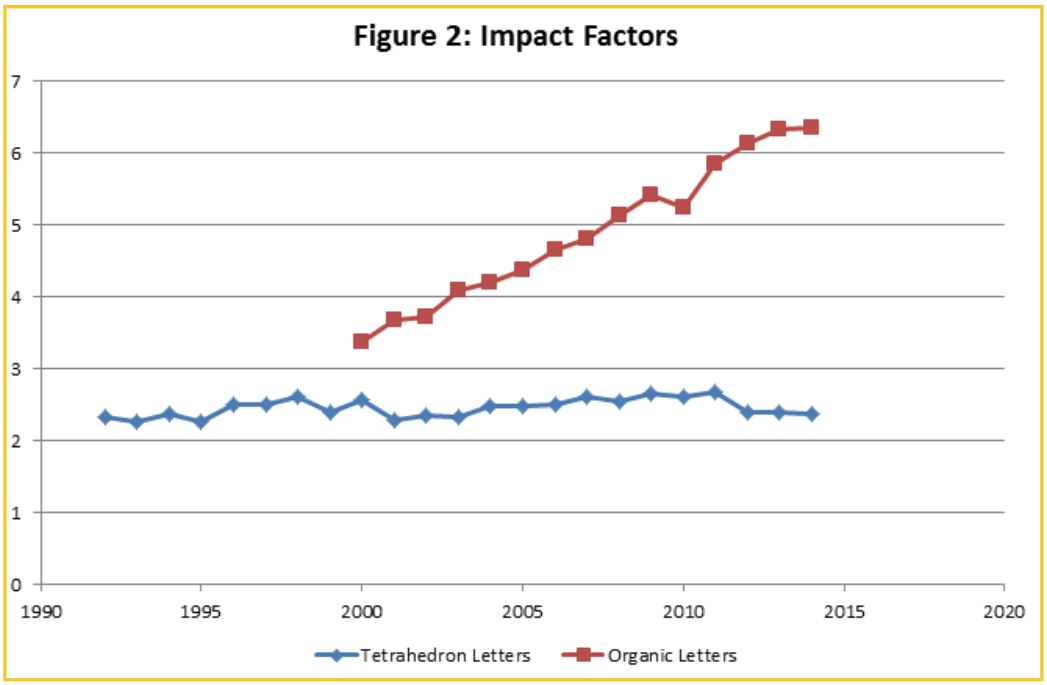
Eighteen years ago, on June 30, 1998, the American Chemical Society (ACS) announced a partnership with the Association of Research Libraries (ARL) to launch a new scholarly journal in the organic chemistry field. This journal, the first of three new journals launched in accordance with ARL's Scholarly Publishing and Academic Resources Coalition (SPARC), would later be given the name *Organic Letters*, the first issue of which appeared in July 1999. SPARC was created as an association of eighty-one ARL member libraries "as a result of the growing concerns among librarians and researchers over the rising cost of academic publications, particularly scientific journals"[1]. Although the press release does not state so explicitly, it seems that *Organic Letters* was intended to be a lower-cost alternative to *Tetrahedron Letters*, an Elsevier publication. Whether through libraries and other institutions deciding to cease subscription to *Tetrahedron Letters* in favor of the new journal, or through authors deciding to send important manuscripts to *Organic Letters* rather than the established journal as a protest against high prices, the existence of a competing journal was supposed to create downward pressure on the price of *Tetrahedron Letters*. Of course, the risk was that SPARC's initiative would simply add another "must have" journal for any institution wishing to keep up with developments in organic chemistry and that the strain on these institutions' library budgets would simply increase.



Now that nearly two decades have passed since the launch of *Organic Letters*, one may ask: has the ACS-ARL-SPARC initiative worked? First of all, has the new journal been diverting papers, and in particular the high-quality papers that drive journal subscriptions, that would have gone to *Tetrahedron Letters*? Fortunately, journal page counts (Figure 1) and impact factors[2] (Figure 2) are readily available on the Internet. Although there is a sudden drop in the page count for *Tetrahedron Letters* between 2007 and 2008, it seems unlikely that this is due to competition from *Organic Letters*, since there is no corresponding increase in the page count for the latter. Regarding impact factors, it appears that while *Organic Letters* has managed to attract highly-cited papers, this has not affected *Tetrahedron Letters*, for which the impact factor has remained steady for the last two and a half decades.

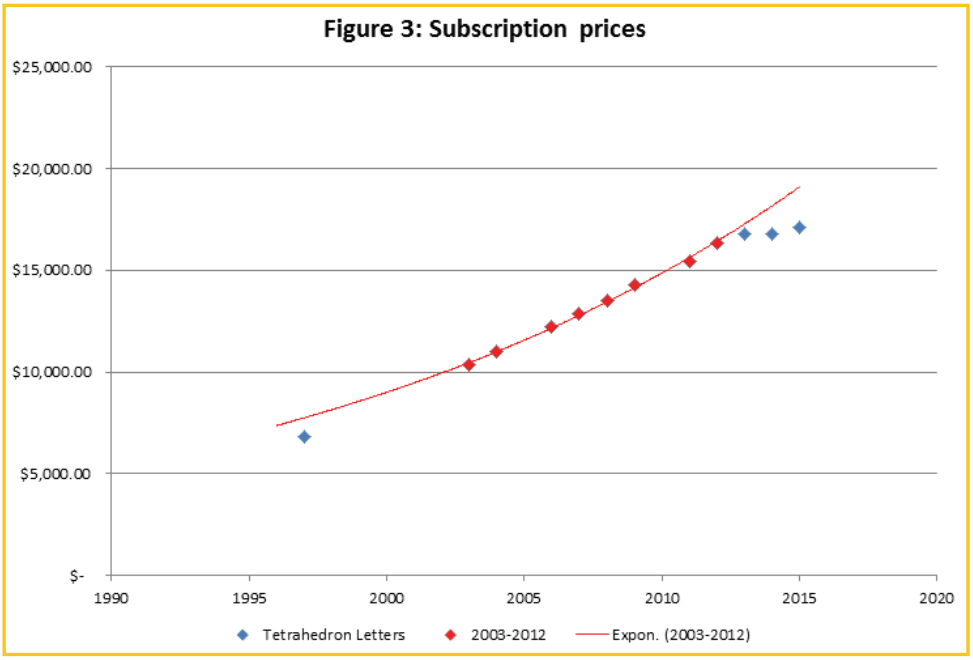
[1] Press release, American Chemical Society, June 30, 1998, archived in the CHMINF-L discussion list by Gary Wiggins on July 1, 1998; Web site accessed April 9, 2016.

[2] https://www.researchgate.net/journal/0040-4039_Tetrahedron_Letters and https://www.researchgate.net/journal/1523-7052_Organic_Letters, accessed February 9, 2014.



Has this had an effect on the subscription prices for *Tetrahedron Letters*? Neither the Wayback Machine[3] nor Elsevier itself[4] was able to give a complete table of subscription prices for the years 1995 to 2016. Figure 3 displays the data we were able to obtain. Unfortunately, we have only one data point that is before the launch of *Organic Letters*, so it is impossible to conclude anything with statistical confidence. It is, however, suggestive that the lone data point for 1997 falls below the trend line (fitted exponential curve) for the period 2003 to 2012, which does not support the idea of a price decrease due to introduction of the new journal.

Data were gathered on the page count and impact factor for *Tetrahedron Letters* and *Organic Letters*. It does not appear that the addition of *Organic Letters* to the set of available journals has led to any compensatory change in the page count or impact factor for *Tetrahedron Letters*. In addition, the institutional list price for *Tetrahedron Letters* for various recent years was obtained. Unfortunately, only one price data point was obtained for the period just before the launch of *Organic Letters*, so no conclusion can be drawn at present. If any reader of this article has records of the institutional list price for *Tetrahedron Letters* for the period 1990-1999 (note that this may be different from the price a particular institution actually paid for *Tetrahedron Letters*), we would like to know, so that the question of the impact of the launch of *Organic Letters* on pricing for *Tetrahedron Letters* may be examined.



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[3] https://archive.org/web/ directed to http:elsevier.com for various dates.
[4] Personal communication from Ramesh Mehto (Elsevier Customer Service).

Technical Program — Symposium Summaries

Global Initiatives in Research Data Management and Discovery

The topic of research data is a major feature of current conversations about science and scholarly communication. Governments and funders are promoting policies and mandates that aim to ensure that research data is properly managed and openly shared. Doing so aids in the validation and reproducibility of results and creates opportunities for reuse of data across disciplines, which, in turn, advances science. The principles and benefits of data sharing are easy to understand, but putting them into practice presents many challenges. These are not specific to chemistry and are shared by other disciplines across the globe.

The CINF symposium in San Diego "Global Initiatives in Research Data Management and Discovery" brought together thought leaders and practitioners from a variety of scientific domains who are engaged in tackling research data challenges on a global basis. This two-day symposium highlighted the experiences of scientists, international and national scientific data organizations, tool vendors, and service professionals. They brought their perspectives on issues of globalization, standards, community practice, technical infrastructure, and cultural shift. One general sentiment that emerged was that chemistry touches every area of science and initiatives in this arena can benefit and contribute to collaborations among a wide variety of stakeholders.

Global organizations and international initiatives represented included the Research Data Alliance; CODATA and the World Data System, both of which were established by the International Council for Science (ICSU); DataCite; FORCE11; and the International Union of Pure and Applied Chemistry (IUPAC). Attendees also heard about disciplinary initiatives, including NIF (neuroscience), the Resource Identification Initiative (biomedicine), and DataOne (earth sciences). Recurrent themes revolved around data publication, interdisciplinary interoperability, persistent identifiers, certifying trust, machine actionability, community engagement, cooperation among initiatives, training, and service support.

