

# CHEMICAL Information

## BULLETIN



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# Chemical Information Bulletin

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Spring 2016 — Vol. 69, No. 2

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Chemical Information Bulletin

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# Message from the Chair

Hello CINF!

I write this during one of the busiest times of year: school years are winding down, grants are coming due, Q2 is ending in industry, and conferences are running full tilt. We are all so incredibly busy! In the midst of all this, let me point out a few items of possible interest.



- At the ACS National Meeting in San Francisco, we faced all of the anticipated issues associated with having our technical sessions located in a remote hotel. This is a challenge for any division not located in the main conference center. Despite our location, we had a rich attendance, and the presentations were excellent. Thank you to everyone who came to speak and helped to organize the symposia!
- If you are not already a subscriber to [CHMINF-L](#), I'd encourage you join. This is the *de facto* mailing list for CINF and other groups and individuals involved in chemical information. Later this year, we will launch a newsletter and discussion board as part of the redesign of the CINF Web site, which we hope will enrich the discussions hosted on this well-established mailing list.
- Outreach is important. One of the main challenges faced by CINF is the notion that division participation requires physical presence at a national meeting. Not so! Starting at the fall national meeting we will hold committee meetings digitally, as well as in-person, so those that cannot come DC can join the discussions around programming, division business, information, and informatics. More and more CINF committees are moving to regular online discussions. I also encourage you to look into and join your local section, as chemical information is relevant *everywhere*, and then let us know! The executive committee is keen to get involved across the globe.
- CINF elections are coming and we need YOU! ACS requires that we cycle through positions on a regular basis, and we need help. If you have a little time to donate to activities like fundraising, treasury, or leadership, please reach out to us to find out more. Physical attendance at National Meetings is not required!

Do you have ideas for CINF and what you would like to see out of your membership? Commentary? Thoughts? Please feel free to e-mail me!

Thanks for being a member!

Erin Davis  
CINF Chair  
[cinfchair@gmail.com](mailto:cinfchair@gmail.com)

## Letter from the Editor

Greetings from sunny Philadelphia.

The month of May has come and gone, and with it the thousand-and-one tasks of the head of an academic chemistry library: giving and grading final exams and term projects, assigning grades, writing budget reports, and enjoying the ever-popular career review season. As I type the last corrections on the last page of the last administrative report and hit the “send” button, the summer opens its doors enticingly, saying, “Come in! Here, there are no classes to teach, no assignments to grade, and very few undergraduates requiring information skills training as they set about their lab reports! You finally have... **spare time!**”



I rejoice. Spare time to work on my projects: it is what I've been dreaming about since January! As I walk through the enchanted doors of summer, however, I start to notice the shadowy corners that I had not seen from the outside. I find that summer harbors surprising denizens: things I didn't have time to do before, things I tried to avoid by being “too busy,” and things that just seemed like a good idea at the time. Lurking to the left are three papers that I started in the fall with the best of intentions but have yet to finish. An unfinished research guide about evaluating information hides to my right, and, when I look up, I am startled to see my research project on what and how chemists read threatening to fall from the ceiling. The phone rings; it is the colleague to whom I faithfully promised a presentation for an upcoming symposium, and she is calling to collect. “But wait!” I cry. “I'm not interested in any of this anymore! I actually want to find out whether or not group work enhances student learning of the material, and I'm sure that the answer to this question will necessitate a complete restructuring of my syllabus....”

The challenge of summer is to air out the dusty corners, critically examine their inhabitants, and perform some soul searching to determine what needs to be done and what does not, what is still interesting and what has outstayed its welcome. And so, I will sift through all of these things to do that I have discovered and invented. I will order them and begin to take a stab at them, feeling a distinct sense of accomplishment when each one is erased from the white board in my office. After all, the three months that stretch gloriously before me will, all too quickly, melt away to be replaced by the structure and rigor of another academic year.

Of course, this only describes **my** summers. Some of you may have tidier corners than I. Your summer projects may already be piled in neatly-prioritized stacks waiting for you to attack them. Perhaps you do not even have stacks at all; maybe your inbox is empty by the end of each day, and your outbox is filled with tidy little packages. If this is the case, I envy you, and, like all envious people, I cannot help but wish to disrupt your process just a little bit.

As disruption, I offer you this issue of the *Chemical Information Bulletin* with a bumper crop of features. For those who did not attend the national meeting in San Francisco and for those who missed talks by running back and forth between the various meeting hotels, seven diligent authors have transcribed the details of their symposia so that you can refresh your memory and be inspired with food for new projects. If you enjoy the subject of food, I invite you to chew over the past and future of the CINF luncheon with Svetlana, and, if the history of our division and discipline interest you, you will enjoy Wendy's historical musing, hopefully the first of many. Finally, just in case your work has not been disrupted enough, Bob Buntrock presents another fine book review of a recent CINF-inspired *ACS Symposium Series* volume, and you can decide whether or not it belongs on your “to read” list.

Now, if you'll excuse me, I simply **must** learn whether group work has pedagogic value or if, as my students seem to think, it is merely a new method of torture devised by instructors in the name of active learning... right after I finish that presentation that I promised to give!

Until next summer.

Judith N. Currano, Editor  
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# Awards and Scholarships

## Scholarship for Scientific Excellence

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) is designed to reward students and postdoctoral fellows in chemical information and related sciences for scientific excellence and to foster their involvement in CINF. Since 2005 the program has awarded scholarships at each of the ACS National Meetings, 70 scholarships in total. The awards at the 253rd National Meeting in San Francisco were sponsored by ACS Publications.

Applicants presented their posters at the CINF Welcoming Reception, where the three winners received their awards, and the Sci-Mix session. Three full scholarships valued at \$1,000 each were awarded to Andrew McEachran, Matthew Seddon, and Christopher T. Lee.

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

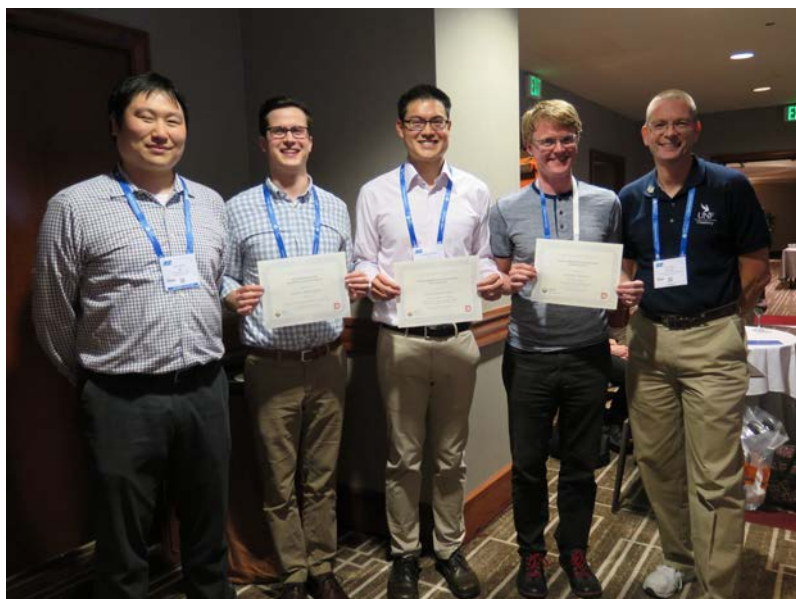
**Andrew McEachran**, National Center for Computational Toxicology, Environmental Protection Agency, Research Triangle Park, NC, USA, “*Mobilizing EPA’s Comptox Chemistry Dashboard data on mobile devices*”  
Co-authors: Kirill Blinov and Antony Williams

**Matthew Seddon**, Information School, University of Sheffield, Sheffield, UK, “*Global spectral and diffusion geometry descriptors of 3D molecular shape for virtual screening*”, Co-authors: David Cosgrove, Martin Packer and Val J. Gillet

**Christopher T. Lee**, Department of Chemistry and Biochemistry, University of California, La Jolla, CA, USA, “*Investigating transport properties with multiscale computable mesh models from heterogeneous structural datasets*”, Co-authors: John B. Moody, J. Andrew McCammon, Michael Holst, and Rommie E. Amaro

The next scholarships are sponsored by ACS Publications and will be awarded at the fall 2017 ACS National Meeting in Washington, DC.

Stuart Chalk  
Coordinator, CINF Scholarships for Scientific Excellence  
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*Scholarship for Scientific Excellence recipients at the CINF Welcoming Reception. Pictured from left to right are: Michael Qiu from ACS Publications; Scholarship recipients Andrew McEachran, Christopher T. Lee, and Matthew Seddon; and Stuart Chalk, the Coordinator for the CINF Scholarships for Scientific Excellence.*

*Photo credit Wendy A. Warr*



## Applications Invited for CSA Trust Grants for 2018

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 2018.



### **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 (e.g. 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 given for activities completed prior to the grant award date.

### **Application Requirements**

Applications must include the following documentation:

1. A letter that details the work upon which the grant application is to be evaluated as well as details on research recently completed by the applicant;
2. The amount of grant funds being requested and the details regarding the purpose for which the grant will be used (e.g. cost of equipment, travel expenses if the request is for financial support of meeting attendance, etc.). The relevance of the above-stated purpose to the Trust's objectives and the clarity of this statement are essential in the evaluation of the application;
3. A brief biographical sketch, including a statement of academic qualifications and a recent photograph;
4. Two reference letters in support of the application. Additional materials may be supplied at the discretion of the applicant only if relevant to the application and if such materials provide information not already included in items 1-4. 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**

Application deadline for the 2018 Grant is March 30, 2018. Successful applicants will be notified no later than May 9, 2018.

### **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](mailto:chescot@aol.com) prior to submission so that she can contact you if the e-mail does not arrive.

## *Chemical Structure Association Trust: Recent Grant Awardees*

### **2017**

**Jesus Calvo-Castro:** University of Hertfordshire, England, was awarded a grant to cover travel to present his work at the Fifth International Conference on Novel Psychoactive Substances, to be held in Vienna, Austria from August 23-23, 2017. He works on the development of novel methodologies for the in-the-field detection of novel psychoactive substances (NPS), where chemical structure and information play a crucial role.

**Jessica Holien:** St. Vincent's Institute of Medical Research, Fitzroy, Victoria, Australia, was awarded a grant to cover travel to present her work at the 2017 Computer-Aided Drug Design (CADD) Gordon Research Conference, scheduled to take place July 16-21, 2017 in Mount Snow, VT, USA. She is a postdoctoral researcher at St. Vincent's and is responsible for a range of computational molecular modelling, including compound database development, virtual screening, docking, homology modelling, dynamic simulations, and drug design.

### **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 23<sup>rd</sup> 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 Isayer:** Division of Chemical Biology and Medicinal Chemistry, UNC Eshelman School of Pharmacy, 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, Spain, 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, 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, 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, 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 ideas from the Integral Equation Theory of Molecular Liquids.

**Sona B. Warriar:** Departments of Pharmaceutical Chemistry, Pharmaceutical Biotechnology, and Pharmaceutical Analysis, NMIMS University, Mumbai, 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, was awarded a 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, U.K., was awarded a 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, was awarded a 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, was awarded a 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, was awarded a grant for travel to work with Professor Ernst Walter-Knappt at the Freie University of Berlin and Professor Jean-Phillipe Vert of the Paris MinesTech to continue his work on the development of atomic partial charge kernels.

### **2010**

**Noel O'Boyle:** University College Cork, Ireland, was awarded a 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, was awarded a grant to do three months of research at the University of Innsbruck, Austria.

### **2008**

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



#### **2007**

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

#### **2006**

**Krisztina Boda:** University of Erlangen, Erlangen, Germany, was awarded a 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, U.K., were awarded a 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, was awarded a grant to purchase equipment needed for her research.

#### **2003**

**Prashant S. Kharkar:** Institute of Chemical Technology, University of Mumbai, Matunga, Mumbai, India, was awarded a 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, Dep. of Chemistry, London, U.K., was awarded a 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.

# Feature Articles

## Twenty-Five Years After

Wendy Warr & Associates was founded 25 years ago in January 1992; see <http://warr.com/15years.html> for other momentous events of that year. By coincidence, the spring ACS meeting that year was held in San Francisco, as was the most recent one, in spring 2017. My first public report on an ACS national meeting covered the meeting held in August 1992 in Washington, DC, and if I produce two reports this year, I will be up to issue number 50!

This year also marks a notable 40-year anniversary for me: the very first ACS national meeting I attended was in fall 1977. Recently I posted a historical note or two on *chminf-l*, and it was suggested that I might like to write an occasional historical item for the *Chemical Information Bulletin*. I hope to start the venture in earnest with the next issue of the bulletin, but here is a short “taster”, focusing on some events of 1991 and 1992.

Tim Berners-Lee posted the first lines of HTML in 1991, and the first sites appeared on the World Wide Web in 1992. Many individuals active in CINF were allocated email addresses by CAS: mine was [waw22@cas.org](mailto:waw22@cas.org) or [waw22@xtrn.org](mailto:waw22@xtrn.org). (A CAS email address had your initials and department number; department 22 was unused internally.) I also had a Bitnet id, but I cannot remember what I used it for.

