Message from the Chair

Greetings from sunny Philadelphia!

I hope that you have all had a relaxing and productive (if desired) summer. As an academic, summer time is generally a time for catching up on projects and attending to the mass of paperwork and less pleasant duties that one has been able to postpone in favor of “more pressing concerns” during the academic year. I would like to thank the Division of Chemical Information for saving me from such a fate this summer by engaging me with preparations for the Fall National Meeting.

The CINF program was exceptional, and I would like to praise Erin Bolstad and all symposium organizers for their hard work in planning excellent symposia and recruiting interesting speakers. For those who were unable to attend the conference, I am delighted to announce that ACS chose to record one of our symposia, “Nature’s Second Act: Revisiting Natural Products,” as part of the Presentations on Demand program. The recordings are available to any ACS member at http://presentations.acs.org/common/sessions.aspx/Fall2014/CINF. In addition, Erin is working hard to collect slides from speakers in all symposia and post them on our Web site; please stay tuned for more content as it becomes available!

The Executive Committee meeting on Saturday dealt largely with the CINF budget, as we attempt to finalize it for the 2015 year. Other business transacted at the meeting included the approval of Donna Wrublewski as the 2015-2016 CINF Membership Chair and approval of the addition of a fully-paid conference registration to the Herman Skolnik Award package. The meeting adjourned prior to the committee dinner. I was sorry that more CINF members were unable to take advantage of the informal setting to learn more about the work of the CINF committees, but those who did attend enjoyed themselves, and some good information changed hands.

I am happy to congratulate the winners of the 2014 CINF elections. Rachelle Bienstock was elected Chair-Elect, Rob McFarland was re-elected Treasurer, Andrea Twiss-Brooks will continue to serve as one of our two Councilors, and Chuck Huber will be the Alternate Councilor. This year’s ballot confused many voters, since Rachelle is currently CINF’s Chair-Elect. A scan of the bylaws indicated that we have no limit to the number of times that an individual may run for an elected office. Therefore, individuals who have already served in any office, including that of Chair, may be recommended or may put their own names forward for the nominating committee’s consideration. As Chair of the 2015 Nominating Committee, I am eager to hear your suggestions of nominees for next year’s elections; please contact me if you wish to be considered or if you want to nominate a colleague!

Awards also dominated this year’s meeting, and I am pleased once again to extend my congratulations to the 2014 Herman Skolnik Award recipient, Dr. Engelbert Zass. The Skolnik Award Symposium and reception were extremely enjoyable, with the award address giving a dynamic and enthralling dissection of a complicated chemical information problem: tracking down the true and complete story of the total syntheses of vitamin B12. I would like to take this opportunity to remind all CINF members to consider nominating a colleague for one of our awards, the requirements for which are listed on the CINF Web site at http://www.acscinf.org/content/cinf-sponsored. In particular, we are seeking nominations for the 2016 Herman Skolnik Award, and the CINF Meritorious Service Award, and we also encourage CINF members to suggest names of outstanding individuals who can be put...
forward for consideration as ACS Fellows (see http://www.acs.org/content/acs/en/funding-and-awards/fellows.html).

I have enjoyed this past year; serving as the Chair of the Division of Chemical Information has been one of the high-points of my career so far. I look forward to my Past-Chair year next year and hope that many of you will consider assisting the Division by agreeing to run for leadership positions and volunteer for committee and committee chair positions in the future. For now, have an excellent fall!

Judith Currano, Chair, ACS Division of Chemical Information

Mark your calendars!

Two more CINF Webinars are coming in 2014, with more details to follow at a later date at CHMINF-L.

Tuesday, October 7, 11:00 am (EDT) Pistoia Alliance (http://www.pistoiaalliance.org/), Ramesh Durvasula

Wednesday, December 3, 11:00 am (EDT) Copyright Clearance Center (http://www.copyright.com/), Stephen Garfield

CINF series of free webinars is archived at: http://acscinf.org/content/webinars
Letter from the Editor

Happy 65th anniversary Chemical Information Bulletin (CIB)!

San Francisco is a special landmark for our Division, as it is where CINF organized its first technical session at the 115th ACS National Meeting in March 1949. After the following fall meeting in Atlanta, the first issue of the Bulletin named “Chemical Literature” with a byline “News Bulletin of ACS Division of Chemical Literature” made its debut in November 1949. (Val Metanomski, Chemical Information Bulletin, Spring 2008, http://digital.library.unt.edu/ark:/67531/metadc5616/m1/10/; this image is the first cover page in color designed for the Fall 1998 issue of CIB).

While the first bulletin was 5 pages long, this winter 2014 issue expands to its largest volume of information at 78 pages. Among its comprehensive content, this “anniversary issue” features a number of other anniversaries, namely: 100 years of the ACS Division of Environmental Chemistry (celebrated by ACS as part of its thematic program during the fall meeting in San Francisco, an overview was written by David Shobe), 100 years of Ullmann’s Encyclopedia (celebrated in 2014, a book review by Frank Weinreich), 100 volumes of the IUPAC Solubility Data Series (a symposium summary and information on the Subcommittee on Solubility and Equilibrium Data by Clara Magalhães), 50 years of work of Dana Roth at Caltech (a symposium summary honoring Dana’s milestone by Donna Wrublewski), 50th anniversary of Harry’s Party (celebrated by CINF in San Francisco, a feature was included in the previous issue http://bulletin.acscinf.org/node/626), the 10th International Conference on Chemical Structures and 10th German Conference on Chemoinformatics (a summary from the Netherlands by Phil McHale).