Examples of scientific community standards of practice in depositing and managing collections of chemistry-related data featured a number of proven data systems, including PubChem, the National Institute of Standards and Technology Thermodynamics Research Centre (NIST/TRC), the Cambridge Crystallographic Data Centre (CCDC), the STRENDA and MIRAGE community standards developed by the Beilstein Institute, and the CODATA Nanomaterials project. An emerging theme was the expressed need for best practices for establishing and sustaining guidelines and for engagement with the research community around data reporting and citation: could this be a role for the global initiatives?

Perspectives on digitally managing scientific data and practically addressing some of these issues “where the rubber meets the road” were presented by a group of researchers, including Henry Rzepa, Simon Coles, Stuart Chalk, and John Kitchin; tool developers, including MestraLab and Dotmatics; and research service providers, including the the California Digital Library (CDL), the Royal Society of Chemistry (RSC), and the Pistoia Alliance. They emphasized development of capabilities and supporting services for data analysis before, during, and after experimental documentation, including downstream scientific use of the data. Such practices involve publishing ‘live’ data; supporting compilation and integration at scale; and supporting workflows that allow individual scientists to manage their data at capture, assembly, analysis, and publication, as well as subsequent organization, delivery, discovery, and functionality for reuse of the data by the broader community.

Many tractable solutions are emerging across this diverse scientific community. The challenges facing academia are fairly similar to those addressed by industry and government, and there is precedent for worldwide, cross-sector collaboration on common issues. Is it time for an international chemistry data interest group to tackle the digital data challenges particular to chemistry standards and community practice and to unpack questions about which data and metadata can be contributed to the pre-competitive, collective chemistry data pool for the benefit of the global enterprise? Are there lower-barrier, higher-impact opportunities for improving usability of chemical data in both research and business, such as machine-actionable and extensible chemical identifiers and

-accessible patent documentation? Do we need to change the chemistry research and reporting culture to enable researchers to share data, or align funder expectations and publishing workflows to scientific workflows? The newly formed RDA Chemistry Research Data Interest Group (CRDIG or DIG Chemistry) aims to connect and promote these conversations through widely spread symposia, networking, workshops, and other venues.

The "Global Initiatives in Research Data Management and Discovery" symposium established the context for the San Diego meeting's program track on chemistry data, which included many other data-related symposia that covered the impact of funder policies on the research data and publication landscape, the challenges of incompatibilities in scientific data, opportunities for linking chemical and biological data, and the role of semantic technologies in enabling richer representation of chemistry data and knowledge. The topic of data management is at once timely and timeless for the field of chemistry, and the conversation is set to continue in several venues, including at the ACS national meeting in Philadelphia, PA, in August 2016, and during International Data Week in Denver, CO, in September 2016.

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Chemistry, Data, and the Semantic Web: An Important Triple to Advance Science (*or Challenges and Opportunities in Chemical Knowledge Management*)

I (Stuart Chalk) agreed to organize this symposium because it was exactly the area I am interested in, the representation of chemical knowledge using semantics and ontologies. I came up with the title on the spur of the moment and had not even thought about exactly whom I would invite. Luckily, I started talking with Stephen Boyer from IBM about the workshop he and Evan Bolton were planning for October 2015 in Basel, and it wasn't long before Evan was on board as co-organizer. It turns out that Evan knows some people.

We invited over 50 speakers to participate in the symposium and in the end we had forty-three speakers present over three days in San Diego, organized into the six sessions below.

- Tuesday morning: Chemical Classification
- Tuesday afternoon: Chemical Information
- Wednesday morning: Informatics Application
- Wednesday afternoon: Knowledge Representation Evolution
- Thursday morning: Informatics Evolution & Use
- Thursday afternoon: Ontology Evolution & Use

Looking back on it now, I am still floored by how many experts in their respective areas contributed to the quality and rigor of the sessions, to the wonderful audience questions (during the sessions and at the breaks), and to the size of the audience. We had audiences of up to eighty for some sessions, and there were even forty on the last day (Thursday). Since the end of the conference, there have been many requests to do more symposia like this at future meetings, and we are certainly working on that.

It would impossible to report about each and every talk at the six different sessions that made up the symposia, so we will not try here. We are planning to write up an editorial with contributions from many of the speakers so

there will be more to read about the perspectives of the presenters and the outcomes of the symposium, but it is appropriate to report the "pain points" that the speakers and the audience contributed. Many folk took photos of the pages we had up on the walls of the conference room (that is how important the issues were), so below is a cleaned-up list of the issues articulated.

Access Issues

⇒ accessing good data that's not published
⇒ data exchange standards, protocols, and best practices
⇒ data locked in text
⇒ extracting data from literature (time consuming)
⇒ interoperability (systems, data sets)
⇒ machine learning for data extraction
⇒ quality of search results
⇒ querying across resources (global search across heterogeneous data sets)
⇒ specificity versus generality
⇒ too many results affect search granularity (consequence of limited metadata?)

Audience Issues

⇒ answering complicated questions
⇒ context of user: perspective on data is important and impacts usage and needs
⇒ speaking the same language: chemistry is different than biology
⇒ targeting data and metadata to specific users
⇒ wide range of users with different backgrounds

Chemical Structure Representation Issues

⇒ dealing with large structures
⇒ different chemical entities in the same crystal
⇒ identifying parts of large structures (partial ids? InChI parts?)
⇒ organic compound stereochemistry
⇒ protein mapping issues
⇒ representation of inorganics
⇒ representation of stereo centers, and cis/trans isomers
⇒ structural representation of organometallics
⇒ symmetry

Community Issues

⇒ agreement on best practices for interoperability (of data, data systems, data formats)
⇒ approaches to normalization
⇒ community agreement on ... everything...
⇒ community standards change
⇒ community standards don't change fast enough
⇒ incentives for generating metadata
⇒ policies for making systems open
⇒ where are the data and metadata resources?

Data Issues

⇒ bioactivity multiplexing
⇒ biological data different from chemical data
⇒ cannot interpret data

⇒ context of chemical data (Complete? Accurate? Usable?)
⇒ data formats not correctly used
⇒ data standardization
⇒ data without context
⇒ finding what we need to find
⇒ help with annotation
⇒ identifier mapping (across different identifier systems)
⇒ integrating legacy identifiers (important for historical data)
⇒ interoperability
⇒ make open data really open
⇒ metadata of experiments
⇒ normalization of data (crosswalking to standard format)
⇒ obvious data gaps
⇒ quality of data (trust in data)
⇒ scale of data; too many data (difficult to find what you need quickly and accurately)
⇒ share your data, please! (including "dark data" the data that "did not work")
⇒ structural multiplexing (equivalent drug forms cause problems in analysis)
⇒ the data is always changing (better versioning needed?)
⇒ time dependent identifiers and classifications
⇒ what are best sources for specific pieces of data?
⇒ units: clean-up needed
⇒ units normalization important for data interoperability

Ontology/Vocabulary Issues

⇒ consistent mapping of terms
⇒ coverage of ontologies (where are the gaps?)
⇒ creating an ontology: coming to agreement on terms
⇒ don't make terms too specific (start by creating more generic terms that can be broadly used)
⇒ finding the (domain) experts to develop ontologies
⇒ gaps in terminology
⇒ harmonization and reaching consensus (of terms)
⇒ how do we deal with ontology evolution? (new terms added, some terms deprecated)
⇒ linking chemical terminology to biological terminology
⇒ ontology convergence (where there are multiple ontologies in the same domain)
⇒ stability of ontologies (are they being actively managed?)
⇒ user friendly vocabularies
⇒ vocabulary clean-up (who does it?)
⇒ (we need to encourage scientists to) invent ontologies for areas where there are none
⇒ what ontologies are out there? knowing which ontologies to use (we need a list of ontologies and coverage)
⇒ who has authority/responsibility to coordinate ontology development? (IUPAC)

Tools to Help Data and Metadata Capture Issues

⇒ best systems? (for storing, accessing data)
⇒ better tools that help data curation (i.e., research data plus metadata)
⇒ consistency of identifiers (naming)
⇒ curation of lists difficult
⇒ effective GUI for data input

- ⇒ globally synchronized data (across multiple sites); availability to third parties
- ⇒ improvements needed in machine learning
- ⇒ limiting options for users so they make sensible choices (provide contextual enumerated lists)
- ⇒ no feedback on tools/usability
- ⇒ old code and legacy systems

To wrap up, if you missed the symposium, you missed an invigorating, stimulating, tour de force of talks addressing all the issues around data and how to glean knowledge from it. We truly believe this symposium, and what follows on from it, will be the catalyst for a lot of activity that will end up changing how we store and represent chemical data and knowledge. Bring it on!

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From Data to Prediction: Applying Structural Knowledge in Drug Discovery & Development

This session brought together a mixture of presentations with a central theme: namely, the authors had a particular interest in using structural data from either 2D or 3D sources to tackle key problems in the drug design arena. The presenters were a mix of end-users of data and providers of data and applications.

3D Methods in Drug Discovery & Development

The session began with a presentation by Marcel Verdonk, who used PDB data to analyze the relative likelihood of atoms being involved in protein binding, given their degree of exposure or flexibility. He highlighted how such information could be useful in ligand design applications. The talk was interesting, very current, and challenged the audience to consider how such information could be used in future to produce better scoring functions.

Matthew Segall (Optibrium) then gave an exposition of how the StarDrop platform can be useful in drug design programs by providing a powerful system for visualizing and understanding data from both 2D and 3D sources, and Christian Lemmen (BioSolveIT) presented an analysis of how their platform, in particular, Hyde scoring, can aid and abet the interpretation of protein structures, specifically focusing on solvent molecules.

Matthias Rarey (University of Hamburg) presented recent work on ASCONA and SIENA, methods for protein binding site alignment and protein ensemble selection respectively. The methods were shown to be useful in tackling complex alignment and selection problems where current sequence-alignment-based methods generally fail.