The early IBM PC read real floppy disks (the ones the mailman could bend). *Tetrahedron Computer Methodology*, a revolutionary electronic journal, using MDL's Chemist's Personal Software Series (CPSS) was issued on these floppy disks. The last issue appeared in 1992, although it was dated 1990 to meet the calendar requirements of a more old-fashioned publishing culture. MDL published its file formats in the *Journal of Chemical Information and Computer Sciences* in 1992, effectively ending the Standard Molecular Data (SMD) file movement, although the Chemical Structure Association was still supporting SMD into 1993. The term “cheminformatics” was not in common use in 1992.

MDL had a year of uncertainty after the death of Robert Maxwell in November 1991 (see Warr, W.A. After the Fat Man Jumped: The Saga of Robert Maxwell. *ONLINE* **1992**, 16(6), 62-67). My notes on the spring 1992 ACS meeting record that relations between MDL and TRIPOS Associates did not improve after the “unfortunate incident in San Francisco”? Can anyone remember what that incident was? It hardly matters now: both companies no longer exist. In 1992, Bob Massie was appointed Director of CAS, and shortly afterwards, Jim Seals departed.

I am happy to receive comments, corrections and omissions. I will include them in my next column, if health, strength, and the demands of my continuing, busy consulting business permit.

Wendy Warr  
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## The CINF Luncheon

Tradition, tradition.... You may find a curious fact that the earliest CINF social event was... a luncheon.

At almost every ACS National Meeting, the division members enjoy having a divisional luncheon, usually on a Tuesday. The tradition was started with the Chemical Literature Group in 1943, long before the division was formed in 1948.

### Speakers

Val Metanomski listed the names of the luncheon speakers between 1943 and 1975 and commented, "The speakers represented a broad spectrum of well-informed individuals with great credentials, mostly from within the ACS membership."<sup>1</sup> Indeed, the early luncheon lecturers were distinguished chemists associated with the society including several future Priestley medalists: Edward R. Weidlein (1848), E. J. Crane (1951), W. Albert Noyes, Jr. (1954), Wallace R. Brode (1960), and Joel H. Hildebrand (1962). Descriptions of the events consistently refer to the luncheon speaker as "the guest of honor." The first speaker, at the fall 1943 ACS National Meeting in Pittsburgh, was Edward Ray Weidlein, who had been ACS president in 1937. This was the year that the Chemical Literature Group was formed within the Division of Chemical Education, and an intriguing description of that luncheon appeared in *Chemical & Engineering News (C&EN)*.

Although the attendance at [the] student breakfast was smaller than usual, there was an overflow crowd (about 110) at the divisional luncheon, at which E.R. Weidlein spoke as one having authority and not as a modern scribe or bureaucrat!<sup>2</sup>

The divisional event attendance of 110 was high, considering that the total meeting registration was 3,537 for that conference. The cost of the 1943 luncheon was \$1.65, which was expensive in proportion to the meeting registration fee of \$3 for a member of the society.

Five years later, at the 1949 spring national meeting in San Francisco, the newly-established Division of Chemical Literature marked another milestone on its path towards its 70<sup>th</sup> anniversary; it organized its first program of three sessions with fifteen papers. The division reported of its social event:

The first meal sponsored by this new division was a luncheon Tuesday noon attended by 43 people. G. Malcolm Dyson of Loughborough, England was the guest of honor. He congratulated the American Chemical Society on the formation of the Division of Chemical Literature, stating he knew of no other chemical organization in the world which had recognized the broad importance of documentation by forming such a sub-division... Membership of the division was at about 300.<sup>3</sup>

Fast-forwarding along the CINF historical timeline to the notable 1970s, another record of high attendance of 102 people was reported at the spring 1975 luncheon in Philadelphia with a keynote address by Eugene Garfield, the founder of the Institute for Scientific Information (now Clarivate Analytics) and the creator of such innovative publications as *Current Contents*, *Science Citation Index*, *Index Chemicus*, and *Current Chemical Reactions*. At the spring 1976 luncheon, Cyrus Levinthal, an outstanding molecular biologist, was a guest speaker, and the first Herman Skolnik Award was given to Herman Skolnik. In 1977, the division luncheon featured presentations entitled "Chemical Information Scientists are really important to Industry Productivity and Profitability" by William Hanford (spring) and "Personal Computing: a Look at the 1980's" by Philip A. Greth (fall). In the following spring, Melvin Calvin, who won the 1961 [Nobel Prize in Chemistry](#) for his research on carbon dioxide assimilation in plants, was an honorable guest presenter. At the fall 1978 ACS National Meeting in Miami Beach, the division tried an experiment where, instead of the usual luncheon speaker, it had a panel discussion on the CINF Tuesday morning's symposium entitled *Retrieval, Analysis, and Indexing of Chemical Reactions*, moderated by Robert Fugmann (a future recipient of the Herman Skolnik Award in 1982). According to the program chair's message, that experiment generated heated feedback comments varying from "how boring" to "it was great; let's do it again!"<sup>4</sup> After a few years, at the fall 1984 national meeting in Philadelphia, CINF had one more unusual luncheon setup with roundtable discussions on topics such as end-user training, office automation, data resource management, copyright, document delivery, full-text searching, and others. (*Chemical*

*Information Bulletin*, Summer 1984, page 20). Aside from those two experiments, the luncheon kept its typical format, with a guest speaker. Val Metanowski carried on his compilation of the CINF luncheon speakers from 1975-1993, and remarked:

The most enduring tradition, Divisional luncheons at the ACS National Meetings, continued throughout that period, almost always capped with a talk by a knowledgeable, interesting, and often witty speaker. Some luncheons were joint with other ACS Divisions such as Computers in Chemistry, and Chemistry and the Law. The subjects covered up-to-date information on general societal concerns, on some of the ACS activities, on new technological developments in information storage, retrieval, and distribution, and on other 'hot' topics.<sup>1</sup>

Since 1993, there have been a few more CINF luncheons featuring keynote presentations by distinguished chemists, namely: Roald Hoffmann, who shared the 1981 Nobel Prize with Kenichi Fukui for their theories, developed independently, concerning the course of chemical reactions (fall 1994); Helen Free, an awardee of the 2010 National Medal of Technology and Innovation and a designee of the 2010 National Historical Chemical Landmark for developing diagnostic strip tests (spring 1996); and Richard Zare, a recipient of the 2010 Priestley Medal for lifetime of scientific achievement and service to chemistry (spring 1997). During the 1990s, CINF began a trend of inviting guest speakers from the region where the national meeting was held. Some examples of institutions invited to speak include the following

- Disney Studios: spring 1995, in Anaheim
- Field Museum (a talk about DNA and dinosaurs): fall 1995, in Chicago,
- Scripps Institution of Oceanography (a presentation by Jeffrey Bada on *Searching for Evidence of Life on Mars*) spring 2001, in San Diego,
- Environmental Protection Agency (a talk by Ted Smith about sustainability of Great Lakes): spring 2007, in Chicago.

Along with adding a regional flavor, the presentation topics began to shift from chemistry and chemical information to popular science and entertainment. There are several possible explanations for this tendency. First, the CINF technical program had become fully packed, prompting a desire on the part of the division chair for a leisurely luncheon. Second, there is no fixed honorarium for the guest speaker, who therefore requires easy transportation to the national meeting site. Luncheons in the 2000s and 2010s hosted more diverse guests, including John Reynolds, who spoke on forensic science and weapons of mass destruction (fall 2006); Michael Capuzzo, who recounted tales from his bestselling publication, *The Murder Room* (with book signing, fall 2010); and Richard Walter, who talked about a notorious serial killer Jack the Ripper (spring 2011). Fortunately for attendees fearing horror stories over lunch, the next series indulged in *Chocolate, Food of the Gods* by Howard and Sally Peters (with delicious samples and prizes, fall 2011); *The Chemistry of Wine* by Kirsten Skogerson (with California wine tasting, spring 2012); and *Science Comedy* by Brian Malow (with jokes and puns, spring 2013). The recent luncheon speakers are listed in the Table 1.

### Awards

In addition to guest lectures and social networking opportunities for division members, the luncheon provides a venue for award ceremonies. Since its inauguration in 1976, the Herman Skolnik Award has been presented to forty-five scientists for their achievements in the theory and practice of chemical information science. The winners are always invited to the CINF luncheon, although the actual award ceremony has recently been scheduled for the conclusion of the Award Symposium. The Meritorious Service Award, renamed in honor of Val Metanowski in 2010, has, since its establishment in 1992, recognized sixteen division members for their outstanding services to CINF. In 2006, the CINF Lifetime Award was dedicated to Val Metanowski and then honored two more members for their long-standing, commendable commitments to the division: Guenter Grethe in 2013 and Bonnie Lawlor in 2015. The spring luncheon was also a good time to thank the immediate past-chair of CINF formally with the presentation of the "ACS Past-Chair" commemorative pin. For a short time in 2009-2010, the Best Presentation Award, funded by the ACS Innovative Program Grant, was also presented at a luncheon.

**Table 1. CINF Luncheon Speakers 2009-2017**

237	Spring 2009	Salt Lake City	Sonja Krane	Highlights of the Journal of the American Chemical Society
238	Fall 2009	Washington	Jeremy Berg	One Chemist's Journey into Informatics
239	Spring 2010	San Francisco	Randy Marcinko	Profitable Publishing: My Journey from Edge Notch to Semantic Edge
240	Fall 2010	Boston	Michael Capuzzo	The Murder Room
241	Spring 2011	Anaheim	Richard Walker	Jack the Ripper Unveiled
242	Fall 2011	Denver	Howard & Sally Peters	Chocolate, Food of the Gods
243	Spring 2012	San Diego	Kirsten Skogerson	The Chemistry of Wine (slides)
244	Fall 2012	Philadelphia	William Brock	The Case of the Poisonous Socks: Tales from Chemistry
245	Spring 2013	New Orleans	Brian Malow	Science Comedy
246	Fall 2013	Indianapolis	Katy Börner	Multi-Scale Maps of Scholarly Activity (slides)
247	Spring 2014	Dallas	Andrew Yeung	Chemistry in Wikipedia: A Personal Perspective
248	Fall 2014	San Francisco	Barend Mons	Data stewardship, Boring or Soaring? (slides)
249	Spring 2015	Denver	David Thomas	19 <sup>th</sup> & 21 <sup>st</sup> Century Malting & Brewing
250	Fall 2015	Boston	Michele Derrick	CAMEO: A Database for Technical Information on Materials in Museums
251	Spring 2016	San Diego	Christopher Tubbs	Dietary Phytoestrogens and Reproduction in Southern White Rhinoceros
252	Fall 2016	Philadelphia	James Voelkel	The Chymistry of Isaac Newton Project and the Chymical Encyclopedia
253	Spring 2017	San Francisco	Andrew Leach	Molecules, Data and Models

Staying true to its mission for supporting students interested in pursuing studies in chemical information and related sciences, CINF has awarded stipends over many years. First, the Student Scholarship Award was established in 1989 and was renamed in 1996 in honor of Lucille M. Wert. Although this stipend is usually mailed to the recipient, there have been several special occasions when it was presented during a CINF luncheon. Second, the Scholarship for Scientific Excellence program was created in 2005, based on generous support from its sponsors: IO Informatics, FIZ Chemie Berlin, Elsevier MDL, Symyx Technologies, Accelrys, RSC Publishing, Springer/InfoChem, and ACS Publications. Since its inauguration, sixty-seven scholarships in total have been awarded via this program, and the scholarship winners are always invited to the division luncheon on Tuesday.

### **Attendance**

Typically, a CINF luncheon gathers about sixty to eighty attendees. The majority of luncheon ticket sales are made through ACS meeting registrations, with the remaining fifteen to thirty tickets sold in person during division social events and given as complimentary tickets to all award and scholarship winners, guest speakers, and sponsors. The available data on ticket sales via ACS registrations and total attendance estimations are listed in Table 2, along with total ACS registrations for each meeting and the price of each ticket.

Getting close to beating its historical record of over one hundred participants, the latest spring luncheon in San Francisco showed the best attendance, with close to ninety diners. Although, there were likely extra "fans" who came only in order to hear the speaker, Andrew Leach, Head of Chemistry Services at EMBL-EBI (The European Molecular Biology Laboratory - The European Bioinformatics Institute), the larger count was drawn from the highest-ever number of total registrants at an ACS National Meeting, 18,850.