Above all, the 2014 Herman Skolnik Award Symposium and Reception Honoring Engelbert Zass was a CINF keynote event in San Francisco. Wendy Warr spoke at the symposium and also wrote an outstanding technical report (20 pages with supplementary information and 20 references) for this issue of the Chemical Information Bulletin. Based on the nature of the presentations at this Award Symposium, someone may consider using Wendy’s “lecture notes” for studying the history of chemical information.

In addition to technical reports written traditionally by CINF symposium organizers, e.g. Rachelle Bienstock, David Martinsen, and Bill Town, this issue has also four stories written by “symposium reporters”: Elsa Alvaro, Phil McHale, Carmen Nitsche, and Donna Wrublewski. Many sincere thanks for their contributions to this issue.

Coincidentally, Elsa Alvaro is featured in this issue’s “Member Profile,” a new column introduced by Donna Wrublewski, incoming CINF 2015 Membership Chair. Carmen Nitsche and Belinda Hurley are praised for their outstanding line-up of CINF Webinar series in 2014. In this issue you will find all other committee updates on CINF Communications and Publications, Education, Membership, ACS Multidisciplinary Program Planning Group (Roger Schenck is a new CINF representative on MPPG), ACS Council, and Joint Board-Council Committee on CAS, and on Publications (with presentation slides by Brian Crawford), as well as new product announcements from our sponsors.

In conclusion, I would like to thank all writers for submitting their articles to this issue. I hope that you will benefit from the information.

Svetlana Korolev, Editor, Chemical Information Bulletin

Chemical Information Bulletin, 2014, 66 (4)
Awards and Scholarships

2014 CINF Scholarship for Scientific Excellence Presented

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) is designed to reward 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 and has awarded 54 scholarships in total. The awards at the Fall 2014 National Meeting in San Francisco were sponsored by the Royal Society of Chemistry.

Applicants presented their posters at the CINF Welcoming Reception and the Sci-Mix session. Four scholarships valued at $1,000 each were presented to the winners at the CINF Luncheon during the same meeting.

The names of the recipients and the titles of their posters are (listed from left to right on the photo):

Alexander R. Geanes, Department of Chemistry, Vanderbilt University, Nashville, TN, USA, “BCL::EvoGen: An evolutionary algorithm for focused library design.” Co-authors: Edward W. Lowe, Jens Meiler.


Huifang Li, Vancouver Prostate Centre, University of British Columbia, Vancouver, B.C., Canada, “Targeting androgen receptor DNA-binding domain using structure-based methods to overcome resistance.” Co-authors: Fuqiang Ban, Kush Dalal, Eric, Leblanc, Paul S. Rennie, Artem Cherkasov.

Katarzyna Odziomek, Faculty of Chemistry, Laboratory of Environmental Chemometrics, University of Gdansk, Poland and Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA, “Towards Quantitative Structure-Activity Relationship (QSAR) models for nanoparticles.” Co-authors: Daniela Ushizima, Tomasz Puzyn, Maciej Haranczyk.

The next scholarships are jointly sponsored by InfoChem and Springer and will be awarded at the Spring 2015 ACS National Meeting in Denver, CO.

Guenter Grethe, Coordinator, CINF Scholarship for Scientific Excellence
The American Chemical Society Division of Chemical Information is pleased to announce Prof. Dr. Jürgen Bajorath as the recipient of 2015 Herman Skolnik Award. The award recognizes outstanding contributions to and achievements in the theory and practice of chemical information science and related disciplines. The prize consists of a $3,000 honorarium and a plaque. Prof. Bajorath will also be invited to present an award symposium at the Fall 2015 ACS National Meeting to be held in Boston, MA.

Bajorath is a world leader in the development and application of cheminformatics and computational solutions to research problems in medicinal chemistry, chemical biology, and the life sciences and has done pioneering work in the area of compound data analysis in chemistry. He is widely recognized for his seminal and prolific research work in molecular similarity analysis and ligand-based virtual screening, fingerprint engineering and advanced machine learning techniques, application of information theoretic concepts to cheminformatics, large-scale graphical analysis and visualization of structure-activity relationships, big data analysis in chemistry, and evaluation of SAR information in medicinal chemistry project progression in novel ways. Bajorath has been active in several areas of scientific enquiry and development that have all helped shape some of the fundamental research issues in chemical information science. Some of these areas include:

- Algorithms to navigate high-dimensional chemical space representations in search of novel active compounds
- Molecular fingerprints for similarity searching that are not affected by molecular complexity and size effects and that are directed against specific compound classes
- Methods for the estimation of recall rates in virtual screening and database rankings
- Prediction of structure-activity characteristics of compound data sets
- Approaches for the analysis of selectivity differences between ligands of members of target protein families and the identification of selective compounds
- Compound data mining and molecular promiscuity analysis
- Activity landscape modeling and systematic exploration of activity cliffs
- Various novel visualization methods for analysis of structure-activity relationships.

Bajorath obtained his diploma (M.S.) and Ph.D. degrees (under Wolfram Saenger, 1988) in biochemistry from the Free University West-Berlin. After postdoctoral work with Arnie Hagler at Biosym in San Diego focusing on DFT calculations on enzyme-inhibitor complexes, he joined Bristol-Myers Squibb (BMS) and spent seven years at the BMS Pharmaceutical Research Institute in Seattle where he became a Principal Scientist. During his years at BMS, Bajorath worked on protein modeling and structure-based design projects and developed his interests in bio- and chemoinformatics research.