Tobias Brinkjost, a third-year PhD student from Oliver Koch's group at the Technical University in Dortmund bravely presented his PhD work using secondary structure information to facilitate searching for ligand sensing cores. His graph-based methods allow very fast comparisons of pockets, not driven by sequence, but based on secondary structure assignment. Tobias showed that his methods could predict cases of non-homologous cavity similarities.

On a different tack, Colin Groom of the Cambridge Crystallographic Data Centre (CCDC) presented the results of the recent CCDC Crystal Structure Prediction blind test and described how structural knowledge from the CSD can be used to aid and abet predictions of crystal structures, a field that still challenges computational chemists. He highlighted how this technology is coming of age and may now be becoming more relevant to the pharmaceutical industry, particularly in drug development.

2D Methods in Drug Discovery & Development

2D methods were illustrated by a number of speakers during the day. Susanne Stalford from Lhasa showed how collaborative efforts between pharmaceutical companies can help in risk assessments associated with mutagenic impurities. Valery Polyakov showed how better random forest algorithms could be applied to large QSAR data sets to derive more meaningful models. In particular, Valery and co-workers have carefully assessed 'novelty' to show the true worth of an underlying model, and have defined methods for picking the best training sets to improve the prospective outcomes of models generated. The results appeared promising; it was surprising (at least to the chair) how much change one could observe in the value of a model by removing seemingly small biases in the underlying training data.

Data Provisioning

Barry Bunin showed how the Collaborative Drug Discovery (CDD) vault was aiding collaborative efforts between research groups across the globe with a number of examples of projects. He explained how data sharing and data security are not necessarily mutually-exclusive.

We had an excellent presentation from Marian Brodney. She has been deeply involved at Pfizer with integrating the disparate data from many projects and many sources in a useful and coherent platform. This presentation really highlighted the challenges faced by large pharma to produce a coherent system that serves a large community with very disparate needs. It also highlighted the breadth of data sources that an information provider has to consider in a large organization.

Finally, despite some technical difficulties, Asta Gindulyte showed how we all could be making far better use of Google for finding chemically-relevant results. The presentation included a demo, where Asta created an on-the-fly search engine to search PubMed in a more targeted way. The session chair will certainly be trying to create his own customized engines in the future!

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Driving Change: Impact of Funders on the Research Data and Publications Landscapes

In the last few years, there has been a renewed emphasis from funders worldwide on making research results more widely-available. In the United States, the Office of Science and Technology Policy (OSTP) released a memorandum in 2013 requiring federal agencies to develop public access plans to federally funded research. Likewise, the Research Councils UK (RCUK) has an open access (OA) policy for the publication of peer-reviewed articles, and Canada recently introduced the Tri-Agency policy, which mandates OA to articles funded by the country's major research agencies. Some private foundations, such as the Gates Foundation, also have OA policies for publications and data.

Roughly coinciding with the third anniversary of the OSTP memorandum, the ACS Division of Chemical Information held the symposium "Driving Change: Impact of Funders on the Research Data and Publications Landscapes" to explore how these new policies and requirements are shaping scholarly communications. Organized by Andrea Twiss-Brooks (University of Chicago), and Elsa Alvaro (Northwestern University), the symposium was part of the CINF program of the 251st ACS National Meeting, and took place on Tuesday, March 15, 2016. The goal of the symposium was to foster a conversation between the stakeholders involved in scholarly communications and to discuss the challenges and opportunities posed by these new policies and requirements.

The symposium opened with talks outlining the public access plans of several US federal agencies. Neil Thakur discussed NIH's public access policy, which requires all peer-reviewed journal articles arising from NIH funds to

be posted to PubMed Central (http://www.ncbi.nlm.nih.gov/pmc/). Dr. Thakur explained the different submission methods that currently exist and how to track compliance at the institutional level. Carly Robinson of the Department of Energy (DOE) explained how public access to DOE publications happens through Public Access Gateway for Energy & Science (PAGES, http://www.osti.gov/pages/). PAGES has centralized metadata, but it has decentralized distribution of full-text articles and manuscripts, relying instead on a partnership with publishers (CHORUS; http://www.chorusaccess.org/) or, in the cases where publishers do not provide public access, a link to the author-submitted, full-text, accepted manuscript. Dr. Robinson also talked about the digital research data management plans, and DOE Data ID Service (http://www.osti.gov/home/doe-data-id-service). Leah McEwen of Cornell University described NSF's open data policy, and her participation in a series of workshops aimed at understanding the community's views on public access to research data in the Mathematical and Physical Sciences (MPS) directorate.

These initial presentations on federal agencies' requirements were followed by talks from different stakeholders, including librarians, publishers, researchers, and tool-makers. Sharon Kipphut-Smith of Rice University and Betty Rozum of Utah State University described an ongoing project aimed at understanding how libraries and research offices are supporting compliance with federal mandates. According to their results, institutions are leveraging existing resources, and there is a general recognition that campus collaboration is important. Ho Jung Yoo of UC San Diego described how the University of California is facilitating public access to scholarly publications and how the Research Data Curation Program (http://libraries.ucsd.edu/services/data-curation/) of UC San Diego Library is supporting public access to research data.

Judy Ruttenberg or the Association of Research Libraries (ARL) talked about SHARE (http://www.share-research.org/). SHARE's mission is to build a free, open data set about research and scholarly activities across their life cycle. Ms. Ruttenberg gave an update on the progress of SHARE Notify, and discussed the progress of Phase II of SHARE, which involves expanding the number of providers, and enhancing the metadata.

ARL's partner for the development of SHARE is the Center for Open Science (COS). Sara Bowman of COS talked about the Open Science Framework (OSF; https://osf.io/), which is a Web application to manage the research lifecycle, including data archiving and dissemination. Dr. Bowman also gave an overview on the Transparency and Openness Promotion (TOP; https://osf.io/9f6gx/) Guidelines and their adoption by different journals.

Darla Henderson of ACS and Ann Gabriel of Elsevier represented the publishers' perspective. Darla Henderson discussed ACS Open Access strategy (http://acsopenaccess.org/), which encompasses the OA journals ACS Central Science and the new ACS Omega, and the programs ACS Editors' Choice, ACS AuthorChoice, and ACS Author Rewards. Ann Gabriel described Elsevier's efforts to comply with the new mandates; their new content types, including data, software, methods articles, and more; and the importance of supporting new workflows (https://www.elsevier.com/about/open-science).

Jeremy Frey (http://www.southampton.ac.uk/chemistry/about/staff/jgf.page) of the University of Southampton addressed the challenges posed by the new landscape from the perspective of the UK researcher. He discussed how this new situation is placing new obligations on the researchers who are securing funding but also is opening up new opportunities.

Bringing the perspective of the data center and database, Amy Sarjeant explained how the Cambridge Crystallographic Data Centre (CCDC; http://www.ccdc.cam.ac.uk/) is supporting researchers who wish to comply with mandates. Dr. Sarjeant outlined the principles of data management, as well as its challenges, including maintaining quality, attribution, funding acknowledgments, and flexibility for the future.

Maryann Martone talked about FORCE 11 (https://www.force11.org/), which is a grassroots movement aimed at accelerating the pace of scholarly communications through technology, education, and community. The membership of FORCE11 includes all stakeholders of scholarly communication, including publishers, scholars, tool builders, and librarians.

Finally, the tool-makers' perspective was represented by Dan Valen of Figshare (https://figshare.com/) and Kortney Capretta of Altmetric (https://www.altmetric.com/). Mr. Valen emphasized that Figshare is building tools that align with funders' requirements to support publishers, researchers, and institutions storing and sharing research outputs. Ms. Capretta introduced the approaches that Altmetric is using to measure and to track the impact of research.

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Linking Big Data with Chemistry: Databases Connecting Genomics, Biological Pathways and Targets to Chemistry

This symposium was concerned with linking disparate sources of database information, primarily linking chemical molecule (drug or toxin) bioactivity and structural information with biological pathway (disease) information and genomic information. There is an increasing amount of genomic information and with growing interest in "personal medicine," there is significant emphasis on correlating genomic information, disease-causing mutations and biological pathway information, with protein targets and drug development. In the past few years there has been significant growth in the number of databases connecting and correlating this type of information, including pathway and network-based processes, prediction of toxicity and bioassay information, and target linkage to disease. This symposium addressed these issues with a group of researchers representing the major database developers on the cutting edge of correlating this type of information: the Cambridge Crystallographic Data Centre, NCBI's PubChem, Elsevier, EMBL-EBI-ChEMBL, IUPHAR/BPS, and others.

Ian Bruno from the Cambridge Crystallographic Data Center (CCDC) spoke regarding "Connecting 3D Chemical Data with Biological Information" and discussed the CRESTANO project – a Common REST API for Structural Annotation. This is a collaboration between the PDB (Protein Data Bank) and the CCDC to improve the small molecule information within the PDB. He also discussed the CCDC's APIs and linking crystal structures to PubChem's data, as only 8% of the structures in the Cambridge Structural Database are currently present in PubChem. The Cambridge Structural Database will also have links to ChemSpider and OpenPHACTS, which will help answer questions regarding the biological pathways with which an entry in the Cambridge Structure database is associated. There are now Biovia Pipeline Pilot components based on the Cambridge APIs.

The talk by YanLi Wang of NCBI, "PubChem BioAssay: Link Chemical Research to GenBank and Beyond," discussed the chemical structure and connectivity information available within PubChem. She discussed data types, metadata, and linking the chemistry data in PubChem to genomics, to the NIH Molecular Library Small Molecule Chemical Probes, and to the biological pathways from KEGG and MedGene. Using NCBI's tools, it is now possible to map BioAssay data to target structures. Assay targets can be aligned to structure, and it is possible to visualize the binding site and interactions between the ligand and protein structure. RNAi BioAssay records and Gene target IDs and kinase selectivity profiling assay are included. There are APIs available to link to CHEMBL ontology, genes, and IUPHAR and KEGG data. PubChem BioAssay data can also be linked to Entrez Gene to verify gene function with RNA data.