**Table 2. CINF Luncheon Attendance 2010-2017**

Mtg.	Year	Location	Tickets sold by ACS	Attendance estimated by CINF	ACS Registrations	Ticket Price
<b>Season: Spring</b>						
239	2010	San Francisco	50	77	18,067	\$15
241	2011	Anaheim	44	70	14,022	\$15
243	2012	San Diego	N/A	60	16,758	\$15
245	2013	New Orleans	N/A	75	15,473	\$15
247	2014	Dallas	32	N/A	13,498	\$15
249	2015	Denver	53	65	13,958	\$15, \$20*
251	2016	San Diego	N/A	70	16,310	\$20, \$25*, \$15**
253	2017	San Francisco	52	85-90	18,917	\$30
<b>Season: Fall</b>						
240	2010	Boston	N/A	75	14,072	\$15
242	2011	Denver	51	85	10,453	\$15
244	2012	Philadelphia	60	80	13,228	\$15
246	2013	Indianapolis	43	N/A	10,803	\$15
248	2014	San Francisco	45	N/A	15,774	\$15
250	2015	Boston	69	80	13,928	\$15, \$20*
252	2016	Philadelphia	60	71	12,989	\$25

\* non-CNF member; \*\* student

### **Ticket price**

During its first thirty years, the ticket price for the luncheon rose from \$1.65 in 1943 to \$5 in the mid-1970s. The price increased sharply to \$8 at the fall 1977 national meeting in Chicago, which raised concerns among members of the CINF executive committee: "Why if the luncheon for the division was subsidized, was the price still \$8, which was equivalent to what the other divisions were paying for their luncheons." It turned out that this luncheon had been held in a higher-priced hotel and incurred additional add-on costs. In the 1980s, the ticket price increased to \$11, remaining under \$14 for several years, with the exception of a jump to \$18 at the fall 1981 national meeting in New York and to \$25 at the fall 1990 national meeting in Boston. During the next decade, the ticket price varied in a range from \$16 to \$28, and then suddenly spiked to \$40 (spring 2000, San Francisco) before reaching its peak of \$42 (spring 2001, San Diego). After managing to keep the ticket price for the next three luncheons at \$30-34 (fall 2001, Chicago through fall 2002, Boston), the CINF executive committee asked its fundraising chair to try to locate a sponsor in order to keep the ticket price below \$30, a goal that was met between 2004 and 2007 thanks to the kind support of MDL and others. In order to keep the ticket price at \$30 for the 2008 spring national meeting in New Orleans, the division luncheon was organized off-site in the Rio Mar Restaurant. At that meeting, the CINF executive committee had a special discussion on "The Future of the CINF Luncheon," reporting that the cost of the luncheon was rising above \$30. The ticket price was driven both by the cost of food and the cost of A/V equipment, which was hundreds of dollars, and the location of the luncheon was almost always dictated by the fact that national meeting programming is very tight. The consensus was that CINF needed to raise about \$2500 - \$3000 in additional funds for each luncheon in order to support a ticket price of \$15, which was deemed a reasonable price. CINF achieved this desired outcome, introduced a special price of \$15 for the fall 2008 meeting in Philadelphia, and has been able to sustain this price for many years thanks to the following generous sponsors:

- Thieme Chemistry (spring and fall 2009)
- Elsevier/Reaxys (spring 2010)
- Bio-Rad Laboratories, CambridgeSoft, and Thieme Chemistry (fall 2010)
- RSC Publishing (exclusively, spring 2011)
- Bio-Rad Laboratories and RSC Publishing (fall 2011)
- RSC Publishing (exclusively, spring 2012-spring 2017).

Recently, the luncheon ticket price has started increasing again. Luncheon tickets at the last three national meetings cost: \$15 member/\$20 non-member (spring 2016, San Diego), \$25 (fall 2016, Philadelphia), and \$30 (spring 2017, San Francisco). Within a decade the ticket price had once again reached \$30, despite the sponsors increasing their contribution to \$4,000. Without this additional support, the ticket price would be \$40 - \$50, as seen for other ACS divisions and committees. Currently, very few ACS divisions organize their luncheons at national meetings; aside from the Division of Chemical Information, the following technical division luncheons were listed in the program for the ACS spring 2017 national meeting:

- Division of the Chemistry and the Law, Drug and Power Luncheon: \$40, off-site
- Division of Chemical Education, High School-College Interface Luncheon: \$45, on-site
- Division of Colloid and Surface Chemistry, Luncheon: \$45, on-site.

Overall, the cost of social events at official ACS national meeting venues has become so outrageously expensive that CINF has discontinued all food services for its long committee meetings on Saturday, paused the traditional "Harry's Party" on Monday, and adapted to a buffet-style luncheon on Tuesday. Erin Davis, the division chair, has been actively exploring off-site venues and joint collaborations with other ACS divisions for social events. She is in favor of mingling opportunities at receptions; for example, she made arrangements with the Computers in Chemistry division to hold a lively joint reception in Jillian's Bar on Saturday night in San Francisco. The CINF luncheon has been a division tradition for seventy-four years, but what is its future? Your feedback is welcome!

### Luncheon photos



Additional photos appear at the following URLs:

Fall 2009: <https://www.flickr.com/photos/cinf/sets/72157623717050810/>  
Spring 2010: <https://www.flickr.com/photos/cinf/sets/72157623720376698/>  
Fall 2010: <https://www.flickr.com/photos/cinf/sets/72157624845342004/>  
Fall 2012: <https://www.flickr.com/photos/cinf/sets/72157631544068782/>  
Spring 2013: <https://www.flickr.com/photos/cinf/sets/72157633296215386/>  
Spring 2015: <https://www.flickr.com/photos/cinf/sets/72157649815681453/>  
Fall 2015: <https://www.flickr.com/photos/cinf/sets/72157658714184736/>  
Fall 2016: <https://www.flickr.com/photos/cinf/sets/72157674179424755/>

### **Sources consulted**

- “50 Years of Chemical Information in the American Chemical Society 1943-1993”
- Brenda Philpot, Lead Program Associate, ACS Meetings & Expositions Services
- Michael Qiu, CINF Social Events Coordinator
- *Chemical & Engineering News*
- *Chemical Information Bulletin*
- *CINF E-news*
- CINF Executive Committee meeting minutes.

### **References**

- 1) Metanomski, V. 50 Years of Chemical Information in the American Chemical Society 1943-1993. [http://web.stanford.edu/group/swain/cinf/50years/html\\_index.html](http://web.stanford.edu/group/swain/cinf/50years/html_index.html) (accessed May 26, 2017).
- 2) Fall, P. H. Chemical Education. *Chemical and Engineering News* **1943**, 21, 1520.
- 3) Casey, R. S. Chemical Literature. *Chemical and Engineering News*, **1949**, 27, 1310-1311.
- 4) Revesz, G. S. From the program chairman’s desk. *Chemical Information Bulletin*, Fall/Winter 1978, p 3.

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# Technical Program

## Assessment of Chemistry Collections and Services Symposium Reflections

Andrea Twiss-Brooks (University of Chicago) and I decided to organize a session on assessment in chemistry collections and services, as there is a growing interest in assessment and data-driven decisions across libraries.

One of the unique aspects of our session was how related the presentations were to each other. The presentations felt like a cohesive collection. This cohesiveness allowed the speakers to revisit content from earlier in the session and allowed audience members to ask questions related to more than one presentation.

The session started with three presentations focused on analyzing chemistry collections through a variety of citation analysis methods. David Flaxbart (University of Texas at Austin) discussed usage trends of chemistry monographs (CINF 155: “What about the books? Usage trends of chemistry monographs among graduate students in an era of transition”), Elsa Alvaro studied research trends by analyzing chemistry article citations and titles (CINF 156: “Matching chemistry collections and user needs: a data-driven approach”), and I discussed research trends through a title analysis of chemistry theses and dissertations (CINF 157: “Assessment of chemistry thesis and dissertation titles for collection development”). In all cases, we learned about research trends in chemistry, citation behaviors, and efforts to use citation data to inform decisions about collections. The take-home message for me was that, by analyzing citation data, we could definitely learn about chemistry research trends and citation behavior, but developing actionable decisions for collections is still a challenge.

Jeremy Garritano (University of Virginia) continued the session with his work on assessing chemistry library space (CINF 158: “Chemistry library as rallying point: assessing how to save a branch library”). The chemistry library at the University of Virginia closed, and the space was redesigned into an active learning classroom environment. Jeremy collaborated with the chemistry department and libraries to help develop an ideal space. One thing that I really liked about Jeremy’s approach was his engagement with the chemistry graduate students. He asked the graduate students to draw a picture of their ideal space and then was able to use elements from the drawings in his planning.

Brian Westra (University of Oregon) presented the closing talk on assessing chemistry data practices and data management plans (CINF 160: “Assessing data management practices and needs through data management plans”). His presentation was an excellent segue into the afternoon Research Data Alliance Chemistry Publisher Forum, which reviewed publisher data requirements and discussed opportunities for increased sharing of chemical data.

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## Information Flow in Environmental Health & Safety

In 2016, the ACS adopted safety as a core value. As awareness for safety increases, it becomes clear that access to chemical safety information will be critical to support a culture of laboratory safety in the chemistry community. As fellow chemistry professionals supporting chemical research and teaching, the Divisions of Chemical Information (CINF) and Chemical Health and Safety (CHAS) have been exploring the state of chemical safety information and its applicability to laboratory safety, particularly in the academic sector. CINF and CHAS have collaborated on Innovative Project Grants and sparked conversations about chemical safety information across the society.

CINF and CHAS regularly co-sponsor symposia on this topic at ACS national meetings, alternating as host division to engage discussion across both communities. At the spring, 2017 meeting in San Francisco, CHAS hosted a program co-sponsored with CINF entitled "Information Flow in Environmental Health and Safety." The symposium presented a variety of use cases for chemical information tools that range from laboratory-specific to widely-applicable. Speakers included chemical safety officers, chemical educators, graduate students, and chemical information professionals. Education, communication, information sharing, and information management were common themes as these communities strive to incorporate risk assessment into their workflows. There are many opportunities to collaborate while meeting these challenges, particularly as the scale of chemical information increases and expectations for safety become more prevalent.

Links to the PDF versions of the following presentations from the symposium are provided on the CHAS Division website: <http://dchas.org/tag/chemical-safety-information/>. Several of these stories will become the core of a special issue of the Journal of Chemical Health and Safety, edited by the CHAS Division and published by Elsevier.

Chemical Safety requires a system, not a solution (CHAS 30)

<https://dchas.org/wp-content/uploads/2017/04/Tues-01-Stuart-System-not-a-solution1.pdf>

R. Stuart (Keene State College, EHS)

Chemical information necessary to establish laboratory ventilation control bands (CHAS 31)

<https://dchas.org/wp-content/uploads/2017/04/Tues-02-Sweet-Chem-info-needed-to-establish-lab-vent-CB.pdf>

E. Sweet (Cornell University, EHS)

Reaction safety information: engaging the community in collecting and sharing of safety learnings (CHAS 32)

<https://dchas.org/wp-content/uploads/2017/04/Tues-03-Nitsche-Reaction-Incident-Information.pdf>

C. Nitsche (Pistoia Alliance)

Chemical management applications for the University of California (CHAS 33)

[Chemical Management Applications for the University of California, P. Painter](#)

P. Painter (University of California, Office of the President)

Talking chemical safety: terminologies and keywords in various information sources (CHAS 35)

[https://dchas.org/wp-content/uploads/2017/04/Tues-06-McEwen-Safety\\_Terminology\\_21070331.pdf](https://dchas.org/wp-content/uploads/2017/04/Tues-06-McEwen-Safety_Terminology_21070331.pdf)

L. McEwen (Cornell University, Library)

Consult the SDS! (CHAS 36)

<https://dchas.org/wp-content/uploads/2017/04/Tues-07-Sigmann-Consult-the-SDS.pdf>

S. Sigmann (Appalachian State University, Chemistry)



Graduate student perspective on the ACS online tool Hazard Assessment in Research Laboratories (CHAS 37)

<https://dchas.org/wp-content/uploads/2017/04/08-Delinger-Grad-Student-Perspective.pdf>

K. Delinger (University of Cincinnati, Graduate)

Unique one-stop access to a multitude of chemical safety resources (CHAS 38)

<https://dchas.org/wp-content/uploads/2017/04/Tues-09-Lederman-Explorit-Everywhere-for-ACS-Chem-Safety.pdf>

A. Lederman (Deep Web Technologies)

EPA CompTox chemistry dashboard: an online resource for environmental chemists (CHAS 39)

[https://dchas.org/wp-content/uploads/2017/04/Tues-10-Williams-EPA-CompTox-chemistry-dashboard-resource\\_CHAS.pdf](https://dchas.org/wp-content/uploads/2017/04/Tues-10-Williams-EPA-CompTox-chemistry-dashboard-resource_CHAS.pdf)

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***Do you want to relive (or experience for the first time) key moments from this spring's meeting?***

Wendy Warr has published her photos from the ACS National Meeting in San Francisco on her Flickr stream. Visit <https://www.flickr.com/photos/cinf/albums> to access the photos. They appear in five albums:

- ACS San Francisco 2017 COMP technical session Tuesday
- ACS San Francisco 2017 Schrodinger reception
- ACS San Francisco 2017 COMP reception
- ACS San Francisco 2017 CINF welcome reception
- ACS San Francisco 2017. Yvonne Martin wins ACS Award. COMP speakers

While you're there, check out the photos from other past national meetings and special CINF events