After leaving BMS, he was involved in starting a biotech company (New Chemical Entities) that ultimately became the AMRI Bothell Research Center. In 1995, he was appointed Affiliate Associate and later Full Professor of Biological Structure at the University of Washington where he developed strong academic ties.
In 2004, after 16 years in the US, he was appointed Full Professor and Chair of Life Science Informatics at the University of Bonn, Germany. He continues to be affiliated with the University of Washington and has also been an invited professor at the University of Strasbourg, France.

Bajorath currently serves as an Associate Editor of the *Journal of Medicinal Chemistry* and is also on several editorial boards (including, among others, *Drug Discovery Today, Expert Opinion in Drug Discovery, Chemical Biology and Drug Design, Molecular Diversity, and Molecular Informatics*) and various scientific advisory boards.

He received the Novartis Chemistry Lectureship Award and was appointed as a F1000 Faculty Member to the Drug Discovery and Design Section.

Jürgen Bajorath has been a dominant force in the fields of cheminformatics, big data analysis, and computational chemistry. He has published more than 450 papers in several prestigious journals, and 4 books and holds 25 issued patents. Some programs and databases that are a result of his scientific research work have been placed in the public domain including SARANE, an open-source Java application for interactive exploration of structure-activity and structure-selectivity relationships.

*Andrea Twiss-Brooks, Chair, CINF Awards Committee*

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**2015 Lucille Wert Scholarship: Call for Applications**

Designed to help persons with an interest in the fields of Chemistry and Information to pursue graduate study in Library, Information, or Computer Science, the Scholarship consists of a $1,500 honorarium. This scholarship is given yearly by the Division of Chemical Information of the American Chemical Society.

The applicant must have a bachelor’s degree with a major in Chemistry or related disciplines (related disciplines are, for example, Biochemistry or Chemical Informatics). The applicant must have been accepted (or currently enrolled) into a graduate Library, Information, or Computer Science program in an accredited institution. Work experience in Library, Information or Computer Science is preferred.

The deadline to apply for the 2015 Lucille M. Wert Scholarship is **February 1, 2015.**

Details on the application procedures can be found at: [http://www.acscinf.org/content/lucille-m-wert-student-scholarship](http://www.acscinf.org/content/lucille-m-wert-student-scholarship).

Applications (email preferred) can be sent to: Andrea Twiss-Brooks <atbrooks@uchicago.edu>

Contact information: Andrea Twiss-Brooks  
Co-Director Science Libraries, University of Chicago  
5730 S. Ellis Avenue, John Crerar Library, Chicago, IL 60615  
Phone: 773-702-8777
The Patterson-Crane Award: Call for Nominations

Do you have a colleague whom you believe should be acknowledged for her/his work in chemical information? The Dayton and Columbus Sections of the American Chemical Society, which sponsor the Patterson-Crane Award, would like to hear from you.

The biennial award consists of a $3,000 honorarium and a personalized commendation and is to be presented in the spring of 2015 at an awards dinner to be held in Columbus, Ohio. The recipient is expected to give an address at the time of the award presentation.

Award Criteria:

Nominees, who need not hold ACS membership, should demonstrate outstanding achievement in the field of chemical information science. Contributions of international significance may relate to:

- Design, development, production, or management of chemical information systems or services.
- Electronic access to and retrieval of chemical information; critically evaluated data compilations.
- Information technology applications in chemistry or other significant chemical documentation, including production of original works, editorial work, or chemical library work.

Nominations for the award must be in writing and may be sent either in hard copy or via email.

They should discuss the nominee's contributions to the field as well as an evaluation of accomplishments. Materials supporting the nomination should include a biography and bibliography of publications and presentations. Seconding letters are required and may also be sent either in hard copy or via email.

Send the nomination materials to Dr. Steven Rosenthal, Chair of the Patterson-Crane Award Committee, (srosenthal@cas.org or CAS, 2540 Olentangy River Road, Columbus, OH 43202-1505) for receipt by 31 January 2015. To receive more information about this award, contact Dr. Rosenthal (614-447-3600, ext. 2070 or srosenthal@cas.org).

Nominations will be judged by a seven-member selection committee consisting of Dayton and Columbus Section members as well as the Chair of the American Chemical Society’s Division of Chemical Information.

The Patterson-Crane Award is international in scope and given in honor of two outstanding members of the sections: Austin M. Patterson (1876–1956) and E.J. Crane (1889–1966), who were both Editors of Chemical Abstracts Service.

Steven Rosenthal, Chair, Patterson-Crane Award Committee
Chemical Structure Association Trust Grant: Applications Invited for 2015

The Chemical Structure Association (CSA) Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program and is now inviting the submission of grant applications for 2015.

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

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

Which Activities are Eligible?
Grants may be awarded to acquire the experience and education necessary to support research activities; for example, for travel to collaborate with research groups, to attend a conference relevant to one’s area of research, to gain access to special computational facilities, or to acquire unique research techniques in support of one’s research.

Application Requirements:
Applications must include the following documentation:

1. A letter that details the work upon which the Grant application is to be evaluated as well as details on research recently completed by the applicant;
2. The amount of Grant funds being requested and the details regarding the purpose for which the Grant will be used, for example, cost of equipment, travel expenses if the request is for financial support of meeting attendance, etc. The relevance of the above-stated purpose to the Trust’s objectives and the clarity of this statement are essential in the evaluation of the application;
3. A brief biographical sketch, including a statement of academic qualifications;
4. Two reference letters in support of the application.