James Rinker (Wuxi Business Development) discussed "Predicting Adverse Drug Events Using Literature Based Pathway Analysis," based on work that he had done while at Elsevier. Elsevier offers Pathway Studio and Reaxys as tools to provide mechanism-based information regarding drug toxicity and targets, including factors influencing adverse events. Pathway Studio (an Elsevier product) can be used for text mining. James presented an example of text mining for JAK kinase family inhibition with a biological target and failed compounds and adverse events. Reaxys can be used to understand target families and to build a network for a target or target class in pathway studies. The literature can be scanned for possible adverse events related to the target with

these tools. James gave an example, scanning the literature for possible adverse events related to target modulation by JAK2.

Chris Southan of the International Union of Basic and Clinical Pharmacology (IUPHAR) discussed "Intersecting Different Databases to Define the Inner and Outer Limits of the Data Supported Druggable Proteome", where he discussed the curated druggable databases sources: BindingDB, ChemEMBL, DrugBank, and the IUPHAR Guide to Pharmacology. UniProt chemistry cross-references and collates these curated sources with complementary selectivity. The IUPHAR/BPS Guide to Pharmacology has curated quantitative interactions between 1300 protein targets and 6000 ligands. The NIH launched the Illuminating the Druggable Genome (IDG) program and the private-public partnership to unlock the untargeted genome, which spearheaded advances in this work.

"Applications of Drug-Target Data in Translating Genomic Variation into Drug Discovery Opportunities" was the topic of a talk by Anne Gaulton (EMBL/EBI), which discussed linking ChEMBL druggability and drug-target data with results of genome-wide association studies to facilitate drug discovery repurposing. She discussed the application of using the combined information to identify non-active site pockets within drug targets, broadening their druggability, and using drug target information for the design of new genotyping arrays around the druggable genome.

"How Can Genomic Databases Be Linked to Chemical Structural Information?" was the topic of the talk given by Rachelle Bienstock, in which she focused largely on a discussion of the Cancer Genome Atlas project and the NCI cancer genomics cloud pilot projects. Three project awards were given by NCI to develop cloud pilots: one to the Broad Institute, one to the Institute for Systems Biology (ISB), and one to Seven Bridges Genomics. The objective of these cloud projects will be to develop tools to navigate the genomic information and link the molecular basis of cancer to cancer target drug discovery and the cancer therapeutics response portal to correlate specific genomic characteristics of tumors with drug treatment outcomes.

Robin Haw (OICR, Canada) spoke about "Reactome Pathway Knowledgebase: Connecting Pathways, Networks and Disease" and presented a systems biology graphical notation, a pathway browser, and protein and chemical structures with external data linkages to ZINC and ChemEMBL. The reactome knowledgebase (http://www.reactome.org) is an open access, public domain bioinformatics resource with reaction and biological pathway information. This data set visualizes interactions of gene products and the application of bioinformatics tools to find patterns in genomic data sets. ReactomeFIVIz is a Cytoscape application which utilizes FI (functional interactions) to correlate pathway and network analysis to identify genes. An example of clustering and annotating The Cancer Genome Atlas Breast Cancer mutations was shown.

Huijun Wang of Merck discussed the "Competitive Intelligence Workbench," a tool developed and used within Merck to integrate multiple sources of data through project dashboards.

"Using Systems Biology in Computational Drug Design Workflows" was the topic of the presentation by George Nicola from Afecta Pharmaceuticals, which is a drug repurposing company. Afecta uses KNIME workflows to enumerate derivatives from patents and generates a combinatorial library of analogues and fingerprints to profile compounds and screen them within a virtual library.

In "Combining Semantic Triples across Domains to Identify New and Novel Relationships and Knowledge," Michael Clark concluded the session by presenting some of the Elsevier Pathway Studio tools to link chemical compound data with biological pathway information.

In summary, the symposium provided state-of-the-art information regarding database searching and linking of diverse chemistry activity and structure information with bioactivity, biological pathway, and genomics information and the use of workflow tools and APIs to integrate and use the data effectively.

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Reimagining Libraries as Innovation Centers: Enabling, Facilitating & Collaborating throughout the Research Life Cycle

This symposium on March 16, 2016, had an exciting variety of presentations focused on collaborative work between libraries and researchers. Some of the topics included new services in libraries, the future of libraries, scholarly communication trends, 3D printing, data visualization, researcher profiles, and chemical safety.

In the morning, Jeremy Garritano (University of Virginia; formerly University of Maryland) first presented "Expanding the Research Commons Model into Disciplinary Instances." Jeremy discussed the ongoing development of learning and research commons from one small space to multiple-location spaces enhanced by virtual portals at the University of Maryland Library. The renaming of the physical space to Research Commons eliminated silos and facilitated collaborations among a variety of disciplines. The virtual presence not only provided integrated library services but also enabled campus partnerships with the Division of Research, IT, and the Library through a virtual portal, Integrated Research Resources on Campus (IRRoC). The challenges of establishing the research commons included no consensus on key terminology, such as research versus search, steep learning curves with grant-funded research for some collaborators, and communication obstacles across units.

Jeremy Frey (University of Southampton) discussed "Libraries for the Future: A Digital Economy Perspective." Jeremy started with a comparison between the traditional view of the library and the current and future roles of librarians and libraries. Researchers turn to libraries for guidance in efficient and accurate access to information, in handling data, and in using information and data. However, libraries can no longer handle the scale required to be the sole quality control center for information. To address this issue, librarians should continue curating information, while teaching other people to curate information, as well. In addition, librarians can help establish amongst researchers a mindset of sharing research, starting from the very beginning of the research process. Libraries will continue to be the focal point of universities and provide connectivity to all.

Kiyomi Deards (University of Nebraska-Lincoln) presented "Leveraging the Interdisciplinarity of Chemistry: Building Interdisciplinary Collaborations." Kiyomi introduced the SciPop Talks! outreach program and other efforts to create collaborations with Nebraska STEM literacy programs. Ensuring speaker-audience engagement and good publicities were key to the success of the science outreach program, SciPop Talks! She also demonstrated how librarians could be involved in state-wide initiatives to facilitate STEM literacy, such as organizing a statewide survey and retreats for supporters to create an opt-in STEM directory, hosting it on a sustainable Web site of a statewide, nonprofit organization.

Ye Li (University of Michigan, U-M) presented "Predicting Local Trends in Scholarly Communication for Decision-Making in Collection Development: An Exploration Beyond Citation Analysis." Ye analyzed a large set of research articles (61,269) from U-M researchers working on chemistry-related topics as an aid to understanding the research community and developing collections. The bibliographic data were retrieved from the Michigan Expert system provided by Elsevier. The analysis revealed the top journals in which U-M chemists choose to publish, due to campus research focus and journal scales, and provided quantitative evidence of the broad distribution of chemistry-related research across campus. The network plot of publications and research themes could help identify units with which to consult for decision-making about a specific journal and to identify the best journals to recommend to local researchers working on a specific field. Ye also attempted to classify journals using time-series clustering in an attempt to predict those journals in which U-M chemists would tend to publish more in the future. The current research suggests increased publishing in PLoS ONE, as the growth of publications in this open access journal was extremely large in recent years.

Vincent Scalfani (University of Alabama) presented "Academic Technologies: A New Library Service to Offer Advanced Software Training." Vin introduced the partnership between the library and other campus divisions in offering robust software training. All science librarians share the responsibility of delivering software trainings for tools, such as MS PowerPoint, MS Excel, QtiPlot, Adobe InDesign, ChemDraw, 3D Printing, MatLab etc. Vin took opportunities to include cheminformatics skills and promotion of library resources into the training, too, including preparing scripts in MatLab to allow interaction with chemistry databases through APIs and performing text analysis with MatLab and Mathematica. The major challenges for the library in hosting the software training

were access, licensing, maintenance of software, impact measures, and time limitations.

Amy Sarjeant (Cambridge Crystallographic Data Centre) presented “Enhanced Chemical Understanding through 3D-printed Models.” Amy introduced how the partnership among CCDC, librarians, and faculty could help develop 3D-prints of molecules to facilitate research and learning. Amy showcased several 3D prints of mechanically-interlocked molecules, molecules with rotatable bonds, and molecules with flexible bonds, all of which could be helpful with real 3D models. Amy also discussed the challenges in converting the 3D models exported from the Cambridge Structural Database System into an appropriate format for a local 3D printer and how librarians could help in the process, aside from providing easy access to 3D printers.

In the afternoon, Danielle Bodrero Hoggan (The Scripps Research Institute) presented “Leveraging the VIVO Research Networking System to Facilitate Collaboration and Data Visualization.” VIVO is a Web platform research networking system initially developed at Cornell University that supports searching, browsing, and advanced visualizations. Danielle and her colleague, Michaeleen Trimarchi, used the VIVO networking system to create profiles for Scripps faculty members. Several interactive graphics were created, including a co-author network and a network of scientific discipline areas. The Science of Science (Sci2) Tool was used to plot the VIVO data into networked visualizations that showed faculty-department collaborative connections.

Grace Baysinger (Stanford University) presented on “Stanford Profiles Created to Support the University’s Scholarly Community.” Stanford Profiles is a Web platform that allows faculty, students, staff, and post-docs to create personal profiles highlighting their research, teaching, and publications. The system auto-populates names, appointments, courses, advisor names, and publication citations. Users are able to search Stanford Profiles via name and keyword queries for research area, thus making communication and collaboration easier. Stanford Profiles also enables users to easily generate a CV, and Stanford University developers to access the data via an API.