## Textbooks & the Practice of Science: Before, During and After Gutenberg

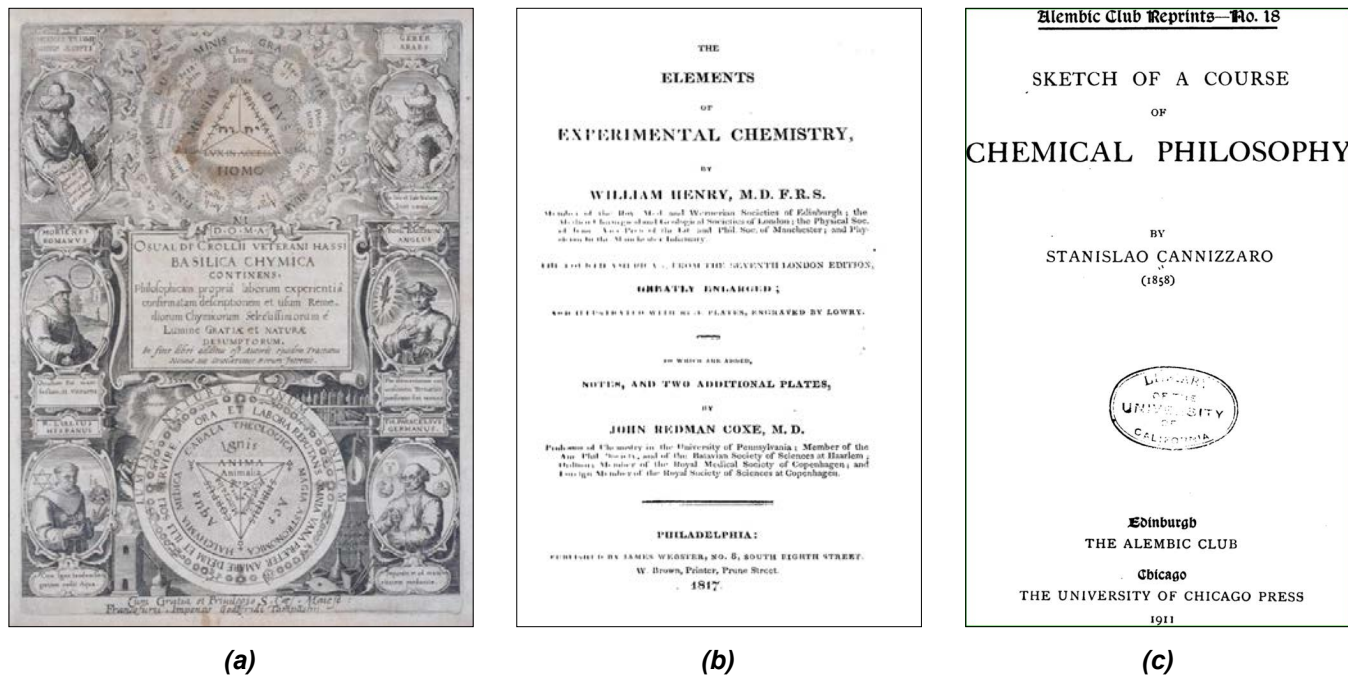
This symposium had three sessions and was organized by Robert E. Belford, Tanya Gupta and Gary Patterson. Gary Patterson presided over the first session, which dealt with historical textbooks. Tanya Gupta and Bob Belford presided over the second and third sessions respectively, and focused more on the textbook in the 21<sup>st</sup> century.

### Session One

The session started with an extended introduction by the organizer and session chair, Gary Patterson. A selection of classic historical textbooks was presented including physical copies of the books. The list included: *De Re Metallica* by Agricola (1561), *Basilica Chemica* (Figure 1a) by Oswald Croll (1609), *Elementa Chemiae* by Herman Boerhaave (1732), *Lectures on the Elements of Chemistry* by Joseph Black (1803), *An Epitome of Chemistry* by William Henry (1801), *The Principles of Chemistry* by Dmitri Mendeleev (1891), and *General Chemistry* (1947) by Linus Pauling.

Gary then delivered a paper on “William Henry and The Elements of Experimental Chemistry” (CINF 36), which included a detailed discussion of a later edition of Henry in an American edition of *The Elements of Experimental Chemistry* (1817). This textbook was an accurate and coherent presentation of chemistry at the time of its writing and was used or copied for over a century (Figure 1b).

The next lecture, “Cannizzaro's *Sunto*: A legendary text of chemistry” (CINF 37), was a discussion by Carmen Giunta of Cannizzaro's *Sunto* (Figure 1c). This classic monograph, which was distributed at the famous Karlsruhe Conference of 1864, became the basis for all the progressive texts that followed it. Cannizzaro taught the entire world of chemistry, from experts to the lowliest student.



**Figure 1:** Images of (a) *Basilica Chemica* by Oswald Croll; (b) *Elements of Experimental Chemistry* by William Henry; and (c) *Sketch of a Course of Chemical Philosophy* by Stanislaw Cannizzaro.

The fourth lecture, “Alexandre Édouard Baudrimont and his *Introduction à l'étude de la chimie par la théorie atomique* (*Introduction to the Study of Chemistry by the Atomic Theory*)” (CINF 38), was by Vera Mainz and described Baudrimont's French textbook (Figure 2a). This early coherent adoption of the best of 19<sup>th</sup> century chemistry was years ahead of the rest of France in 1854. Jean Perrin finally convinced almost all French chemists of the truth of the atomic theory in 1911, although some still doubted.

The fifth lecture, “Chemistry for a popular audience: Josiah Parsons Cooke's *The New Chemistry*” (CINF 39) was by Roger Egolf on a popular textbook (Figure 2b) by Josiah Cooke of Harvard, *The New Chemistry* (1872). It was based on Cooke's Lowell Institute lectures in Boston.



(a)

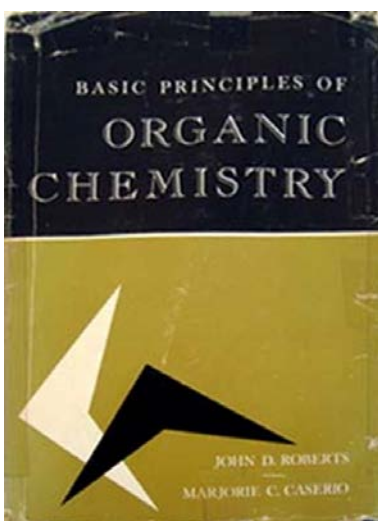
CONTENTS.	
LECTURE	PAGE
I. MOLECULES AND AVOGADRO'S LAW . . . . .	9
II. THE MOLECULAR CONDITION OF THE THREE STATES OF MATTER—THE GAS, THE LIQUID, AND THE SOLID . . . . .	37
III. HOW MOLECULES ARE WEIGHED . . . . .	63
IV. CHEMICAL COMPOSITION—ANALYSIS AND SYNTHESIS—THE ATOMIC THEORY . . . . .	84
V. ELEMENTARY SUBSTANCES AND COMBINING PROPORTIONS . . . . .	104
VI. ATOMIC WEIGHTS AND CHEMICAL SYMBOLS . . . . .	122
VII. CHEMICAL REACTIONS . . . . .	149
VIII. CHEMICAL CHANGES CLASSIFIED . . . . .	175
IX. THE THEORY OF COMBUSTION . . . . .	195
X. CARBONIC ACID AND NITRO-GLYCERINE . . . . .	216
XI. QUANTVALENCE AND METATHESIS—ALKALIES AND ACIDS . . . . .	238
XII. ELECTRO-CHEMICAL THEORY . . . . .	265
XIII. ISOMERISM, AND THE SYNTHESIS OF ORGANIC COMPOUNDS . . . . .	296

(b)

**Figure 2:** Images of (a) Introduction to the Study of Chemistry by the Atomic Theory by Alexandre Édouard Baudrimont; and (b) The New Chemistry by Josiah Cooke.

The sixth lecture, “Basic organic textbook: from its beginning to its (digital) end” (CINF 40), was a discussion of the creation and publication of the classic organic textbook, *Principles of Organic Chemistry* (1964) by one of its authors, Marjorie Caserio. Although it is now out of print, it is still the best elementary textbook in organic chemistry and CaltechAUTHORS have made it available online, <http://authors.library.caltech.edu/25034/>.

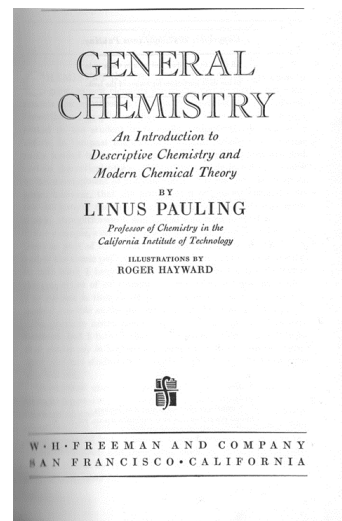
The seventh lecture was by Jay Labinger on Basolo and Pearson’s epoch-making inorganic chemistry textbook: *Mechanisms of Inorganic Reactions* (1958), and was entitled “Mechanistic turn in inorganic textbooks: Basolo and Pearson’s *Mechanisms of Inorganic Reactions*” (CINF 41). This textbook influenced all later books and is still worth reading.



(a)



(b)



(c)

**Figure 3:** Images of (a) Basic Principles of Organic Chemistry by Roberts and Caserio; (b) Mechanisms of Inorganic Reactions by Basolo and Pearson; and (c) General Chemistry by Linus Pauling.

Gary Patterson’s presentation “Edgar Fahs Smith and elements of chemistry at Penn” (CINF 42), the eighth lecture, was a consideration of the 20<sup>th</sup> century elementary textbook by Edgar Fahs Smith (Figure 4), *Elements of Chemistry in Lecture Form* (1915). Smith was Provost (President) of the University of Pennsylvania, twice-elected President of the American Chemical Society, and the founder of both the Division of the History of Chemistry and the Division of Chemical Education. This textbook included a few more elements than Henry’s early 18<sup>th</sup> century textbook, but was at a much lower level. It was agnostic with regard to atoms, ignored Mendeleev’s Periodic Table, and generally was a waste of time.



**Figure 4:** Edgar Fahs Smith beside his statue on the Penn campus

The session concluded with a panel discussion of issues raised during the day. The major conclusions of the discussion were that a good elementary textbook should treat all of the fundamental paradigms of chemistry in its day, present enough good examples to convince the students that the paradigms do work, and include enough real problems to equip them to be real chemists. The only real book of this kind in the 20<sup>th</sup> century was *General Chemistry: An Introduction to Descriptive Chemistry and Modern Chemical Theory* by Linus Pauling.

## Session Two

This session included papers on various topics, such as the evolution of textbooks from ancient historical artifacts to current digital texts, with a focus on Open Educational Resources (OERs). It also incorporated presentations on integrating laboratory safety and process skills and addressing misrepresentation of science and fads in the age of social media and fake news.

The symposium began with an introduction by the organizer Robert (Bob) Belford from the University of Arkansas, Little Rock. In his introductory remarks, Bob briefly discussed best practices for digital media, annotating text and engaging in online discussions, and innovative ways of sharing electronic content to make it accessible to audiences across the globe. Tanya Gupta, of South Dakota State University, presided over the session.

The first presentation, by Bob Belford, was on the “Extensible Electronic Notebook” (CINF 73). During his presentation, Bob provided a detailed description of the electronic textbook that was used during the intercollegiate Online Chemistry Course (OLCC) on Cheminformatics, which was offered for the first time in the fall of 2015 and offered again during the spring of 2017. Bob demonstrated the electronic textbook used for OLCC course and provided a brief description of features like embedded Teaching and Learning Objectives (TLOs) that provide the ability to integrate new ideas and information as the course evolves during instruction. He showed videos that capture the essence of the electronic textbook and demonstrated ways in which the discussion of literature and related cheminformatics content could be aggregated at the bottom of each chapter of the e-textbook using the hypothes.is annotation service (<https://web.hypothes.is/>).

The second presentation was entitled “Supporting transmission of knowledge for chemical safety: an information workflow supplement to the laboratory textbook,” by Leah McEwan (CINF 74). Leah’s presentation focused on important aspects of laboratory instruction that include laboratory safety, environmental aspects of laboratory instruction, and the effectiveness of lab instruction in teaching research skills. She provided information on emergent chemical safety educational resources and information technologies and how these resources provide an opportunity to build on the core scientific concepts that are important components of laboratory manuals.

Leah shared information on the role of chemistry librarians and environmental health and safety staff and described how their collaboration with laboratory instructors fosters the planning process based on the RAMP model. The key features of RAMP are **R**ecognizing hazards, **A**ssessing risks of hazards, **M**inimizing hazards, and **P**reparing for emergencies. Effective implementation of RAMP in a laboratory curriculum can serve as a stepping-stone for preparing students to perform independent research, due to its emphasis on laboratory processes and safety. RAMP is integrated in the recent ACS Committee on Professional Training (CPT) guidelines for information management and for implementing safety standards in the laboratories.

The third presentation of the session (CINF 75), by Brad Fahlman, was entitled “Chemistry in Context: how do we most effectively engage the non-science majors.” This focused on the popular ACS textbook *Chemistry in Context*, which was developed in 1993. It has been used since its inception to present chemistry fundamentals to students and has a conceptual framework at its core. Brad discussed the theme of each edition of the text since 1993 and showed how the cover art of each text carries an image of a specific element from the periodic table and its significance in the real world. Since its introduction, the text has evolved to meet the needs of students. Students can access online homework, videos, and examples of applications of various chemistry concepts contained in the text. Brad highlighted the need to capture the interest of non-science majors in chemistry by providing opportunities for students to engage with the content of the text through interactive tools. Each chapter has an accompanying video and interactive simulations and activities on the subject of a global issue that puts the chemistry in context for learners.