Additional materials may be supplied at the discretion of the applicant only if relevant to the application and if such materials provide information not already included in items 1 - 4. Three copies of the complete application document must be supplied for distribution to the Grants Committee.
Deadline for Applications:
Applications for the 2015 Grant are due by March 13, 2015. Successful applicants will be notified no later than May 2 of the relevant year.

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

Recent Grant Awardees:

2014

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

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

Dr. David Palmer: Department of Chemistry, University of Strathclyde, Scotland. He was awarded a Grant to present a paper at the fall 2014 meeting of the American Chemical Society on a new approach for representing molecular structures in computers based upon on ideas from the Integral Equation Theory of Molecular Liquids.

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

A complete list of the previous grant awardees is at: http://bulletin.acscinf.org/node/590

Bonnie Lawlor, Chair, CSA Trust Grant Committee
Thanks to everyone for attending ACS San Francisco and helping make it one of CINF’s BIGGEST meetings yet! We had about 130 talks, 20 Sci-Mix posters, 5 competitor posters for the CINF Scholarship for Scientific Excellence: all organized into 13 multi-tracked sessions including the Herman Skolnik Award Symposium. With San Francisco continuing the trend of high attendance, it was a very full and busy meeting.

The program was very diverse, ranging from a brand new symposium (Epidrugs) to one of our largest symposia on a classic CINF topic (Chemistry Text Mining). With the rapidly developing field, we see new technology and research presented every time we host this popular symposium.

We are very pleased to report that our symposium “Nature’s Second Act: Revisiting Natural Products” was selected for ACS Presentations on Demand. This was a surprising symposium with a very diverse array of presentations, which all tied in together well to the topic. An excellent organizing job, Roger Schenck! Check out a selection of these talks at Presentations on Demand (http://presentations.acs.org/common/tracks.aspx/Fall2014). While you’re there, be sure to also check out CHED’s Sustain-Mix symposium, a collection of talks on sustainability across the Society from the perspectives of many divisions. CINF’s own Chair, Judith Currano, contributed an excellent presentation on the sustainability and utility of an ever expanding scholarly record. (Editor’s note: due to technical issues Judith Currano’s presentation recording is currently not available at the ACS website. To see her presentation slides, please follow this link at: http://bulletin.acscinf.org/PDFs/maintaining-sustainable-scholarly-record.pdf).

The fall meeting also saw some in-depth and exciting discussions within CINF and among the attendees. The “Inspiring the Next Generation To Pursue Computational Chemistry and Cheminformatics” led to some long and interesting discussions about informatics education, as well as newfound plans for outreach across other divisions for CINF and the student body. This is something we plan to focus on for the upcoming Denver and Boston meetings.

CINF’s regular Tuesday Luncheon had an exciting keynote address presented by Prof. Dr. Barend Mons (short bio and presentation abstract, slides) discussing an open initiative to get data into a standard and consumable format for easy searching and connecting (Datafairport.org). This falls under a rapidly evolving area of semantic technology, a subject very important to CINF, and to electronic information in general.

Despite CINF being placed quite far from the conference center, our attendance was still high, which led to some fabulous discussions across this broad array of symposia. We are still in the process of collecting the presentation slides from speakers so that we can share them with you: check back soon for these at the CINF website (http://bulletin.acscinf.org/node/621).

Thanks again to everyone who put so much work into making this San Francisco meeting a resounding success!

Erin Bolstad, Chair, CINF Program Committee
Computational Methods and the Development/Production of Biologics and Biosimilars

For a long time the pharmaceutical industry has been dominated by the production of small organic molecules as drugs. This has changed recently with the introduction of biological medicines or biologics. Biologics, as opposed to synthetic organic small molecules, are derived from living cells and are typically larger-sized molecules. As a group they include therapeutic and fusion proteins, monoclonal antibodies and DNA vaccines. They are much more difficult to manufacture and characterize than typical small molecular organic drugs and are almost always taken by injection (as opposed to orally). The development of biologics, hormone therapies and targeted monoclonal antibodies, has contributed greatly to enhanced cancer treatments for patients. Biosimilars are similar, but not identical copies of a biologic drug. Generic drugs are identical copies of small organic molecules but, because biologics are much more complex, biosimilars cannot be identical copies of them. The manufacturing of biologics and biosimilars adds a level of complexity because biologics are not made with a standard set of starting materials like typical drugs, but are made by genetically engineered living cells. A number of steps involved in creating a biological drug are much more complex than for a typical drug and any slight process variation can affect the biological product in terms of stability, efficacy and immunogenic properties. In 2009 the World Health Organization developed guidelines for regulating biosimilars and biological pathways, and for ensuring that their manufacturing process should meet the same standards as required for the originator products. However, even simple issues such as naming conventions and compound registration systems can be of concern. This symposium sought to initiate discussion on some of these issues.

Dr. Roger Sayle of NextMove Software gave a presentation entitled “Classification, representation, and analysis of cyclic peptides and peptide-like analogs,” which described some of the difficulties involved in naming nonstandard amino acids, as well as defining macrocyclics due to the diverse ways in which peptides can form cyclic linkages. The naming and machine-recognition of synthetic macrocyclic peptides provide significant informatics challenges. For example, covalently cross-linked side-chains may have multiple possible (degenerate) primary sequences, requiring the selection of a preferred canonical form during biological registration. In this presentation, Dr. Sayle described the development of a software program “Sugar and Spice,” which can provide some assistance in standardization and machine-recognition of non-standard amino acids. There is a need for standardized naming conventions and notations, which currently are not in place for designed and engineered non-alpha-amino acids, acyclic peptide backbones, and different types of peptide disulfide bridges.