Linda Galloway (formerly of Syracuse University; now at Chapman University) presented on “Managing Researchers’ Reputations throughout the Research Life Cycle.” Linda discussed the changing landscape of scholarly communications and how discovery of literature is changing (e.g., discovery via social media). Social networks such as Academia, LinkedIn, Mendeley, and ORCID are becoming very popular with researchers, as they allow control over shared materials and help to promote scholarship, but Linda discussed some drawbacks to social media platforms: users must monitor them frequently, be aware of copyright policies, and understand their metrics. Finally, best practices for managing social media profiles and accounts were highlighted.

Leah McEwen (Cornell University) presented on “Anatomy of the Chemistry Research Enterprise in the Academic Sector: Serving the Underserved in a Large Research Institution.” Leah talked about creating a digital data culture. Interestingly, much of the chemistry data is still typed manually and organized by researchers (e.g., NMR shifts, mass spectral data). Workflows and systems should make this process easier and more efficient for researchers. How can service groups (e.g. instrument labs, health and safety, and libraries) support researchers with digital management of data? Different levels of chemistry data management were discussed, including highly-curated post-publication data, at-publication data, and pre-publication laboratory data. Lastly, several case studies were discussed highlighting potential methods of supporting chemistry data management. The future will likely need to focus on methods that improve accuracy of data collection, verification of data, streamlined report generation, and increased communication.

Ralph Stuart (Keene State College) presented “The Safety Use Case for Chemical Safety Information.” Limitations in finding chemical information were discussed, including the use of generic safety information in textbooks followed by the notation, “see MSDS,” outdated links on Wikipedia, and no clear description of the rationale for choosing a particular source. Ralph discussed a project on which he is working, comparing the safety

information in Wikipedia to PubChem using the following methodology: locating chemicals in the PubChem Laboratory Chemical Safety Summary (LCSS), converting the PubChem CIDs into InChI keys, and using these InChI keys to compare the LCSS to Wikipedia data. Future directions include studying the Wikipedia chembox structure, developing a Wikipedia-PubChem link for safety information, and evaluating which chemical safety data should be included within the Wikipedia chemboxes.

Yanli Wang (NCBI, NLM, NIH) presented "PubChem BioAssay: Grow with the Community." Yanli discussed the current PubChem BioAssay tools and how PubChem has grown in depositions since 2005. Usage of the PubChem database and citations to PubChem also continue to grow. Next, Yanli discussed the benefits of data sharing, such as increased discoverability, value-added integration, data management, and building collaborations. Finally, the PubChem data submission tool was discussed, as well as the increasing number of journal publishers requiring deposition of data into PubChem.

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Future Thematic Programming at ACS National Meetings

252nd, August 21-25, 2016, Philadelphia, PA: Chemistry of the People, by the People and for the People
Rudy Baum, r_baum@acs.org

253rd, April 2-6, 2017, San Francisco, CA: Advanced Materials, Technologies, Systems and Processes
Kathryn Beers, kathryn.beers@nist.gov

254th, August 20-24, 2017, Washington, DC: Chemistry's Impact on the Global Economy
Nancy Jackson, nbjacks@sandia.gov

255th, March 2018, New Orleans, LA: The Food, Energy, Water Nexus

256th, August 2018, San Diego, CA: Nanotechnology

257th, March 31-Apr. 4 2019 Orlando, FL: Chemistry for New Frontiers

258th August 25-29, 2019, San Diego, CA: Chemistry of Water

259th, March 2020, San Francisco, CA: TBD

260th, August 2020, Philadelphia, PA: Chemistry from Bench to Market

Committee Reports

Report from the Council Meeting Held on March 16, 2016

The Council of the American Chemical Society met in San Diego, CA, on Wednesday, March 16, 2016, from 8:00am until approximately 11:30am in the Sapphire Ballroom of the Hilton San Diego Bayfront Hotel. The Council opened with the passing of resolutions in memory of deceased Councilors. Below is a summary of the meeting that followed.

Nominations and Elections

President-Elect: The Committee on Nominations & Elections (N&E) identified four nominees for the office of 2017 ACS President-Elect. They were as follows: Peter K. Dorhout, Thomas R. Gilbert, C. Bradley Moore, and Gregory H. Robinson. The four nominees answered questions at the Town Hall meeting held on Sunday, March 13, and made brief presentations to the Council. Council voted to select Peter K. Dorhout and Thomas R. Gilbert as the final two candidates whose names will appear on the fall ballot, along with any petition candidates who may arise.

Other Elections

The Committee on Nominations and Elections announced the results of the election held prior to the San Diego meeting to select candidates from the list of nominees to serve as Directors from District II and District IV on the Board of Directors for the term 2017-2019. By Internet ballot, the Councilors from these districts selected George M. Bodner and Christina C. Bodurow as District II candidates; and Rigoberto Hernandez and Larry K. Krannich as District IV candidates. Ballots will be distributed on September 29, 2016, to all ACS members in District II and District IV for election of a Director from each District.

N&E also announced the election of Directors-at-Large that will be conducted in the fall. The candidates for a 2017-2019 term are Joseph A. Heppert, Kristin M. Omberg, Dorothy J. Phillips, and Kathleen M. Schulz. Ballots for the election of two Directors-at-Large from among those candidates and any selected via petition will be distributed to the Council on September 29, 2016.

N&E has established the Vote 20/20 Task Force, charged with examining all aspects of nominations and elections for ACS national offices and designing an enhanced process to be in place by the year 2020. The committee welcomes ideas from all members as to how nominations and elections should be handled. Send comments to vote2020@acs.org

ACS Dues for 2017

Council voted to accept the recommendation from the Committee on Budget and Finance with regard to the 2017 membership dues (an increase of $4.00 - from $162 to $166).

Petitions for Vote

Approval of the "Academic Professional Guidelines"

The Committee on Economic and Professional Affairs (CEPA) presented the revised "Academic Professional Guidelines" for consideration at the Council meeting in Boston on August 13, 2015. After approving an amendment to the proposed revised *Academic Professional Guidelines* (Council Agenda, pp. 75-89), the Council approved the revised guidelines, subject to approval by the Board of Directors. The guidelines apply to those members of the academic community whose job function impacts directly or indirectly on scientists practicing the profession of chemistry.

Budget and Finance

In 2015, ACS generated a Net from Operations of $16.6 million, which was $3.2 million favorable to budget. Total revenues were $511.7 million, essentially on budget. Expenses ended the year at $495.1 million, which was $3.1 million or 0.6% favorable to budget. This variance was attributable to a continued emphasis on expense management across the Society. The Society's financial position strengthened in 2015, with Unrestricted

Net Assets, or reserves, increasing from $144.7 million at December 31, 2014 to $163.3 million at year-end 2015, although this amount is still below the recommended financial guidelines.

Additional information can be found at www.acs.org, at bottom, click 'About ACS', then 'ACS Financial Information'. There you will find several years of the Society's audited financial statements and IRS 990 filings.

Meetings and Expositions

The Committee on Meetings and Expositions (M&E) reported that the 2017 registration fee for ACS national meetings will be $440 ($415 will be the early bird rate). The attendance at the San Diego national meeting, as of the morning of the Council meeting, was as follows:

Students:	5,979
Exhibitors:	1,094
Exhibition only:	473
Guests:	383
Regular:	8,398
Total:	**16,327**

Spring National 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:	18,067
2011: Anaheim, CA:	14,047
2012: San Diego, CA:	16,864 (as of Tuesday evening, March 27, 2012)
2013: New Orleans, LA:	15,596 (as of Tuesday evening, April 9, 2013)
2014: Dallas, TX:	13,680 (as of Tuesday evening, March 18, 2014)
2015: Denver, CO:	13,930 (as of Tuesday evening, March 24, 2015)
2016: San Diego, CA:	16,327 (as of Tuesday evening, March 16, 2016)

The last National ACS meeting in San Diego was held in the spring of 2012 and attendance at that meeting totaled 16,864 for the same time period noted. San Francisco has had the highest attendance for ACS National Meetings, at least since 1997 (1997: 18,042; 2010: 18,067; and 2000: 18,336).

Membership Affairs Committee

The Committee on Membership Affairs (MAC) reported that ACS membership declined 1% in 2015 to slightly under 157,000, despite the fact that 25,000 new members were added. The overall membership retention rate is 84% and there has been a 3.85% growth in foreign new membership.

Committee on Economic and Professional Affairs

The Committee on Economic and Professional Affairs (CEPA) reported that the unemployment rate for newly-graduated chemists has increased from 12.4% to 13%. The overall unemployment rate for all ACS chemists is up from 2.9% to 3.91%. The overall U.S. unemployment rate is 5.5%.

Divisional Activities Committee

The Committee on Divisional Activities (DAC) reported that it will be providing more training for division chairs on member recruitment and retention. It will also be actively encouraging all divisions to develop business plans.

Committee on Constitution and Bylaws

The Committee on Constitution & Bylaws (C&B) certified twenty-nine unit bylaws in 2015. With regard to the Petition to Extend the Unemployment Members' Dues from two to three years, C&B is concerned with the assumption in the explanation that, without the waiver extension, the Society would lose those members who would benefit from the waiver extension. The financial implications of this petition are still being assessed.

Petitions to Amend Constitution & Bylaws

New petitions to amend the Constitution or Bylaws must be received by the Executive Director no later than May 4 to be included in the Council agenda for consideration at the fall 2016 meeting in Philadelphia. Contact C&B with any questions or requests for information at bylaws@acs.org

Actions of the Board of Directors

The Board's Executive Session

The ACS Board of Directors met March 11 - 12, 2016, and considered a number of key strategic issues and responded with several actions. These are as follows:

Board Development

ACS is a large, highly complex, global organization, with two major businesses – Chemical Abstracts Service and ACS Publications – and a significant professional membership organization component. The Board sets aside substantial discussion time at each meeting for the most important strategic issues facing the Society.