The fourth paper was presented by Anita Tseng and was entitled “Facts versus foundation – the evolution of learning needs for contemporary science students” (CINF 76). In this paper, Anita presented a theoretical perspective on the correctness of the scientific information available via social media and various other online resources and the ability of students to evaluate the scientific facts available through such media. Students are vulnerable to misunderstanding and misinterpreting scientific content because they do not check the veracity of online information, accepting these sources as inherently reliable.

Anita closed her presentation with a call for a greater emphasis on developing the evaluation skills of students. To develop evaluation skills, students need content knowledge to balance their understanding of science and of



information presented through various media. She suggested that students' own scientific reasoning skills could be established by giving them opportunities to identify and analyze errors and flaws in scientific experimentation, including errors in textbooks, and by addressing the concept of scientific bias during instruction. She specifically identified four key skills that need to be developed among students to evaluate content presented through various sources: data interpretation and analysis skills, understanding the nature of science and its social context, critical reading skills, and questioning and critiquing errors or anomalies.

The fifth paper, "Alchemy to chemical science: the advance of texts for over 5,000 years in China from the oracle bones to e-learning resources and methodologies" (CINF 78), was presented by Ron Rusay and Ben Koo. Their presentation started with the oldest writings in China (about 5000 years ago), which were bones and shells that contained symbolic inscriptions. The bones were commonly used for medication until the 19<sup>th</sup> century, when Wang Yirong realized that they were ancient writings. Their preservation has helped to chronicle the journey of science in China from ancient times.

Rusay and Koo highlighted contemporary use of textbooks in China, which are mainly used for exam preparation. They described the intricacies of textbook publishing in China; until 1992, all textbooks were produced by a single publisher, directed by the Ministry of Education and adopted by the national curriculum. Today, there are multiple approved publishers involved in publishing curricula for higher education. In their closing statement, the authors described progressive teachers who are the change agents for modern education in China, challenging the quality of existing textbooks and resources and adapting quality Open Educational Resource (OER) materials, such as LibreTexts, for use in their classrooms. The use of LibreTexts and ABC (Application Oriented, Business Orientation, and Context Specific Courses) curriculum is gaining momentum in Chinese education, due to the efforts of a few progressive educators.

The last paper was on "Instructor support is key to adoption of open educational systems: How LibreTexts is growing to meet the needs of instructors" (CINF 79), and it was presented by Joshua Halpern. This paper focused on the rising costs of the textbooks, open source electronic materials from LibreTexts as a viable alternative to expensive textbooks, and the need to rise to the challenge of providing instructor-tailored textbooks for students that fit their classroom needs.

Josh showed charts correlating the increase in student enrollment with an increase in the cost of textbooks for college, especially for STEM majors. He made a point that major reasons for instructors' textbook preference included the time involved in preparing a course and their universities' increased expectations for teaching, research, and service. He then pointed out that traditional textbooks seem to be losing their appeal for both faculty and students, based on the increase in demand for the Open Educational Resources (OERs). OERs have several advantages over expensive textbooks, including ease of availability, flexible content development for specific instructional needs, and versatility to include different interactive activities, such as videos, animations and simulations.

### **Session 3**

The final session was moderated by Bob Belford and started with a presentation on an OER by Delmar Larsen, "Developing and Assessing Effective Cyberlearning with the LibreText Libraries", <http://libretexts.org/> (CINF 96). Delmar described the information architecture of the LibreText hyperlibrary while also providing data on its usage (>50 million visits last year) and various ways faculty can adopt it for their classrooms. He also presented some use-case examples of schools that have used LibreText and assessment data for some classes that adopted it as their sole textbook.

This was followed by Mark Bishop of Chiral Publishing, presenting, "Textbooks in Transition: It's all About Options", <http://preparatorychemistry.com/> (CINF 97). Mark has been a pioneer in the field of e-textbooks, and he presented multiple business scenarios for self-publishing. He also gave an overview of many of the tools that he has used to develop multimedia content throughout the years.

Brett McCollum presented the third paper, entitled "Democratization of Learning and Re-Embedding the Textbook" (CINF 98). Brett used LibreText outside of class for reading and notetaking, and then started class with



an Academic Reading Circle (ARC), followed by clicker activities and ending with a short lecture.

The fourth paper, “MindTap General Chemistry: Integrating Scientific Exploration and Problem-Solving within a Textbook” (CINF 99) by Bill Vining, gave an assessment of student study habits in the digital age and problems with student usage of printed textbooks to gain conceptual understanding. His work on MindTap (<http://www.cengage.com/mindtap>), an advanced commercial e-textbook, directly connected textbook concepts with graded problem-solving activities through interactive reading.

John W. Moore followed this with his talk, “What Should a Textbook for 21<sup>st</sup> Century Students Look Like?” (CINF 100). He started with ideas that were introduced with the [FIPSE Lecture Series](#) of the late 1980s, which examined technology influence on curriculum, and then focused on student learning in Digitally Enhanced Active-Learning (DEAL) systems. He also presented data indicating student preference for flipped classroom activities accompanied by a printed textbook over the traditional lecture, work which has been submitted to the *Journal of Chemical Education* for publication.

The next paper, “High School Students and Critical Reading of Inaccurate Science Claims on the Internet” by Anita S. Tseng (CINF 101), dealt with information literacy issues in today’s classroom. Students pull information that may or may not be valid from online sources. Anita’s work indicates that, in addition to learning scientific “facts”, students need to learn the characteristics of appropriate scientific reasoning, in contrast to that of persuasive media.

The final talk, by Peter F. Rusch, was entitled “Textbooks and the SI base units: a challenge for authors and editors” (CINF 102), and it dealt with the need to update textbooks in 2018, when the definitions of the SI base units will change. This paper included a history of the SI base units, a description of the current definitions, and their 2018 revisions, which are based on physical constants that are considered to be invariants of nature.

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## Text-mining and Natural Language Processing for Chemical Information: From Documents to Knowledge

This was a well-attended session at the recent national meeting in San Francisco. The full-day session, sponsored by the Division of Chemical Information, was attended by fifty to sixty people throughout the day and saw presentations on a diverse and interesting range of topics in text mining.

Several themes were consistently mentioned in the talks. User interfaces were shown and discussed. Certainly, ease of use was a major consideration for applications. Extracting data from PDFs continues to be an issue because document formats are often not maintained. In particular, table extraction was a consistent issue, with different techniques being adopted to extract relevant information keyed to specific column and row headers. When extracting chemical compounds, structure errors must be identified and corrected. Sometimes these errors may be found through name-to-structure conversions. Image-to-structure conversions are being employed more frequently, but efforts are confounded by the presence of Markush structures and R-group representations. These formats are especially problematic in patents and are very much an active area of research.

The session started with Jeffrey Nauss from Linguamatics giving an overview of text mining in “From documents to knowledge” (CINF 104). By building queries and including natural language processing, one is able to progress from the simple identification of interesting documents through the pin-pointing of precise information of interest, to finally linking information within and between documents. The presentation helped set the mood and perspective for subsequent talks.

Next, Evan Bolton from the National Center for Biotechnology Information (NCBI) presented “Improving chemical names matching for verification, rating, and validation of PubChem compound records” (CINF 105). Using PubMed as the corpus and PubChem as a dictionary or “name corpus,” he showed that only a small percentage of chemical compounds mentioned actually were tested for bioactivity. A variety of techniques was employed to improve the link between PubMed and PubChem, offering an opportunity to enhance searches by considering word frequency and context. The group at NCBI also presented PubTator, a web-based tool for manual literature curation which uses text-mining and has a RESTful API to programmatically access annotations. PubTator supports semantic search of genes, diseases, and chemicals.

Roger Sayle of NextMove Software delivered “Advanced grammars for state-of-the-art Named Entity Recognition (NER)” (CINF 106). The text mining engine, LeadMine, is used to extract important terms from documents with great efficiency. Dictionaries are employed, but advanced users specify regular expressions to identify unique entities. Combinations of grammars and Hearst patterns allow for a potentially infinite number of terms. The techniques can be used in areas like precision medicine to quickly search a variety of gene variations.

Alexander Tropsha from the University of North Carolina presented “Mining protein interactions from biomedical literature using semantic similarity” (CINF 107). Using many data analysis techniques from QSAR and drug design, descriptors of semantic context were used to generate vectors in multi-dimensional space. A time course study of the vectors showed that term usage and context will vary over twenty years but also will converge to steady-state context as described by the vectors. This approach could be used to account for variations in terminology for corpora spanning several decades.

The problem of extracting bioactivity data from patents was very nicely explained by Daniel Lowe from NextMove Software in “Automatic extraction of bioactivity data from patents” (CINF 108). Using the XML format of U.S. patents, data were extracted from tables and compound structures. When ChemDraw sketches were provided, they were used to correct structural errors and to interpret labels. Text-mining was used to resolve compound identifiers in various formats. A Naïve Bayes classifier was trained and used to identify targets or assays associated with the extracted data.

Using text mining to help monitor chemical toxicities for the EPA was the topic of Nancy Baker’s presentation “Text-mining strategies to support computational research in chemical toxicity” (CINF 109). In a very nice overview of text mining, a key point made was that in order to use text mining effectively, one must know the question; in other words, one must know precisely for what one searches. In their work at the EPA, researchers use MeSH headings in MEDLINE for rapid screening. More intense text-mining is used to determine the inference.

A user-friendly data visualization was very useful for successful searches.

A very interesting talk was presented by Sabine Kuhn (CAS) and John Tinsley (Iconic Translation Machines.) in “Making the old new again: modern technology provides access to historical chemical information” (CINF 125). After converting to PDF the entirety of *Chemisches Zentralblatt*, a German-language science abstract collection from 1830 to 1969 containing 3 million abstracts, techniques were applied to translate over 800,000 documents and make them available through a SciFinder add-on product called ChemZent. Trends over time were observed for spelling and abbreviations. Challenges included optical character recognition and abstract formats. The work will be useful for the study of the history of chemistry.

The SciFinder theme continued, with Philippe Ayala presenting “Evolution of SciFinder to meet the changing needs for scientific information” (CINF 126). Among the trends observed over the years has been an increasing requirement for precision. However, the key point for both precision and recall is relevance. Relevancy can vary from user to user and query to query. User interaction with results through facets allows them to focus better on relevant results. Extensive user testing is used to evaluate recall and precision and for testing relevancy algorithms.

Jeff White from the Royal Society of Chemistry presented “Trends and relations” describing an article recommender. Log file processing from previous searches was considered to recommend additional articles. Four different methods were developed and tested. Further work is on-going to refine the methods.

The presentation “ChemAnalyzer: a text analytics platform for chemical surveillance” (CINF 128) by Sanket Gaurav (University of Illinois – Chicago) was next. ChemAnalyzer is a tool to extract data from chemical incident reports. PubChem was used to develop chemical ontologies and keyword tables. Natural language processing (NLP) and machine learning were used to extract information in five key areas: chemical, organization, amount of spill, location, and number of people affected. A clean user interface allows users to quickly search large reports and cross-reference the information.

Josef Eiblmaier from InfoChem described functions for patent searches in “Addition of chemical search capabilities to PATENTSCOPE: turning a full-text search system into a chemistry database” (CINF 129). Chemical images were converted to structures and InChIKeys with several conversion programs. Chemical annotation was accomplished using InfoChem’s ICANNOTATOR. InChIKeys were added to the patent database to search via Solr for exact structures. A chemical drawing interface was incorporated to do structure search. Results from one document are promising, but a more thorough survey is needed.

The final talk of the day was presented by Stuart Chalk (University of North Florida) who collaborated with Springer Materials in “ChemExtractor: enhanced rule-based capture and identification of PDF based property data” (CINF 130). ChemExtractor can extract data from the Landholt-Börnstein database. Using OCR and regular expressions, tabular data were extracted from the database documents. The regular expressions were used to capture both chemical compounds and an entire row of data from tables. The data is then stored in a MySQL database for easy retrieval.

The session was well-received and provided a broad view of how text-mining can be used. Work is still needed, and, as a result, we will have more to look forward to in the future.

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## The Write Thing to Do: Ethical Considerations in Authorship and the Assignment of Credit

The ACS Committee on Ethics (ETHX) partnered with the Division of Chemical Information (CINF) to present “The Write Thing to Do: Ethical Considerations in Authorship and the Assignment of Credit.” This half-day symposium, organized by Judith Currano of the University of Pennsylvania and Pam Mabrouk of Northeastern University, aimed to highlight ethical issues that affect authors. The organizers were pleasantly surprised when the ACS Committee on Patents and Related Matters expressed great interest in the topic of the symposium and quickly broadened the scope to include two papers that expanded on the ethical considerations put forth for authors, placing them in the context of patent inventorship.