Dr. Suman Sirimulla, St. Louis College of Pharmacy, gave a talk entitled “Non-covalent interactions in protein-ligand interactions: Applications of halogen bonds and carbon bonds in designing PTSD drugs,” in which he presented the significance of considering non-covalent protein-ligand interactions in drug design. There is a growing need to consider the significance of halogen bonds and carbon bonds in protein-ligand interactions. He presented an application in designing drugs for post-traumatic Stress Disorder (PTSD) with the nociceptin receptor as a target, and the design and development of nociceptin analogues using halogen-bond information and halogen-amino acid interaction data to search and mine the Protein Data Bank.

Dr. Sandeepkumar K Kothiwale, Chemistry, Vanderbilt University, Nashville, Tennessee, presented “BCL:Conf A knowledge based ligand flexibility algorithm and application in computational drug discovery like online drug design game Foldit,” on a derived fragment conformational database created from frequently sampled experimental structures within the Crystallographic Structure Database (CSD) and the Protein Data Bank (PDB). The likely sampled fragments were stored as a rotamer library. A hierarchical search algorithm was used to perform substructure searching: a random Monte Carlo conformational sampling.
onformer generation using multiple threads allows easy integration into high-throughput docking experiments using RosettaLigand.

All the talks presented illustrated the development of novel computational methods to the area of biologics drug design.

Rachelle Bienstock, Symposium Organizer

The Future of the History of Chemical Information
Editors: Leah McEwen, Robert Buntrock
Volume 1164
Sponsoring Division: ACS Division of Chemical Information
Publication Date (Web): August 6, 2014

The aim of this collection is to critically examine trajectories in chemistry, information and communication as determined by the authors in the light of current and possible future practices of the chemical information profession. Along with some additional areas primarily related to present and future directions, this book contains most of the topics covered in the meeting symposium held on August 20, 2012, at the 244th American Chemical Society Meeting in Philadelphia, PA.

Presentation titles, abstracts and slides (#47-51 & 59-65) are listed at: http://bulletin.acscinf.org/node/347.

This symposium set out to explore how the public communication of science influences the interaction between science and policy development in the regulation of the environment, food, health and transport. It presented a series of case studies illustrating the impact of science communication on policy development. The controversy surrounding the science behind the study of global warming and the resulting focus on the reduction of carbon dioxide emissions by international agreement and by national and international regulation is one example of such an area where science communication and policy development are inextricably intertwined. The symposium was one of a series which is seeking to identify other areas where science-based policy development is of increasing importance. The first symposium, held in Philadelphia in 2012, has recently been published as an ACS Symposium book *Science and the Law: Analytical Data in Support of Regulation in Health, Food, and the Environment*, Editors: William G. Town, Judith N. Currano, Volume 1167, ISBN13: 9780841229471, eISBN: 9780841229488.

Our first speaker, Fred Stoss, gave a presentation entitled “Coming out from under the cloud of “Climategate”: Are scientists effectively communicating with the public on climate change?” The strategies, resources, and tools of the groups that challenge scientific communication with the public, were discussed and various STEM-based information, communication and education resources described. Communicating with the public is not a traditional role of scientists, but is of increasing importance in today’s virtually connected world. It is incumbent that the public understands the basic scientific principles of the environments in which they live, work, learn, and play.

Climate change emerged in the 21st century as one of the most complex and controversial environmental problems. Enhanced scientific communication by scientists and their proxies was a response to the theft of emails and documents from the University of East Anglia in November 2009. These emails were strategically “leaked” days before the United Nations Framework Convention on Climate Change in Copenhagen. Climate change deniers attacked researchers, and Conservative radio talk shows dispersed allegations of fraud, withholding and manipulation of data, and suppression of publications. “Climategate” neutered the UN negotiations and, more lastingly, created public confusion and mistrust about the scientific consensus on climate change.

Scientific organizations challenged scientists to evaluate their roles as communicators and set the stage for increasing the proactive discussion of their research. In particular, they needed to explain how their research contributes to a more informed decision-making process which is necessary if we area to transform our ways of thinking: from living in a greenhouse gas-constrained world to a world not constrained by greenhouse gases.

The second speaker, Hanna Breetz, experienced logistical problems and was unable to deliver her talk on “Carbon accounting for indirect land use change (ILUC) in biofuels policy.” Fortunately, we had advanced notice of the logistical problems which were caused by Hanna’s new university position and Fred was able to fill the gap in the program without any difficulty.

Our final speaker before the intermission, Jim Solyst, described strategies for “Communicating the risk of nicotine delivery products.” The rapid increase in the use of electronic cigarettes by smokers of tobacco cigarettes has highlighted the risk perception and communication challenge facing the US
Food and Drug Administration (FDA) in characterizing nicotine delivery products. Tobacco smokers believe that by switching to electronic cigarettes they are reducing their risk level. This is likely to be true, but the scientific evidence is only now being collected. FDA is a public health and science-based agency, and cannot communicate the risk reduction potential of electronic cigarettes until they have sufficient evidence, regardless of the intuitive risk reduction potential of the product.

The 2009 Tobacco Control Act provides authority to the FDA Center for Tobacco Products to regulate tobacco products, including electronic cigarettes. Section 911 of the Act, Modified Risk Tobacco Product (MRTP), provides a scientific evidence-based process by which a company can apply for and receive a MRTP order. If a product can be demonstrated to reduce harm to the individual and benefit the overall public health then it may be characterized as modified risk and FDA may communicate that information to the public.