Strategic Issues and Retreat

The Board held a conversation focused on strengthening the process utilized for strategic issues discussions, and a discussion on timing and topics of a possible facilitated retreat for all Board members during 2016. Also, the Board is committed to development and discussed ways to continuously improve its effectiveness in the service of ACS as individual board members, and as a collective body.

The Board's Committees

The Board received input and discussed reports from its Committees on Grants and Awards, Executive Compensation; and the Joint Board-Council Committee on Publications. On the recommendation of the Committee on Grants and Awards, the Board voted to approve an endowment to support the E. Bright Wilson Award in Spectroscopy.

Also on the recommendation of the Committee on Grants and Awards, the Board voted to approve language to be included in the guiding documents for the National Awards and Fellows Program to allow for the rescission of national awards and the ACS Fellows designations where reasonable grounds exist.

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.

On the recommendation of the Joint Board-Council Committee on Publications, the Board voted to approve the reappointments of Editors-in-Chief for two ACS journals.

The Executive Director/CEO Report

Executive Director and CEO Thomas M. Connelly, Jr. discussed ACS membership programs, reviewed the information technology area, and offered personal reflections on his first year as Executive Director and CEO. His direct reports updated the Board on the activities of Chemical Abstracts Service (CAS), the ACS Publications Division, the Office of the Treasurer and CFO, and the Society's Secretary and General Counsel.

Presidential Succession

The members of the presidential succession briefed the Board on their current and planned activities for 2016. President Donna Nelson highlighted presidential programming at the San Diego meeting on employment and

diversity in the chemical sciences and on organic chemistry education. Also, a special discussion topic on the U.S. employment of chemists will be conducted at the Council meeting.

The Board's Open Session

The Board held a well-attended open session which featured Amy Harmon, a reporter for the New York Times, who covers the social implications of science and technology. Ms. Harmon's topic was "Telling Science Stories: Dispatch from the Conflict Zone."

Prior to the presentation, members of the presidential succession and the Executive Director and CEO offered brief reports on their activities. The officers provided more extensive reports on their activities and/or future plans as part of their written and oral reports to the Council.

Contact the Board

Your Board of Directors is elected by and acts in the best interests of the members of our Society. Please contact them with your comments, concerns, ideas, and suggestions at secretary@acs.org.

Additional Information

The following is a list of URLs or email addresses presented in reports or on slides at the Council meeting

Donna Nelson, President	djnelson@ou.edu
Allison Campbell, President-Elect	a.campbell@acs.org
Diane Grob Schmidt, Immediate Past President	d.schmidt@acs.org
Budget and Finance	www.acs.org → About ACS → ACS Financial Information
Career Navigator	www.acs.org/careernavigator
Chemists with Disabilities	www.acs.org/cwd
Committee on Education	chemidp.org
Committee Preference Forms	https://www.yellowbook.acs.org
ConC Subcommittee on Diversity	www.acs.org/conc → Committee Information
Constitution and Bylaws	bylaws@acs.org / www.acs.org/bulletin5
Highlights of ACS Achievements	www.acs.org/acshighlights2015
Local Section Activities	www.acs.org/getinvolved
Nominations and Elections	nomelect@acs.org / Vote2020@acs.org
Office of Secretary & General Counsel	secretary@acs.org

Respectfully submitted March 28, 2016

CINF Councilors

Bonnie Lawlor
Andrea Twiss-Brooks
Svetlana Korolev

Note: The Council Agenda Book can be accessed at: http://www.acs.org/content/dam/acsorg/about/governance/councilors/council-agenda-3.16.pdf.

CINF Education Committee

The following are the minutes of the ACS CINF Education Committee Meeting, which occurred on March 12, 2016, at the San Diego Convention Center. Grace Baysinger (chair), Jeremy Garritano, Chuck Huber, Ye Li, Marion Peters, and Teri Vogel were in attendance.

Report on the Meeting and Activities of the Society Committee on Education (SOCED) – *Jeremy Garritano*

- SOCED is planning to work on a graduate education Website, giving guidance on topics such as looking for and selecting graduate schools.
- By the end of the year, they plan a big survey about online instruction (e.g. MOOCs and virtual labs). It is assumed that this will be distributed to department chairs.
- They have been asked to look into recognizing chemistry programs in other countries (e.g. RSC programs)
- A representative from the Committee on Chemical Safety spoke. CCS has plans for a ChemLuminary award for promoting chemical safety. The two-volume *Safety in Academic Chemical Laboratories* will be updated this year (last updated in 2003). CCS also plans to issue safety guidelines for demonstrations.
- There was a soft launch of ChemIDP.org. One hundred people have already created independent development plans. ChemIDP.org is free to use but requires an ACS login. The "Explore Careers" module is the most popular; it is mostly geared towards graduate students, but undergraduates are also showing interest. The hope is to get more funding to further develop this.
- The National Research Council just released "Effective Chemistry Communication in Informal Environments." It includes a framework and guide.
- There was discussion about a practitioner's statement regarding the importance of laboratory activity, but the committee opted not to develop one at this time. They are more interested in crafting something about effective learning and teaching techniques, perhaps one or more articles that can be written up in the *Journal of Chemical Education* (JCE).
- SOCED is also looking at guidelines and performance expectations for general chemistry, a multi-year project. They want to make it cross-disciplinary, describing expectations of both chemistry majors and non-chemistry science and engineering majors.

XCITR Repository

- XCITR is currently offline, due to security concerns from the Royal Society of Chemistry (RSC). RSC hosted it for a few years until their Drupal upgrade. The account creation site was heavily spammed, resulting in a moratorium on new accounts. Current account holders have added little content.
- The site will be up long enough for Stanford University to archive it, and they will offer public access. Internet Archive has also archived some of it.
- Ideas
  - ⇒ Set up a Google custom search. Grace Baysinger has seen this done for government documents.
  - ⇒ LibGuides links could be added to the Chemical Information Sources Wikibook (ChemWiki Book), and we could link to documents if the archive copy is available via URL.
- Questions
  - ⇒ What is the utility of the content currently in XCITR? (Out of date? Non-English language materials?)
  - ⇒ How many people were searching and using the content, and who are they?
  - ⇒ Are there communities (creators, depositors, and readers) to support the work?
  - ⇒ The group decided that the ChemWiki Book should be the bigger priority, and they can add selected links from LibGuides, as well as archived, deposited documents.

Chemical Information Sources Wikibook (ChemWiki Book)

- The committee will hold further discussions about the Wikibook at a virtual meeting later this spring.
- The WikiBook is being read, and the Committee on Professional Training (CPT) points to it.

- The committee needs to review current chapters and determine whether additional ones are needed, reach out to past authors, and seek new editors.
- The community needs "support" from the Education Committee to continue contributing. In particular, the committee should try to devise a way to give credit to editors (or authors). This includes reviewing the content and the level of accountability.
- Recommendations:
  - ⇒ Request that the Executive Committee adopt the Wikibook as a formal "publication of CINF."
  - ⇒ Identify rights, responsibilities, and roles for the editor-in-chief, editors, and authors.
  - ⇒ Work with Martin Walker to add more functionality to the interface, which will also help contributors.
  - ⇒ Develop a roadmap/to-do list.
- *Action Items*
  - ⇒ *The entire Education Committee will review the organization, structure, and chapters of the Wikibook and send comments to Chuck.*
  - ⇒ *By May 2, committee members should send Grace items that should go into the road map. This will be followed by a conference call later that week.*
  - ⇒ *Ye will serve as interim technical editor so as to gain this level of expertise; eventually, a permanent technical editor will be appointed.*
  - ⇒ *Submit a piece for the Fall CIB to Teri Vogel by mid-to-late July.*

CINF Education Page

- The page is completely out of date and needs an overhaul. Grace Baysinger has already revised the Chemical Information Literacy page in response to articles in the *JCE* special issue linking to the page.
- The meeting minutes have been moved into the ACS network.
- A question arose about whether someone on the committee can get access to edit the Web pages, or whether all changes must go through the Webmaster.
- *Action Item*
  - ⇒ *Grace Baysinger will send out a charge for the committee to review and submit comments, as well as a draft of the updated page for comment.*

Graduate Student Information Literacy Guidelines

- The committee aims to complete this project by the fall meeting, focusing on learning objectives, not lists of links and resources.
- The GradIDP mentions data/database management, but nothing else about database searching or other information literacy skills.
- Grace brought up the issue of SciFinder certification with the new chair of the Joint Board-Council Committee on Chemical Abstracts Service. Ye Li mentioned digital badges.

ACS Style Guide

- The committee is interested in having the References chapter updated so that the guidelines for citing online resources align more closely with the ways in which these sources are actually cited in articles.
- Committee members were reminded that access to the *ACS Style Guide* is free with an ACS ChemWorx account.
- *Action Item*
  - ⇒ *Marion Peters will check in with Michael Qiu, and perhaps this can be added to the agenda for the next Academic Roundtable Meeting.*

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CINF Careers Committee

The CINF Careers Committee has the goal of promoting careers in chemical information and providing practitioners with information that will be beneficial to building their careers. They have sponsored symposia at national meetings and are in the process of developing useful, Web-based materials for new and seasoned chemical information professionals. The Careers Committee is always looking for interested individuals to join the team; geography is immaterial, and travel is not required; the committee meets virtually several times per year, with current members located across the United States. The following is a brief report of recent committee activities.

Preparing for ACS National Meetings

If you are new to the division or you know someone who is, please see our handout about "Preparing for the CINF Division of the ACS National Conference"

http://acscinf.org/PDF/Preparing_for_CINF_at_ACS.pdf

Career Resources

The committee is also in the process of reviewing and updating our "Resources in Careers in Chemical Information".

http://www.acscinf.org/content/resources-careers-chemical-information#overlay-context=content/careers

We would welcome suggestions of recently published books and articles about careers in chemical information.