Lida Anestidou (National Academy of Sciences) was to have begun the session with a presentation entitled, “Authorship issues in academia of low and lower middle income countries” (CINF 88); unfortunately, an unanticipated business trip meant that she was unable to present her paper. She did, however, send slides and notes to the session organizers, who were able to present an abridged version of the talk. Since 2011, the U.S. National Academies, including the National Academies of Science, Engineering, and Medicine, have sponsored a program entitled “Educational Institutes in Responsible Science.” The Educational Institutes incorporate active learning techniques to teach responsible conduct of research (RCR) in the Middle East, Northern Africa, South Asia, and Southeast Asia. Many of the countries in these regions lack formal definitions or regulations surrounding the responsible conduct of research, and the absence of ethical standards makes it extremely difficult to navigate the morass that is authorship and the assignment of credit. The goal of the National Academies’ program is to create a network of researchers who can teach RCR in an interactive way and who consider the principles taught to be central to the professional conduct of science. To date, these programs have reached almost five hundred participants and have awarded fifty-one grants for further work.

Heather Tierney (American Chemical Society) followed this talk with her presentation, “What constitutes authorship? Guidance from the Committee on Publication Ethics (COPE)” (CINF 89). COPE was established in 1997 as a small forum of medical editors to discuss ethical issues. It has since expanded to include physical and life scientists, but it is not and never has been an adjudicating body. On its Web site, COPE includes guidelines and discussion documents on many subjects in the realm of publication ethics, including one entitled “What constitutes authorship?” The definition of an “author” varies from community to community, but it usually involves being the creator of an idea or the individual who writes the idea in tangible form. The medical community has an extremely detailed definition with four key requirements: contribution to the design or data analysis of the study, writing the paper, approving the final version, and maintaining accountability for the final piece. The physical sciences, on the other hand, require only that one “make a significant contribution” to the science. Heather presented four basic problems surrounding authorship: individuals who are not authors of papers believe that they should be listed as such; individuals who have not made a significant contribution are granted “gift authorship;” authors dispute the ordering of authors on a paper; and authors wish to be removed from authorship of a paper for a variety of reasons. COPE stresses that editors should not be adjudicators and that authors in conflict should work with one another and their institutions to resolve the issue.

Now that some of the basic ethical considerations for authorship had been highlighted, Judith Currano (University of Pennsylvania) discussed some of the problems that students have understanding these ethical norms in her paper, “Teaching students where credit is due: Attribution 101 for the mash-up generation” (CINF 90). She began her presentation with a picture of the world of today’s students, in which musical variations, mash-ups, and shares and retweets of anything that one finds interesting are the norm. This forms a stark contrast to the world of scholarly communication, in which the reuse of information is governed by strict rules, and students do not always understand what they need to do to be ethical authors. In particular, Judith noted three cases of the reuse of published information that frequently cause students problems: the appropriate reuse of written material, the reuse of previously-published images, and the reuse of material that one has written one’s self. At the end of the talk, she suggested two lesson plans for teaching correct attribution to undergraduate students and graduate students. At the undergraduate level, she recommended teaching why, what, and how to document previously published work, and at the graduate level, she recommended going in detail into the duties and responsibilities of an author of a scientific journal article, indicating the most common ethical pitfalls and holding group discussions about how to surmount them.

Following on the theme of authorship and undergraduate and graduate education, Amy Andes, an undergraduate from Northeastern University, presented a paper that she had coauthored with Aneri Pattani and Pam Mabrouk, entitled "Influence of Graduate Students on Authorship Decision-making in Undergraduate Research Partnerships" (CINF 91). Research on the subject of what undergraduates know about authorship has been sparse, and the authors sought to remedy this. In order to do this, they instituted a study of undergraduate students performing research and their faculty and graduate student mentors. They learned that graduate students actually have a great deal of influence when mentoring the undergraduates, so, they expanded the study, to examine the relationships between all three groups in responsible authorship practices. In particular, they sought to learn what responsible conduct of research (RCR) training each group received, what influence each group had on the authorship of a paper, and what possible barriers exist and must be removed before they could put responsible authorship into practice. Through the course of interviews with each party in the triad, they learned that there was little consistency in definitions of authorship and decision trees for who was an author; and RCR training, while desirable, was uneven, to say the least. The authors recommended having authorship checklists for everyone, as well as train-the-trainer sessions in RCR for the graduate student mentors.

Jeffrey Seeman (University of Richmond) presented the results of a fascinating survey of academic chemists in his paper, "Authorship issues and conflict in the U.S. academic chemical community" (CINF 92). He began his talk by discussing the claim of plagiarism that Corey made against Woodward in the 2000s, stating that he, and not Woodward, had originated the Woodward-Hoffmann rules. This led to a discussion of the importance of a good and complete literature search, with the author's opinion being that repeated failure to perform one constitutes misconduct. Jeffrey's survey gathered about six hundred responses from American academic chemists on questions involving authorship and the assignment of credit to others, and it unveiled some rather surprising trends. More chemists were willing to give credit to their own students than to individuals outside of their research groups, despite the fact that the "rules" and norms of responsible authorship state no context dependency. The survey results reveal that chemists would give their own students coauthorship in situations where they would only grant acknowledgement to a student from a different lab. The older the chemist, the more likely he or she was to assign credit to someone else, and individuals were more likely to give credit based on their feelings or on things that they learned from other people.

Cory Craig (University of California, Davis) presented a paper with a slightly different spin. Rather than focusing on the rules involving the assignment of credit, she talked about "ORCID iDs and project credit: contributor badges and getting credit for your work" (CINF 93). She began by explaining what an ORCID is and what one can do with it. The ORCID is a unique author identifier that "unifies the 'beyond the pdf' aspects of your scholarship," allowing individuals to direct others to their complete body of publications through such diverse means as Twitter, an e-mail signature file, and from a publication itself. Individuals establish an ORCID profile at [www.orcid.org](http://www.orcid.org) and then can apply their ORCID to all of their publications. She then introduced CRediT (Contributor Roles Taxonomy), a project of CASRAI (Consortia Advancing Standards in Research Administration Information). Under CRediT, there are fourteen different roles that an individual can have in a project, and each has a badge assigned to it. Authors can apply a badge next to their name and ORCID on a journal article so that readers can know the exact contribution of each author. Currently, *Cell* is using CRediT. Cory closed with a reminder to all authors to hold discussions about the expected contributions of each researcher prior to the commencement of writing.

At this point, the symposium shifted in focus from authorship to inventorship. Xavier Pillai (Leydig Voit Mayer) spoke about the importance of accurately assigning inventorship to a patent in his talk, "Do not lose your invention by improperly naming inventors on the patent" (CINF 94). If all inventors are not listed on a patent, any "undocumented" inventor could grant permission to another body to use the invention. Since one inventor cannot sue another over patent rights, the documented inventors will have little legal recourse in such a situation. Xavier presented an interesting case study of Burroughs Wellcome vs. Barr Labs and Novopharm. In this case, six patents on areas related to the use of AZT for HIV treatment were challenged. Burroughs Wellcome had sent some substances to NIH for testing without telling the NIH scientists what they were. As soon as they had the NIH test results, they filed an application for a patent. According to the U.S. Code, an inventor is defined as the one who conceived the invention and completed the mental picture of it. It is not necessary to complete the work in order to be the inventor, provided one has a complete mental picture of the invention. The defendants



held that the NIH employees should have been inventors on the patent and therefore had the right to license the technology to others, but the courts ultimately decided that, since the first draft of the patent had been written by Burroughs Wellcome before any of the NIH scientists began work on the project, the NIH scientists did not qualify for inventorship.

The second inventor-related presentation, and the final talk of the session, was “Hey – You stole my invention! Avoiding ethical pitfalls in determining inventorship, authorship, and honoring Non-Disclosure Agreement (NDA) obligations” (CINF 95), delivered by Justin Krieger (Kilpatrick Townsend). Justin began his talk with a comparison of authorship to inventorship, building on points made by previous speakers. He then presented an interesting case study, a mechanism for performing an “anti-gravity illusion” that was patented by Michael Jackson, Michael L. Bush, and Dennis Tompkins for use in one of Jackson’s music videos. After a rigorous examination of the requirements of inventorship, which involve both conceiving the idea and developing a method of putting it into practice, Justin determined that Jackson should not have qualified for inventorship unless his contribution to the project went beyond merely identifying the problem: “Hey. Wouldn’t it be cool if I could lean way over and then right myself without falling!” This led to a discussion of joint inventorship and what individuals must contribute in order to be considered joint inventors. Justin closed his presentation with a discussion of non-disclosure agreements, again returning to Michael Jackson’s “anti-gravity” stunt. He presented a hypothetical situation in which Jackson enters a NDA with Velcro, during which he asks them to create closures for the boots that he was to wear during the stunt. During the course of discussions between the two parties, Jackson discloses the details of the trick and the two parties discuss the desired properties of the boot closures. Justin’s talk closed with a discussion of what patenting rights Michael Jackson and Velcro would have over their respective technologies as a result of the non-disclosure agreement that they signed.

Many of the speakers were able to remain for the entire session, and the presiders spent the last slot of the session moderating a lively question-and-answer forum. Audience members asked questions of individual speakers and of one another, and many volunteered information from their own experience. This was a wonderful close to the afternoon, especially as more questions arose during the various presentations than their presenters had time to answer. It is to be hoped that the audience (and speakers) left the symposium with a high level of knowledge about ethical issues in authorship, and, even if they did not learn the answers to all of the questions, at least they had an extensive collection of questions to ask.

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# Committee Reports

## Report from Council to the Division of Chemical Information 253<sup>rd</sup> ACS National Meeting San Francisco, California April 2 – 6, 2017

The following summary is adapted from selected talking points for Councilors provided by the ACS Office of the Secretary. Consult the full agenda book for the [ACS Council \(https://www.acs.org/content/dam/acsorg/about/governance/councilors/council-agenda-4-17.pdf\)](https://www.acs.org/content/dam/acsorg/about/governance/councilors/council-agenda-4-17.pdf) meeting for more details on these and other items of Council business at the 253<sup>rd</sup> ACS National Meeting

### *Actions of the Council*

#### **Election Results**

##### *Candidates for President-Elect, 2018*

- The Committee on Nominations and Elections presented to the Council the following nominees for selection as candidates for President-Elect, 2018:

Nominee	1 <sup>st</sup> Round	2 <sup>nd</sup> Round	3 <sup>rd</sup> Round
*Bonnie A. Charpentier	200	210	242
Mark D. Frishberg	73	80	-
Anne M. Gaffney	26	-	-
*Willie E. May	132	141	158

- 431 valid electronic ballots were cast, with 216 being the majority. The results of the first preference vote totals are shown in the 1st round column. No nominee attained a majority. Following the procedures approved by Council, second-preference votes were distributed in two subsequent rounds. Bonnie A. Charpentier and Willie E. May were declared elected as candidates. These two candidates, along with any candidates selected via petitions, will stand for election in the fall national election.

##### *Candidates for Districts III and VI*

- The Committee on Nominations and Elections announced the results of the election held prior to the San Francisco meeting to select candidates from the list of nominees for directors from District III and District VI on the Board of Directors for the term 2018-2020. By Internet preferential ballot, the councilors from these districts selected Alan B. Cooper and Teri Quinn Gray as District III candidates; and Rita R. Boggs and Paul W. Jagodzinski as District VI candidates. Ballots will be distributed on or before October 1 to all ACS members in District III and District VI for election of a director from each district.

##### *Candidates for Directors-at-Large*

- The Committee on Nominations and Elections announced the selection of the following candidates for directors-at-large for 2018-2020 terms: Kenneth P. Fivizzani, Wayne E. Jones, Bonnie A. Lawlor, and Barbara A. Sawrey. The election of two directors-at-large from among those candidates and any selected via petition will be conducted in the fall. Ballots will be distributed to the council on or before October 1, 2017.

#### **Other Council Actions**

##### *Amendments to the ACS Bylaws*

- A recommendation by the Council Policy Committee to approve the Petition for the Removal of Officers and Councilors (Bylaw III, Sec. 1, i; Bylaw VII, Sec. 1, c; Bylaw VIII, Sec. 4, d) failed. The council had voted to approve the related Procedures for Removal of a Councilor or Alternate Councilor, contingent upon approval

of the Petition for the Removal of Officers and Councilors. As the petition subsequently failed, given the interdependence of the petition and related procedures, the procedures will not take effect.

- The council approved the Petition on the Rights of Affiliates (Bylaw II, Sec. 1, a, 2, a, 3, b, (3) and (4)).

#### *2018 Member Dues*

- The council voted on the recommendation of the Committee on Budget and Finance to set the member dues for 2018 at the fully escalated rate of \$171. This rate is established pursuant to an inflation-adjustment formula in the ACS Constitution and Bylaws.

#### *Distribution Formula for Division Funding*

On the recommendation of the Committee on Divisional Activities, the council approved a formula for allocating dues funds to divisions, effective with allocations for 2017 division performance. The allocation formula is based on these categories of division metrics and activities:

Innovative Project Grants:	10%
Base:	15%
Per Member:	12.5%
Number of Attendees at Oral Sessions:	31.25%
Number of Division Members at National Meetings:	15.625%
Number of Division Posters Presented at National Meetings:	15.625%

#### *Continuation of Committees*

- The council approved the recommendation of the Committee on Committees that the Committee on Project SEED be continued; and that the committees on Chemists with Disabilities, on Public Relations and Communications, and on Women Chemists be continued contingent on approval of the Board of Directors.