There are products, for example, Swedish snus (a smokeless tobacco powder), for which there is a great deal of human health evidence and may at some time be granted a MRTP order; but there is no such human health evidence for electronic cigarettes due to the recent introduction of the product to the market. So what does FDA say to the tobacco smoker who is considering switching to electronic products? The best advice is not to use nicotine products at all, but does FDA have an obligation to inform smokers of the obvious benefits of switching, even if the evidence is not complete?

Our first speaker after the intermission was George Lunn from the FDA who presented “PEPFAR - a US Government program that is helping to keep millions alive around the world.” This was a good news story. PEPFAR, the President’s Emergency Plan for AIDS Relief, was announced by President George W. Bush in 2003 with the aim of preventing infections, treating infected people, and caring for infected individuals and orphans in resource-limited countries.

In a unique arrangement, low-cost manufacturers submit to the FDA New Drug Applications or Abbreviated New Drug Applications for antiretroviral drugs to treat AIDS and these applications are reviewed to the same standards as applications for products that are destined for the US market. To expedite the preparation and submission of these applications, the FDA has reached out to the manufacturers, distributors, and other interested parties. At the beginning of 2014 the FDA had taken an action on 168 applications and 6.7 million people worldwide are being treated with these antiretroviral drugs. George described the communication challenge that resulted from this outreach program.

Our next speaker was Neil Ravenhill of Weber Shandwick (who was a late substitute for Tamora Langley) and he discussed the topic “Does science or communications have greater influence in formulating policy? A UK perspective.” The dynamics and principles of the scientific environment are starkly at odds with the dynamic of the political environment in which policies are made or broken. While a scientific approach is rational, evidence-based, and formed through consensus of experts, the political environment is emotional, driven by communications, and adversarial. Although decision makers aspire to evidence-based policy-making, in contested areas the side with the most effective communications often seems to “win.”

The recent economic crisis in the UK and across mainland Europe has necessitated drastic cuts in public spending, impressing on officials the need to make savings and squeeze more value out of public resources. In the UK, the government marked out the health budget as one of only two areas of public spending to be shielded from the cuts. Still, relatively flat health spending has been outstripped by rising demand for services, and so any new policies requiring additional resources remain in theory unaffordable. Where new health policies have been introduced, such as the Cancer Drugs Fund (CDF), they have been driven not by scientific developments so much as by public opinion and
political decision-making. Similarly, attempted policy change driven by or expressed in terms of economic or rational imperatives (such as attempts to reconfigure health services, or attempts to change statutory regulation of dispensing medicines), have failed in the face of patient and professional campaigns. To conclude that those who shout loudest will always win is to over-simplify. Besides, in some policy debates, patient and professional advocacy groups are divided. Even if policies are pushed through by noisy campaigns, they can be reversed or stalled by the public officials who “outlive” their political masters and realize they are in practice unworkable or inefficient. The answer? Begin with the science, but recognize that the communication of science is just as critical.

David P. Richardson, described some of the pitfalls in the “Consumer communication of nutrition science and impact on public health.” Dietary interventions for vulnerable groups such as the elderly, women of childbearing age, children and adolescents can contribute beneficially to help reduce the risk of suboptimal intakes and deficiencies of micronutrients, to control costs of healthcare, and to promote the health and quality of life of people globally. Examples presented included the communication of the scientific evidence for (a) the use of folic acid/folate to reduce the risk of neural tube defects, (b) the reduction in prevalence of iron-deficiency anemia, (c) the relationship of calcium and vitamin D to bone health and reduced risk of osteoporosis, and (d) the modulation of the age-related decline in most organ functions and reduction in the development and/or progression of many chronic diseases. Richardson highlighted the need for evidence-based healthcare and communication policies, including the use of nutrition and health claims on food products to raise awareness of the role of diet in health.

The final speaker, Sarah Cooney, illustrated the problems of “Communicating controversial science: The case of tobacco harm reduction and the ethics of blanket censorship” and the difficulties encountered when publishing research from the tobacco industry. It has long been accepted that cigarette smoking causes serious disease and death, and public policy has focused on reducing tobacco use. In the US, the FDA has had regulatory jurisdiction over tobacco products since 2009 and is committed to an evidence-based approach for regulatory decision-making anchored by sound science. In an effort to generate much more data about tobacco science, the FDA has established an interagency partnership with the National Institutes of Health (NIH), which is making available billions of research dollars to study priority questions about tobacco science to inform FDA regulations. This new funding should attract many new researchers, creating a larger and more diverse, transparent and results-orientated tobacco science community.

The FDA has set an example in acknowledging tobacco manufacturers both as an important stakeholder and as a potential source of valuable scientific expertise. Perhaps as a result, there is a general increase in scientific publications resulting from research undertaken by tobacco industry scientists. Additionally, most tobacco manufacturers are even more committed to developing products substantially less risky than cigarettes, and the science to evaluate the potential of such products to promote harm reduction. At the same time there is an increase in the number of scientific journals introducing blanket bans on publishing science from tobacco manufacturers, with the BMJ (British Medical Journal) being a recent example. Cooney described the ethical dilemmas surrounding scientific censorship and the role of peer review in protecting scientific integrity.

The session concluded with a panel discussion with active participation of the speakers and the audience. The layout of the room precluded the normal format of a panel discussion with all the speakers on a podium, but this worked to our advantage and may have inspired more active involvement of the audience, many of whom had followed the whole symposium.