Upcoming Events

We are planning our next Careers program for the ACS meeting in San Francisco (April 2-6, 2017)

Information about the Careers Committee can be found at http://www.acscinf.org/content/careers.

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Calling All Committee Members!

Do you belong to a CINF committee, an ACS national committee, or a committee of another ACS division that discusses issues related to chemical information or cheminformatics? Consider submitting a brief summary of your committee's activities to the *Chemical Information Bulletin*, to be placed in the Committee Reports section. Submissions may be of any length and should be sent directly to the editor of the issue in which you wish them to appear; a list of editors appears in the **CINF Officers** section of this issue of the *CIB*. This is a great way to disseminate the news of your committee's activities to the broader chemical information community!

ACS Committee on Ethics (ETHX)

The governance of the American Chemical Society is complex, as befits a large member institution, but nowhere is its complexity better exemplified than through its committee structure. There are five different types of committees, and the following is a brief description of their purpose and composition; for more information, please refer to the governing documents of the Society (http://www.acs.org/content/dam/acsorg/about/governance/charter/bulletin-5.pdf?_ga=1.211259733.1512377879.1423839481).

- **Council Committees** (*Council Policy Committee, Committee on Nominations and Elections, Committee on Committees*): elected committees of the Council, with members elected by and from the body of Councilors;
- **Standing Committees of the Council** (*Committee on Membership Affairs, Committee on Meetings and Expositions, Committee on Divisional Activities, Committee on Local Section Activities, Committee on Economic and Professional Affairs, Committee on Constitution and Bylaws*): other Council committees, whose members are councilors appointed by the President of the Society, with input from the Committee on Committees;
- **Society Committees** (*Society Committee on Education, Society Committee on Budget and Finance*): special committees whose members are councilors and non-councilors appointed by the president of the Society, with input from the Committee on Committees;
- **Joint Board-Council Committees** (*examples include the Joint Board-Council Committee on Publications, the Joint Board-Council Committee on Chemical Abstracts, Service, and the Committee on Professional Training*): committees developed to serve a specific purpose, whose members may be any member of the Society and are jointly appointed by the president of the Society and the chair of the Board, with input from the Committee on Committees;
- **Other Committees of the Council**: These committees are also established to serve a particular purpose and are evaluated by the Committee on Committees. Their members, who may be any member of the Society, are appointed solely by the president of the Society, with input from the Committee on Committees.

The Committee on Ethics (ETHX) is an "Other Committee of the Council." Its charge is as follows:

> *To coordinate the ethics-related activities of the Society, serve as an educational resource and clearinghouse, but not as an adjudication body, for ACS members seeking guidance on ethics issues; raise awareness of ethics issues through meeting programming and columns/editorials; review recognition opportunities for acknowledging ethical behavior; and to develop and oversee 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.*
>
> http://www.acs.org/content/acs/en/about/governance/committees/ethics/about.html

CINF enjoys dual representation on this committee; Leah McEwen is a full member, and Judith Currano is a new associate member. Much of the work of the committee is done in its subcommittees, and ETHX has three subcommittees, devoted to Communication and Awareness, Education and Materials, and Programming and Screening.

ETHX is particularly interested in cosponsoring programming at ACS National Meetings focused on ethical issues; as a result, it will be cosponsoring a symposium on the ethics of authorship and inventorship with CINF at the San Francisco meeting in the spring of 2017. While some of the talks will be invited, we will also post a general call for papers, so, please keep an eye open for it!

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ACS Joint Board-Council Committee on Chemical Abstracts Service (CCAS)

The Joint Board-Council Committee on Chemical Abstracts Service (also known as CCAS) met twice in 2015 and met again at the Spring National Meeting in San Diego. The Committee consists of members from academia, industry, and government, and continues to fulfill its charter by serving as a channel for the flow of information between CAS management, ACS members, and users of CAS products and services. At each CCAS meeting, committee members held open dialogue on a range of topics, including synthetic chemistry dissertations, junior college solution options, and the SciFinder Future Leaders in Chemistry program and provided input on new products and services.

At both 2015 meetings, CAS management provided the committee with an overview of financial performance as well as product and service news. At the fall meeting in Boston, committee members learned that CAS continues furthering its leadership position in the scientific community, exemplified by the registration of the 100 millionth chemical substance in CAS REGISTRY, in the 50th anniversary year of the world's largest database of unique chemical substances. CAS is also becoming a robust solutions provider with exciting new products. Members were pleased to learn about MethodsNow, a new workflow solution for analytical, pharmaceutical, and biotech scientists that will provide access to the largest collection ever of analytical procedures, indexed and organized by CAS, and will save researchers time in the lab, as well as provide advancements for researchers in commercial, government, and academic organizations. This highly-innovative benchtop solution features the world's largest collection of templated protocols in analytical chemistry and reaction science. MethodsNow will be offered as a "stand-alone" product, and selected capabilities will be offered as an add-on within the SciFinder experience.

CAS successfully launched three new products and services in 2015 including PatentPak, NCI Global, and CHEMCATS. These new offerings expanded CAS's product portfolio with an innovative workflow improvement for scientists, a solution for regulatory professionals, and a new business model for chemical suppliers whose products are promoted to hundreds of thousands of scientists around the world via SciFinder. In 2016, CAS introduced PatentPak in STN for intellectual property professionals.

CAS databases continue to grow at record pace: a new record of more than 13.5 million new substances were added to the CAS REGISTRY in 2015, which now includes more than 105 million small molecules. This exceeds the prior record set in 2014, when 13.1 million new CAS RNs were assigned. As in recent years, growth in 2015 was driven by prophetic substances identified in patents, chemical supplier offerings in CHEMCATS, and organic growth for indexing of the literature.

The CCAS Committee met in Executive Session on March 11, 2016, where CAS management reported on highlights from 2015, including financial and strategic updates. CAS President, Manuel Guzman, reported that CAS' sustained solutions performance continues to support ACS initiatives. The new products released in 2015 are being well-received by customers around the world as CAS continues to expand its global reach through support for the scientific enterprise, adding dedicated resources in the following seven countries: Japan, South Korea, Brazil, Mexico, Taiwan, Singapore, and Australia. Expansion efforts now total thirty new team members in eleven countries, bringing direct representation to nearly twenty countries.

I am pleased to report that the Committee on Chemical Abstracts Service continues to fulfill its responsibilities in a purposeful manner. Committee members provide important feedback, suggestions and questions regarding CAS solutions. We welcome input from ACS members and all CAS users through the ACS Member Network. I encourage you to stop by the CAS booth at the Convention Center to learn more about the numerous exciting initiatives underway at CAS.

Wendy Cornell
Chair, Joint Board-Council Committee
on Chemical Abstracts Service

Book Reviews

Better late than never? For this issue of the *CIB* I review two books on bibliometrics, deferred from appearing in the wnter issue of the *CIB*. I discovered these books when researching my article on citations and bibliometrics in the March issue of *J. Chem. Educ.* (http://pubs.acs.org/doi/abs/10.1021/acs.jchemed.5b00451), a special issue devoted to chemical information. Both are highly recommended for those interested in further study of the entire field of bibliometrics or of constituent portions.

Beyond Bibliometrics: Harnessing Multidimensional Indicators of Scholarly Impact, B. Cronin, C. R. Sugimoto, Eds., MIT Press, Cambridge, MA, London, Eng., 2014, 468 p. +viii, ISBN 978-0-262-02679-6 softcover $37.

This multi-authored monograph is an excellent review and resource covering the rapid growth of the study of bibliometrics. Subject matter for this field has expanded from books in medieval times to journals and journal articles, references, citations, authors and institutions, patents, personnel management (performance reviews, hiring, firing, and promotion), and into the universe of the Internet including "gray literature", less formal publications, social media, etc. Thirty authors have written twenty-one chapters grouped into categories including history, critiques, methods and tools, alternative metrics (altmetrics), and perspectives. All aspects of the field have been and continue to be controversial, and these controversies are well covered.

"Beyond bibliometrics" refers to discussion of even younger "descendants" of bibliometrics, viz. webometrics and scientometrics. The rapid growth of all of these fields has been facilitated by the parallel growth in the Web, social media, and the associated venues. However, increased quantity is not always better than the arguably-associated quality. Since "metrics" means quantitative measurement, one must be sure that one is measuring the correct phenomena or making appropriate applications.

The first two chapters cover the history of scientific communication and bibliometrics. The second section covers, in four chapters, critiques, including ethics and criteria. Section three (seven chapters), covers methods and tools including finding, evaluation, and recommending articles. Alternative metrics, covered in the six chapters of section four, discusses altmetrics, Web impact, and readership. The final section (two chapters) covers perspectives of the publishing industry and determination of science policy. Every chapter concludes with references and the book concludes with a list of authors and brief biographies and an index for the entire volume.

Scholarly Metrics Under the Microscope: From Citation Analysis to Academic Auditing, B. Cronin, C. R. Sugimoto, Eds., ASIS&T/Information Today, Medford, NJ, 2015, p. 963 + xii, ISBN 987-1-57387-499-1 hardcover $149.50.

In preparing their previous book (reviewed above), the editors discovered a large gap in the literature covering many of the topics on bibliometrics. Bibliometrics has been critiqued, due to the fact that many have used it to "pick winners" in any number of subjects, a misuse forecast by Garfield in early years. This volume cannot be a "one-stop resource," but the editors attempt to assemble in one volume much of the literature that critiques bibliometrics and highlights the limitations in its use. The result is this tome, consisting of 55 reprinted articles, divided into six sections. Part 1 covers Concepts and Theories, Part 2, Validity Issues; Part 3, Data Sources; Part 4, Indicators; Part 5, Science Policy; and Part 6, Systemic Effects. In addition to the introduction to the entire volume (which also includes Eugene Garfield's original 1955 article), the editors have written introductions to each section, as well as an overall epilogue. If they were not already in digital form, the 55 articles were digitized by OCR, edited in Word, and had all references converted to endnotes.