### **Special Discussion**

The council conducted a special discussion, “ACS Yesterday and Today: Paving the Way to Tomorrow,” to gather input for the Joint Board-CPC Task Force on Governance Design. Forty councilors approached the floor microphones to share observations, comments, and suggestions to assist the task force in identifying opportunities and issues for governance improvement. The task force offered three questions to guide the discussion: What should the society and its governance do differently to achieve its objects? If you could change one thing about ACS governance, what would it be? What should the task force leave “as is”? A poll conducted at the conclusion of the discussion revealed that 57% (222) of the councilors disagreed that the current governance structure, processes and procedures are already optimal to achieving the objects of ACS in the 21<sup>st</sup> century, 16% (54) agreed, and 27% (104) needed more information. Three-hundred and six (84%) said they would be willing to provide additional input and feedback to the task force. They will be contacted by the task force in the coming weeks.

### **Highlights from Committee Reports**

#### *Nominations and Elections*

The Committee on Nominations and Elections solicits councilors’ suggestions of qualified individuals for the offices of president-elect and directors. Suggestions may be sent to [nomelect@acs.org](mailto:nomelect@acs.org).

#### *Budget and Finance*

In 2016, ACS generated a net from operations of \$23.8 million, which was \$7.2 million higher than 2015. Total revenues were \$526.8 million, increasing 2.9% (\$15 million) over 2015. Expenses ended the year at \$503 million, which was 1.6% (\$7.8 million) higher than last year. This was attributed to a continued emphasis on expense management across the organization. The society’s financial position strengthened in 2016, with unrestricted net assets, or reserves, increasing from \$163.3 million at December 31, 2015, to \$206.5 million at year-end 2016.

Additional information can be found at [www.acs.org](http://www.acs.org). At the bottom, click “About ACS”, and then click “ACS Financial Information.” There, you will find several years of the society’s audited financial statements and IRS 990 filings.

### Membership

As of December 31, 2016, the ACS membership was 156,129, which is 0.5% less than on the same date in 2015. The number of new members who joined in 2016 is 23,700. The society's overall retention rate is 83.5%. The Committee on Membership Affairs also reported that the number of international members has increased to 27,388, exceeding the committee's target by 5%. Retention of graduate students increased by 2% to 76.2%. ACS has recently hired a new director for membership, Kate Fryer, previously with the Society for Neuroscience.

### Meeting Attendance

As of Tuesday, April 4, the San Francisco meeting attendance was as follows:

Attendees	9,797
Students	6,914
Exhibitors	1,198
Expo Only	475
Guest	466
<b>Total</b>	<b>18,850</b>

Total attendance figures for all spring national meetings since 2004 are 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)
2017	San Francisco, CA	18,850 (as of Tuesday evening, April 4, 2017)

The last National ACS meeting in San Francisco was held in the fall of 2014, and attendance at that meeting totaled 15,761. San Francisco has had the highest attendance for ACS National Meetings, at least since 1997 (1997: 18,042; 2010: 18,067; 2000: 18,336; 2017, 18,850).

### Highlights on CAS and ACS Publications Activities from various reports

ACS Symposium Series Books are planned for two topics which may be of interest to CINF members. First, a book will compile the results of activities addressing employment of chemists and will be entitled *The Present Employment Status of Chemical Professionals in the United States and Actions Needed for Its Improvement*. Material included will be activities of the Presidential Task force on Employment in the Chemical Sciences, ACS members who e-mailed comments and ideas, bloggers who wrote on employment in the chemical sciences and spoke to the Task Force, and so on. Second, a book based on the symposium "Diversity – Quantification – Success?" will include contributions from its speakers and other contributors. It will focus on data-driven analyses of the status of women and underrepresented minorities at all levels in STEM disciplines, including chemistry and chemical engineering.

Both CAS and ACS Publications had very strong years in 2016. CAS launched its rebranding, introducing new graphics and an added emphasis on delivering solutions, rather than simply information. CAS launched new products such as MethodsNow and *Chemisches Zentralblatt*. The roll-out of SciFinder<sup>n</sup> also occurred before year-end 2016.

ACS Publications launched *ACS Sensors*; *ACS Energy Letters*; *ACS Omega*, a global, open-access journal; and *ACS Earth and Space Chemistry*. ACS also announced its intent to explore ChemRxiv, a chemical sciences preprint server. *C&EN Global Enterprise*, a new *C&EN* electronic product for ACS Publications' institutional subscribers, went live with the first January 2017 issue.

CAS registered a record number of new substances, 21,542,278 in total, during 2016, bringing total substance registrations to over 125 million. More than 1.36 million indexed records were added to the CA/CAPLUS family of databases. Patents continue to grow as a percentage of the total indexed records, now attributing greater than 1/3 of all records indexed by CAS scientists in 2015. Nearly 1.7 million new single-step reactions were added to the CAS reaction collection, with reactions drawn from more than 100,000 journal and patent documents.

### **Other Highlights**

ACS Webinars produced 44 weekly webinars for members and prospective members in 2016. The live broadcasts drew more than 50,000 registrants and 25,000 participant sites combined, with an estimated 10% of sites having multiple individual participants. 22 of the weekly webinars were delivered as part of two industry series focused on drug discovery and advanced materials. Notably, over 2/3 (69%) of participants surveyed stated that they are more likely to join or renew their ACS membership as a result of ACS Webinars. In addition, the overall satisfaction rate for weekly webinars was over 90%.

The Education Division and Web Strategy and Operations, in collaboration with the ACS Committee on Chemical Safety, launched a new website with a rich collection of methods and tools for assessing hazards in research laboratories at <http://www.acs.org/hazardassessment>. The site is based on *Identifying and Evaluating Hazards in Research Laboratories*, a resource created in response to a recommendation by the U.S. Chemical Safety Board for ACS to develop guidance on assessing and controlling hazards in research laboratories.

## **Actions of the Board of Directors**

### **The Board's Executive Session**

The ACS Board of Directors met March 31 – April 1, 2017, considered a number of key strategic issues, and responded with several actions.

### **The Board's Committees**

The Board of Directors received and discussed reports from its committees on Executive Compensation, Strategic Planning, Corporation Associates, Professional and Member Relations, and the Joint Board-Council Committee on Publications.

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 several ACS journals.

On the recommendation of the Committee on Professional and Member Relations, the board approved screened lists for the 2018 Priestley Medal and the ACS Award for Volunteer Service. From these lists, the board will select the recipients of these awards.

### **The Executive Director/CEO Report**

The board received a report from the Executive Director and CEO on issues relating to the Information Technology area, the Executive Leadership Team retreat, ACS financials, and Board Regulations on the Governing Board for Publishing. His direct reports updated the board on the activities of the Membership Division, Chemical Abstracts Service (CAS), and the ACS Publications Division.



## Other Society Business

The board heard reports from the Presidential Succession on their current and planned activities for 2017.

As part of its ongoing commitment to consider the most important strategic issues facing the society, the board held a discussion and provided input to its Strategic Planning Committee on context setting and change drivers to be addressed during the strategic planning process.

The board is developing a statement based on the society's core value of diversity and inclusion in response to the repeal of the North Carolina law known as House Bill 2 ('bathroom bill') and similar proposed legislation in Texas. It is assembling a representative group of stakeholders to advise it on actions relating to the location of society meetings.

## Board Retreat

The board held a discussion on timing and topics of a possible facilitated retreat for all board members during 2017. The board regularly holds these retreats to consider strategic issues in depth or for ongoing development.

## Board Resolution

The board passed a resolution expressing appreciation to Denise L. Creech for her 27 years of service in the Membership and Scientific Advancement Division, which she led as Director for nearly 14 years.

### *The Board's Regular (Open) Session*

The board held a well-attended open session which featured two "TED type" presentations. Dr. Joseph M. DeSimone, CEO and co-founder of Carbon, Inc.; Chancellor's Eminent Professor of Chemistry, UNC-Chapel Hill; and William R. Kenan, Jr., Distinguished Professor of Chemical Engineering at NC State University and of Chemistry at UNC, spoke on "Future Fabricated with Light: The Launching of Carbon."

Anne Milasincic Andrews, Professor of Psychiatry and Chemistry & Biochemistry; Semel Institute for Neuroscience & Human Behavior, Hatos Center for Neuropharmacology, and California NanoSystems Institute; University of California, Los Angeles, spoke on how "The Brain is More Than a Computer."

Prior to the presentations, 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](mailto:secretary@acs.org).

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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!

## Book Reviews

**Science and the Law: How the Communication of Science Affects Policy Development in the Environment, Food, Health, and Transport Sectors;** Town W. G., Currano, J. N., Eds; ACS Symposium Series 1207; American Chemical Society: Washington, 2015. 199 p. + x, ISBN 9780841231078 Hardcover \$150.

This book is the second in the series. The first book (reviewed by Pamela Scott) includes material presented at a symposium at the fall 2012 ACS meeting in Philadelphia (1); the current book is based on a second symposium held at the fall 2014 ACS meeting in San Francisco. Both remain timely, especially given the continuing political developments in these areas. Of the ten chapters, six are by authors in the United Kingdom.

In the first chapter, co-editor Bill Town outlines the topics to be covered in the book and describes how the scope is expanded beyond that of the first book, before recounting his extensive experience with these subjects. He also describes several developments on the ever-important topic of communicating science and scientific research to various audiences. Scientific advice has become increasingly important and is widely requested; simultaneously, it is more contested and challenged than ever. (For additional discussion of this topic see “The War on Science” (2).) A number of subjects have become “hot” topics: climate change (and Climate Gate), cybersecurity, poverty, pandemics, food technology, fracking, etc, and many federal organizations require scientific information to inform policy in many areas, including federal budget policy (often controversial), energy, climate change, and stem cell research. In addition, the general population assimilates scientific information and forms its own views, which often include misconceptions and sometimes outright hostility. The introductory chapter also discusses science communication channels, including science communication cycles and the role of social media.

In Chapter 2 (Impact of the Communication of Science on Government Policy – The Perspective from the United Kingdom), Neil Ravenhill discusses the history of the topic, from the Age of Enlightenment to the present, and highlights our increasing dependence on evidence and critical thinking (whether adopted or ignored). He presents three cases studies, the Cancer Drug Fund, Meningitis B vaccine, and illegal drug policy, and stresses the role of the informed public.

David Richardson describes informed policies for health care and nutrition in Chapter 3 (Consumer Communication of Nutrition Science and Impact on Public Health), another hot topic. He discusses WHO and EC policies, including three examples: (1) folic acid/folate for improved pregnancy nutrition, (2) calcium and vitamin D influence on bone health and osteoporosis, and the effect on the outcome of falling, and (3) benefits of omega-3 fatty acids on cardio health.

Prevention of smoking in the United States forms the basis for Chapter 4 (The Role of Regulatory Science in reducing the Public Health Impact of Tobacco Use), written, surprisingly, by authors from British American Tobacco, U.K. The FDA established the Center for Tobacco Products (CTP), which funds research on regulatory policies. The authors present risk continua of the various products (including e-cigarettes) and list harmful components of tobacco and tobacco smoke, including toxicity data. They also describe *in vitro* toxicity testing, clinical studies, and modeling.

Chapter 5 (FDA’s Communication of Nicotine Science) also discusses tobacco. The chief information source on this subject is the CTP; however, communication of relevant data and information is directed towards federal regulatory processors rather than the general public, especially on the FDA website. E-cigarettes and smokeless products are seldom discussed. The FDA uses other media to fill these gaps. The authors also discuss addiction vs. toxicity of nicotine and provide a risk continuum and harm reduction.

Chapter 6 (Communicating Controversial Science: The Case of Tobacco Harm Reduction and the Ethics of Blanket Censorship) is the third and final chapter of the book that addresses tobacco. The FDA has regulated

tobacco since 2009 and has partnered with the NIH, which yields more funding for research. The authors present levels of hazard from the various components of tobacco and tobacco products and the risk/hazard continua for the various products. Tobacco companies are developing less hazardous products, but several journals ban publication of results from these companies, a situation that prompts the authors to discuss the ethics of censorship.

Indirect land use change, referring to deforestation and land use expansion, is the subject of Chapter 7 (Science, Value, and the Political Framing of Indirect Land Use Change (ILUC)). The controversial driving force of increasing crop prices complicates the issue. Arguments between stakeholders and scientists occur at all stages: advisory reports, rule-making documentation, and public comments. The end results are not straightforward.

Chapter 8 (The importance of Exposure Dose in communicating the Ecotoxicity of Engineered Nanomaterials) addresses policy formation regarding engineered nanomaterials. The authors use the case of the use of nanoparticles of titanium dioxide to illustrate the control of these materials used by consumers and in disposal, and they discuss the adequacy of the ecotoxicity literature to help formulate policy. Questions remain.

Chapter 9 (Risk Analysis Approaches for Establishing Maximum levels of Essential Nutrients) in Fortified Foods and Food (Dietary) Supplements covers risk analysis for safe levels of essential nutrients in food. The authors determine the risks of too little or too much of these nutrients, their maximum tolerance and non-adverse effect levels (including RDAs), and the nutrient levels in conventional foods. The derived models can be used to protect both adults and children.

The U.S. President's Emergency Plan for AIDS relief (PEPFAR) is discussed in Chapter 10 (PEPFAR—a U.S. Government Program That Is Helping to keep Millions Alive Around the World). In the 11 years since its announcement, the program of distribution of medicines has been very successful, with 7.7 million people under treatment worldwide. The authors give a brief history of the program, describing the role of the FDA and their communications to manufacturers and others.