William Town, Symposium Organizer

Chemical Information Bulletin, 2014, 66 (4)
The International Conference on Chemical Structures (ICCS: http://www.int-conf-chem-structures.org/) is a leading chemical informatics meeting, held every three years since 1987, and this year it was combined with the 10th Annual German Conference on Chemoinformatics (GCC). CINF is one of the sponsoring organizations for ICCS. This combination of two 10th anniversaries worked well, and although the subjects covered tended more towards computational chemistry and QSAR, with a reduced emphasis (compared with previous ICCS sessions) on informatics per se, data analysis and integration, the result was interesting and an eclectic mix of papers with plenty for anyone involved in chemical structures and informatics to learn from.

The conference was well-attended with 204 participants from 20 countries. There was a reasonably balanced demographic: 37% academic (including 12 students supported by bursaries), 10% government/non-profit, 24% commercial, and 28% vendors.

The conference received 144 abstract submissions from 20 countries, and the scientific advisory board selected 34 plenary and 83 poster presentations. Papers were presented in the following thematic sessions:

- Cheminformatics
- Structure-based drug design and virtual screening
- Analysis of large chemistry spaces
- Dealing with biological complexity
- Integration of chemical information with other resources
- Structure-activity and structure-property prediction

Where abstracts were submitted, they are available at http://www.int-conf-chem-structures.org/fileadmin/user_upload/program/Book.of.Abstracts.pdf; and for those authors who choose to submit them, their papers will be published (subject to satisfactory peer review) in a special edition of Journal of Chemical Information and Modeling due for publication in early 2015.

In addition to these rather staid and 20th century methods of communication, the minute-by-minute goings on during the conference were live-tweeted by some participants, the most active (the “tweetiest”?) being Wendy Warr and Egon Willighagen, who kept the Twittersphere informed almost on a slide-by-slide basis.

In the majority of the papers, the focus was (correctly) on the science, experimental studies and results, and there was very little mention of informatics products or solutions per se as the focus of any talks, again correctly; but wearing my vendor hat briefly, it is always interesting to see when off-the-shelf products can be used, and when organizations feel compelled to build their own proprietary solutions.

There is now a growing set of open source offerings to complement/compete with the commercial vendors. One example that was mentioned by several speakers was Open PHACTS (http://www.openphacts.org/) which is being widely used in industry and academia in Europe as a source for integrated published pharmacological data. It can be accessed via an API (https://dev.openphacts.org/), a simple forms-based application Open PHACTS Explorer (http://www.openphacts.org/explorer), and some other third-party applications such as...
ChemBioNavigator (www.chembionavigator.org), and PharmaTrek (www.pharmatrek.org), for exploring pharmacological space.

In addition to the plenary papers, there was a small exhibition with 17 exhibitor companies, and there were two poster sessions. All these were well-attended and provided the backdrop for serious discussions, networking, rumor-mongering and light-hearted social chit-chat.

And on the light-hearted social front, one highly anticipated part of ICCS is the afternoon excursion. This year’s was no exception, and included a tour of the newly re-opened Rijksmuseum in Amsterdam, surviving a brief torrential downpour, a fascinating guided boat tour of Amsterdam’s canals, and a sumptuous conference dinner in an old converted church.

All told this was a very successful conference. The three year cycle for ICCS means that enough “new stuff” has happened between conferences to make attendance almost mandatory to keep abreast; and the injection of the GCC in 2014 added new content and different speakers, resulting in a detailed and up-to-date snapshot of the state of chemoinformatics.

Phil McHale, Conference Reporter

Photo credit: pic.twitter.com/avN8DCMGDJ

The 2014 CSA Trust Mike Lynch Award presented to the “InChI Team” at the 10th ICCS/GCC Conference, Noordwijkerhout, Netherlands
The Impact of the IUPAC InChI on Finding and Linking Information on Chemicals

With the inception of the internet and the proliferation of vast and scattered resources of chemical information on the web, it became evident that the community needed an open identifier to allow for a free and meaningful discoverability and exchange across this body of data. So back in 2000 IUPAC began a project to establish just such an identifier, releasing the first version in 2005. This fall’s symposium on InChI, taking place over 10 years since that effort began, clearly demonstrated that the original goals of the IUPAC efforts have succeeded, as most chemical database producers support or use InChI in one way or another and the exchange of chemical compound information across web resources is now commonplace and successful, thanks to InChI.

The symposium covered many aspects, from ideas for improvement of the existing implementation, to ideas and actions to expand coverage to include new compound types, to examples of how InChI is being used at various organizations today to improve and foster data exchange, and how it could be used in the future.

InChI Expansion

We heard from the InChI Trust (Richard Kidd, Treasurer) and several working groups, whose mission it is to maintain and further develop the InChI algorithm. Polymers are next on the list to be handled by InChI. The specifications have been completed and the standard will be programmed by end of this year. The organometallics proposal is out for comment. For now, funding is still being sought for inorganics and Markush structures.

A fair amount of work has also been completed on the RlnChI: a chemical Identifier to handle reactions (update given by Guenter Grethe). Efforts in the biomolecules project are moving forward, with an InChI working group holding a requirements-gathering meeting at NIH later this Fall. (update provided by Keith Taylor). Don Burgess of NIST described a project underway to use the existing InChI structure and expand the tiers to capture conformer, electronic state, and a quantum enumeration layer to create a representation for elementary reactions (InChI-ER).