Is a collection of reprints worth $150? That is for each interested individual to decide, but the additional commentaries may make it so. Of course, finding and accumulating all of the included articles is a daunting and expensive task for any individual. An alternative to purchasing the book is using a library copy, but this collection, like the original references, will not always be available. The nearby Fogler Library, at the University of Maine, does not have a copy, nor does any other library in Maine. Fortunately, I was able to obtain a review copy, and I suggest that interested individuals request that their library obtain a copy.

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Announcement from the ACS Committee on Professional Training (CPT)

"**Future of the ACS Directory of Graduate Research (*DGRweb*)**
The ACS Directory of Graduate Research (*DGRweb*) will no longer be published. The 2015 DGRweb and its archive will remain on the Web site (www.acs.org/dgrweb) through the end of 2016 for free online searches. Thank you for supporting ACS Directory of Graduate Research (*DGRweb*) over the last 63 years. "

Source (in News and Announcements): http://www.acs.org/content/acs/en/about/governance/committees/training.html (accessed May 27, 2016).

Sponsor Announcements

Division of Chemical Information Sponsors, Spring 2016

The American Chemical Society Division of Chemical Information is very fortunate to receive generous financial support from our sponsors to maintain the high quality of the Division's programming and to promote communication between members at social functions at the ACS Spring 2016 National Meeting in San Diego, CA, and to support other divisional activities during the year, including scholarships to graduate students in chemical information.

The Division gratefully acknowledges contribution from the following sponsors:

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Please feel free to contact me if you would like more information about supporting CINF.

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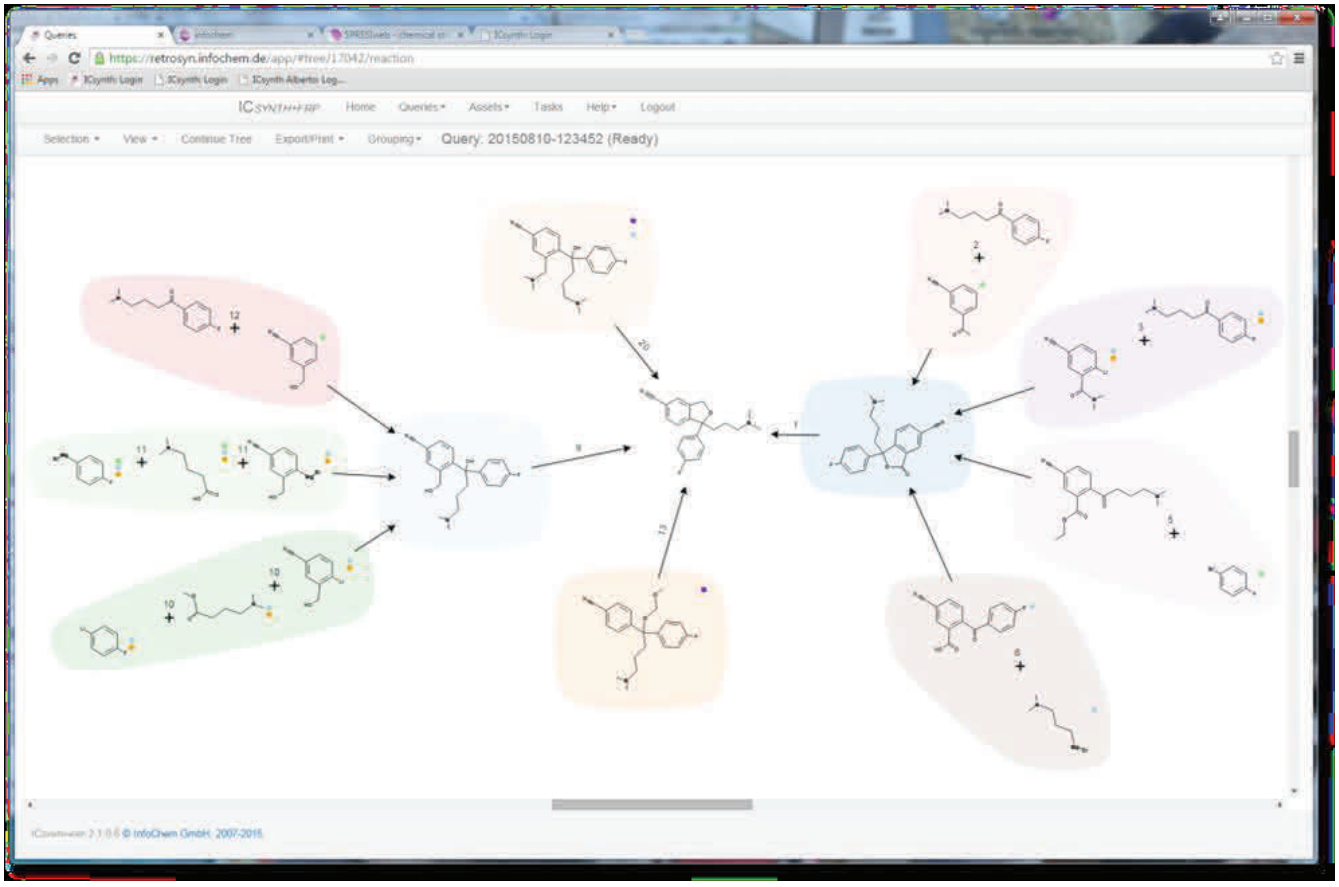
The ACS CINF Division is a non-profit tax-exempt organization with taxpayer ID no. 52-6054220.

IC*SYNTH* Version 2.2 Launched

InfoChem is proud to announce the release of IC*SYNTH* version 2.2 in in Q1 2016.

IC*SYNTH* is a powerful synthesis-planning tool able to define synthesis strategies based only on fully algorithmic chemical knowledge and not on synthesis path analysis. The system builds multistep, interactive synthesis trees, taking advantage of automatically-created transform libraries. The user is able to interact with the software, selecting different synthesis strategies and defining the number of precursors and steps.

IC*SYNTH* Version 2.2 now offers a reaction layout view, in addition to the known tree view. This new layout shows the target molecule in the middle of the screen, with all selected precursor reactions visible around it. In addition, all the visible chemical structures are highly interactive, enabling easy browsing of the retrosynthetic analysis results. Furthermore the algorithm responsible for the precursor search has been successfully improved, resulting in better pathway suggestions.



For more information about IC*SYNTH*, please visit our homepage (http://infochem.de/products/software/icsynth.shtml) or contact us (info@infochem.de).

Springer Nature to extend content sharing!

Springer Nature will now provide authors with shareable links to view-only versions of their peer-reviewed research papers, starting with authors of *Nature* and the Nature research journals, such as *Nature Chemistry*. This initiative will also be extended to authors of all other Springer Nature-owned primary research journals, and ultimately to all authors of Springer Nature published primary research journals. These links can be posted anywhere, including via social channels and on other highly-used sites, institutional repositories, and authors' own Web sites, as well as scholarly collaborative networks, which many researchers are using to collaborate and to share both publicly and privately.

This comes after a year-long nature.com content sharing trial to enable its research articles to be freely-shared with all researchers and the wider public via its authors, subscribers, and global media partners. The successful trial, covering around 50 journals and 6,000 articles, resulted in over 1.3m additional article accesses. The results of this trial were released in December 2015.

You can follow this story on Twitter, using the hash code #scishare.

SpringerOpen Blog: Insights into our open access publications in chemistry!

SpringerOpen is Springer's portfolio of fully open access journals and books. As content in SpringerOpen covers research from all areas of science, we aim to highlight each of these areas on the SpringerOpen blog. In this newsletter we wanted to share with you some of our recent highlights in chemistry available at http://blogs.springeropen.com/springeropen/category/chemistry/.

We have an incredibly diverse set of fully open access chemistry journals in the SpringerOpen portfolio that demonstrate the interdisciplinary nature of chemistry and how it can be applied to many different and sometimes surprising areas.

We have some fantastic examples of this on the SpringerOpen blog including our blog on what effect different methods of recording data have on recalling chemistry experiments and our recent post on the use of imaging spectroscopy to analyze works of art.

Take a look, and sign up for to receive the latest SpringerOpen chemistry posts straight to your inbox.

Charlotte Hollingworth, Editor SpringerOpen
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Wiley ChemPlanner Awarded Best of Show at Bio-IT World Conference & Expo

Hoboken, NEW JERSEY – May 27, 2016 – Wiley ChemPlanner was awarded “Best of Show” for the Research & Clinical Data Management category at the Bio-IT World Conference & Expo 2016. Judged by leading industry experts and Bio-IT World editors, this award distinguishes Wiley ChemPlanner as an exceptional innovation in technologies used by life science professionals today.

Wiley ChemPlanner is a state-of-the-art workflow product that helps chemists find the best selection of diverse and viable routes for their synthesis. Its unique combination of predictive reactions and curated information delivers the best of both worlds, computer-aided synthetic design backed by millions of empirical reactions. Wiley ChemPlanner has the potential to help pharmaceutical chemists improve efficiency and creativity while synthesizing molecules. “We are thrilled to receive this recognition for ChemPlanner. Our team has worked very hard to turn the dream of computer-aided synthesis design into a reality,” said Dave Flanagan, Director of Lab Solutions at Wiley. “To be recognized by the Bio-IT World judges as Best of Show 2016 is powerful confirmation of the feedback we have gotten from our customers, that computers can predict viable synthesis routes to target molecules, enhancing the creativity and productivity of users.”

Wiley ChemPlanner was launched in September 2015 and is currently sold as a Software as a Service (SaaS) solution and hosted on secure servers, with a local installation version coming this year.

About Wiley

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