The book has an index, but it is very inadequate and has entries only for subjects beginning with E-G, I, N, and R-T. As a result, searching directly for "climate change" is not possible. That, together with the delayed delivery of books for review, indicate the inadequacies in what is left of the ACS Books division.

### References

- 1) *Science and the Law: Analytical Data in Support of Regulation in Health, Food, and the Environment*; Town W. G., Currano, J. N., Eds; ACS Symposium Series 1167; American Chemical Society: Washington, 2014.
- 2) Otto, S. *The War on Science: Who's Waging It, Why It Matters, What We Can Do About It*; Milkweed Editions, Minneapolis, 2016.

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# Sponsor Announcements



Division of Chemical Information Sponsors, Spring 2017



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 2017 National Meeting in San Francisco, 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:

<b>Gold</b>	<a href="#"><u>ACS Publications</u></a>
<b>Silver</b>	<a href="#"><u>Journal of Chemical Information &amp; Modeling</u></a> <a href="#"><u>Royal Society of Chemistry</u></a>
<b>Bronze</b>	<a href="#"><u>Journal of Cheminformatics (Springer Nature)</u></a> <a href="#"><u>Collaborative Drug Discovery</u></a> <a href="#"><u>PerkinElmer</u></a> <a href="#"><u>Thieme Chemistry</u></a>
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Please feel free to contact me if you would like more information about supporting CINF.

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Chair Pro Tem, Fundraising Committee 2017  
Email: [Sponsorship@acscinf.org](mailto:Sponsorship@acscinf.org)  
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# ACS REAGENT CHEMICALS

## ACS Reagent Chemicals

### What is ACS Reagent Chemicals?

The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials. These specifications have become the *de facto* standards for chemicals used in many high-purity applications, with agencies like the US EPA and ASTM referencing these specifications and methods. In addition to detailing these specifications, ACS Reagent Chemicals provides general physical properties and analytical uses for all reagent chemicals, as well as guidelines for standard analytical methods.

The eleventh edition of *ACS Reagent Chemicals*, originally released in print, became the version of record in June 2016. In January 2017, the online edition based on the eleventh edition became available, and this version reflects the content of the eleventh edition. The first round of supplements and updates were also published online and will soon be incorporated into the content of the online edition. All content is under regular review by the Committee, and additions and updates to existing content will be integrated in the online version beginning in 2017. New mechanisms are being added for capturing the historic record moving forward.

### Who benefits from access?

Academic and research institutions gain access to standards that are utilized by top organizations (the U.S. EPA and U.S. Pharmacopeia, for example) for analytical procedures. Students also benefit from access to easy-to-follow methods and highlighted handling instructions for chemicals. They also can easily find physical constants, equations, and other data in the monographs for each chemical.

Industry professionals use *ACS Reagent Chemicals* to check that reference materials are of an acceptable purity for the test being performed and ensure that starting materials are of high enough purity for product synthesis. Manufacturers use *ACS Reagent Chemicals* to ensure that their inventory of analytical and Reagent Grade chemicals meet the committee's standards for purity.

### What's new for 2017?

The content of the new online edition is delivered on the same platform as ACS journals, providing a consistent experience for users. Additional benefits include:

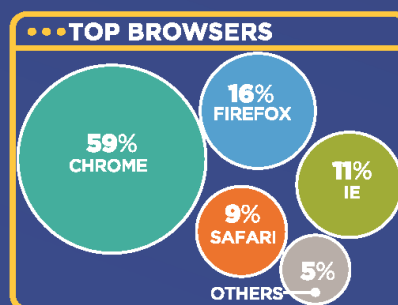
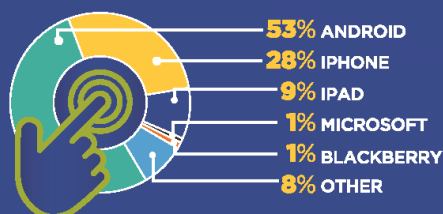
- Better user interface, paired with expanded accessibility, including mobile friendliness, helps readers find the information they need easily from wherever they are.
- DOIs for each monograph and method.
- All content is under regular review by the committee, with regular online additions and updates starting in 2017.
- Each monograph will show a summary of historic changes moving forward, giving the reader full awareness of changes and a link to prior versions.
- Internal references are hotlinked, helping readers to locate all the information they need quickly.
- HTML and printable PDF formats help readers use the content in the format that is most convenient for them.
- Usage, denials, and abstract data at the chapter level help librarians track utilization.



# 2016 BY THE NUMBERS

**27** MILLION UNIQUE VISITORS **51** MILLION SEARCHES

**9** MILLION VISITS FROM MOBILE DEVICES



**94** MILLION ARTICLE REQUESTS **25** MILLION CHINA **20** MILLION USA **19** MILLION EUROPE



**41,000+** ARTICLES PUBLISHED



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**476,000+** UNIQUE ACS ID REGISTRANTS



**181** MILLION ABSTRACTS VIEWED





***USPTO Issues Collaborative Drug Discovery, Inc. (CDD) Patent***

**CDD has been awarded a U.S. utility patent for a “Hybrid machine-user learning system and process for identifying, accurately selecting and storing scientific data” (U.S. Patent No. 9,594,743, issued March 14, 2017).**

From the desk of Mark A. Harper, Ph.D., Partner, Dinsmore & Shohl LLP, Legal Counsel (CDD’s Patent Lawyer)

The United States Patent and Trademark Office (USPTO) officially issued U.S. Patent No. 9,594,743 assigned to CDD on March 14, 2017. The CDD patent is directed to a hybrid machine-user learning system and process for identifying, accurately selecting, and storing scientific data. This includes use in screening runs measuring drug candidates or medical knowledge bases that go into more detail about the biological systems being assayed. After examination of the application by the USPTO, which included a review of the application, a search of prior art and a comparison of the claims of the application with the prior art uncovered during the search, the USPTO noted that the prior art “does not disclose, teach or suggest” the invention as recited in the claims. Particularly, the USPTO noted that the scoring and ranking of possible annotations assigned to Part of Speech (POS)-tagged blocks as taught in the application and recited in the claims was novel and not obvious in view of the prior art.

The full patent abstract, images, description, and claims can be cleanly viewed in Google Patents here:

<https://www.google.com/patents/US9594743>

For more information on the new BAE product using this patented technology to annotate your assays more efficiently in machine-readable, semantically marked-up formats, please see the [BioAssay Express \(BAE\)](http://www.bioassayexpress.com/) (<http://www.bioassayexpress.com/>) website or schedule a free demonstration via email to [sales@collaborativedrug.com](mailto:sales@collaborativedrug.com).

(Reproduced from <https://www.collaborativedrug.com/buzz/2017/04/11/uspto-issues-cdd-patent/>)

*Journal of Chemical Information and Modeling*

**JOURNAL OF  
CHEMICAL INFORMATION  
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The *Journal of Chemical Information and Modeling* is excited to be sponsoring the Division of Chemical Information, and our team looks forward to working with many of its members in the coming months. In the past, I mentioned changes at the journal which involved creating two new manuscript types: reviews and application notes. We have published several application notes describing software appropriate to chemical information and other areas, and we are currently in the process of publishing several reviews. If you have an idea for a review please contact me at [eic@jicm.acs.org](mailto:eic@jicm.acs.org), and we can discuss your idea further. We also are expanding our support in the area of molecular simulation and materials informatics, so please consider sending your manuscripts in these areas to the journal. All the best in 2017!

Kennie Merz  
Editor-in-Chief, *Journal of Chemical Information and Modeling*



April 3, 2017

### ***New Cloud-Based PerkinElmer Signals Notebook Helps Scientists Accelerate Drug Discovery Research***

#### ***ELN Leverages Cloud- and Web-based Technology to Streamline and Centralize Scientific Data***

**WALTHAM, Mass. – April 3, 2017 –** [PerkinElmer, Inc.](#), a global leader committed to innovating for a healthier world, today announced the launch of the [PerkinElmer Signals Notebook](#) at the American Chemical Society (ACS) Spring National Meeting and Exposition (Booth #619). PerkinElmer's new cloud-based electronic laboratory notebook solution (ELN) powers smarter science through collaboration.

Researchers and lab managers can utilize the platform to quickly compile, report, and share data to accelerate drug discovery by leveraging the PerkinElmer Signals Notebook cloud to access, manage, and author notebooks or experiments in real-time. The PerkinElmer Signals Notebook also enables R&D to help accelerate the pace of innovation.

“Scientists and lab managers must have the most effective and modern data management tools at their fingertips to meet the evolving demands of drug discovery today,” said David Wang, Vice President and General Manager, Informatics, PerkinElmer. “The PerkinElmer Signals Notebook provides powerful tools to enable users to focus on achieving breakthroughs at an accelerated pace with collaborators. Further, the new cloud-based solution can be implemented immediately for a quick return on investment.”

The PerkinElmer Signals Notebook allows for simple navigation that helps researchers seamlessly store, organize, share, and find data. The platform is fully-integrated with Microsoft Office and Microsoft Office Online applications to further streamline processes such as directly attaching documents to experiments. The PerkinElmer Signals Notebook also offers cloud storage that is safe, secure, and convenient for recording observations and synthesis attempts.

For more information on the PerkinElmer Signals Notebook, please visit PerkinElmer [www.perkinelmer.com/product/signals-notebook-signalsn](http://www.perkinelmer.com/product/signals-notebook-signalsn).

#### **About PerkinElmer**

PerkinElmer, Inc. is a global leader committed to innovating for a healthier world. The company reported revenue of approximately \$2.1 billion in 2016, has approximately 9,000 employees serving customers in more than 150 countries, and is a component of the S&P 500 Index. Additional information is available by calling 1-877-PKI-NYSE or at [www.perkinelmer.com](http://www.perkinelmer.com).

Follow us on Twitter [@PKILifeScience](https://twitter.com/PKILifeScience).

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## Royal Society of Chemistry

### **Royal Society of Chemistry**

Advancing excellence in the chemical sciences

We are the world's leading chemistry community, with a membership and professional society of over **53,500 members**.

We publish **high quality** chemical science research. Our average journal Impact Factor<sup>1</sup> is now **6.105** and continually increasing.



### **2017 Highlight: RSC Advances is open access (OA)**

*RSC Advances*, the largest chemical sciences journal in the world has become a **gold open access** (<http://www.rsc.org/journals-books-databases/open-access/gold-open-access/>) journal. This provides researchers free access to a broader scope of high quality research and offers new, affordable open access publishing options for authors around the world.

In January, we published our **first fully gold open access issue** (<http://pubs.rsc.org/en/journals/journalissues/ra#!issueid=ra007001&type=current>) of *RSC Advances*, featuring 75 articles from authors in 28 countries.

*RSC Advances*' article processing charge (APC) is £750, one of the lowest in the industry. For the first two years, this charge will be discounted to £500, with further discounts and waiver options also available.

Our aim is to support the scientific community and advance excellence in the chemical sciences. Converting a journal of this size and reputation to open access cements our influence in OA publishing, and puts us in a strong position to shape its future for the benefit of our community.

### **References**

- 1) 2015 *Journal Citation Reports*, (Clarivate Analytics, June 2016)

*Thieme Chemistry launches SynOpen*

**The new open access journal for chemists**



Stuttgart – *SynOpen*, the Thieme Publishing Group's latest addition to its range of open access journals, reports on current research results in the field of chemical synthesis. The new English-language journal gives interested authors in chemistry the option to publish their articles in open access format. Manuscripts are currently being accepted.

The new open access publication, *SynOpen*, rounds off Thieme's range of journals for synthetic chemists. "The launch of *SynOpen* gives chemical researchers the possibility to choose between publishing in an open access or a traditional subscription journal," says Dr. Susanne Haak, Managing Editor at Thieme Chemistry. "This option is of increasing importance for our authors, as the requirements of financial backers and funding bodies are becoming more and more complex in this regard," adds Haak.

Thieme encourages authors to submit full papers, letters or practical synthetic procedures (PSPs) in the field of chemical synthesis for publication in *SynOpen*. The journal covers all areas relating to organic synthesis, including catalysis, organometallics, medicinal chemistry, biological chemistry, and photochemistry, as well as related disciplines, such as materials science. Researchers are also invited to publish the primary data of their experiments. All submitted manuscripts are peer-reviewed by experts to ensure the same high level of quality that readers have come to expect from the Thieme subscription journals *Synthesis*, *Synlett*, and *Synfacts*. The publishers were able to bring an experienced editor, Professor Laurence M. Harwood, on board for the new journal, whose work at the University of Reading, U.K., includes the development of new synthetic methods and their application to the synthesis of natural and unnatural products. For some years he has also been working in the field of nuclear chemistry.

Authors interested in publishing articles in *SynOpen* can find all the information they need at [www.thieme-chemistry.com/synopen](http://www.thieme-chemistry.com/synopen).

The Thieme Publishing Group's product range in the field of chemical synthesis also includes the English-language journals *Synthesis*, *Synlett*, and *Synfacts*. Each journal has its own board of internationally renowned editors to ensure that chemists have access to the latest high-quality research results in their areas of specialization.



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