InChI Improvements

The NCI/CADD group has worked with InChI since the beginning as part of their free web services. Marc Nicklaus presented an interesting analysis of the current state of tautomers within the InChI 1.x algorithm. With this data they are putting together a proposal to improve the algorithm so InChI can achieve its original design goal of being a “tautomer-invariant” identifier.

Community Use of InChI

Major database producers updated us on their uses of InChI. Tony Williams of the Royal Society of Chemistry discussed how InChI has allowed them to integrated disparate compound databases, and how it supports the pursuit of their open source drug discovery platform. He held out the hope that more chemists outside of the CINF Division would become more aware of InChI and related topics. Evan Bolton of National Center for Biotechnology Information discussed how InChI is fundamental for their cross-resource correlation within PubChem and how they have started offering programmatic services that include InChI. Users can import, export, and compute InChIs, in addition to searching by them. He also discussed the PubChemRDF project, which allows users to download slices of related PubChem data. Ian Bruno of the Cambridge Crystallographic Data Centre discussed how they were using InChI to identify the overlap between the Protein Data Bank (PDB) and the Cambridge Structural Database (CSD).
Future Uses of InChI

One interesting application of InChI was as part of the information incorporated into a QR code, discussed by Don Cruickshank of University of Southampton. This could be a good way to deliver emergency information as well as speed up inventory management. Even labels damaged up to 30% are still readable.

InChI Keys also lend themselves to text mining, and Tom Griffin of IBM reported on processing full text documents and assigning InChls and InChIKeys (“entity insertion”) to make the originally text-based chemical information indexable and retrievable.

One question that kept coming up in various guises at the Q&A sessions was why the “same compound” often seemed to have “different” InChls. This tended to do with the way a molecule was normalized rather than with a failure of the algorithm. While the vendors have always understood the challenges of normalization and representation rules, I believe this forum allowed the wider audience to appreciate the rich and nuanced intricacies behind our taken-for-granted chemical drawing tools. Please visit http://bulletin.acscinf.org/node/621 for the full program with abstracts and slides, where available.

Carmen Nitsche, Symposium Reporter

Global Challenges in the Communication of Scientific Research

Science is global now: it is not only carried out in more places than ever, but also addresses worldwide problems and is increasingly collaborative. Forty years ago, about two-thirds of publications had an author from one of the G7 countries (Canada, France, Germany, Italy, Japan, the United Kingdom, and the United States). Nowadays, the contributions of other countries to the research landscape have increased, especially from the so-called BRICKS countries (Brazil, Russia, India, China, South Korea, and South Africa).

The ACS CINF Symposium “Global Challenges in the Communication of Scientific Research” addressed this new geography of science from different perspectives. How are publishers reaching out to new audiences? How are developers shaping their products to exploit the cheaper technologies and the interconnected world? How can we facilitate international science? And ultimately, what are the challenges ahead of us in the scholarly communications arena?

The symposium was organized by David Martinsen and Norah Xiao, and chaired by David Martinsen. The morning sessions featured talks centered around two broad themes: tools and resources that can facilitate global science, and global cross-cutting issues. In the first group, Steven Muskal described the efforts of Eidogen-Sertanty to use cloud-based mobile app development and pipelining technologies to meet global needs; Tony Williams and Valery Tkachenko talked about the Royal Society of Chemistry (RSC) efforts to build a chemical data repository that can enable storage, validation, standardization, and sharing of data, and that can also enhance scientific publishing; Charlie Weatherall presented an overview of CDD Vault, which is a tool to manage, visualize and share chemical and biological data and described some examples of its use in team science; Andrey Yerin described the new IUPAC organic nomenclature and the concept of Preferred IUPAC Name (PIN) and how ACD/Labs is working to incorporate it into the newest iterations of their products. Global issues broached in this session included the state of photovoltaics in the world, by Colin Perry.
from the University of North Texas, and the need of open data for drug discovery of rare and ultra-rare diseases, by Sean Ekins of Collaborations in Chemistry.

The afternoon sessions focused on how the changing global landscape of science affects scholarly communication. A common issue raised by several speakers was how the global nature of science is pushing publishers to engage with new audiences and creating new markets for companies offering services to international authors. Thus, Amy Beisel of Research Square described some of the challenges that international authors face when submitting articles to English-language journals: preparing and formatting the manuscript, making sure that the topic fits the journal scope, responding to reviewer comments, and understanding the correspondence from editors and reviewers.

Talks by ACS and RSC staff brought the chemistry publisher perspective and highlighted their focus to reach globally. Steve Hansen and ACS journal editors Kirk Schanze and Prashant Kamat presented an overview of the expansion of the well-established ACS on Campus program to Mexico, China, and India. They also summarized what they have learned about participants of those programs, including their desire for information and advice on the peer review and publication process, their value of recognition and eagerness to see their research published, and their concerns about the fairness of the peer review system. Along the same lines, Stephen Hawthorne and Daping Zhang presented RSC efforts for supporting and facilitating the development of research beyond the scientific powerhouses in chemistry, such as their community engagement in Far East Asia and Latin America, and their focus on developing skills in Russia, Africa, and India.

Chinese journals are also seeking to increase their international influence. Xiaowen Zhu of University & Higher Education Press described the situation of chemical journals in China from the Chinese publisher point of view. Increased financial support by the government, international editorial boards, and collaboration with international publishers were some of the strategies mentioned.

New trends in scientific publishing are also likely to have a global impact. Thus, the session also included two talks centered on new trends in scholarly communication by open access publishers. Frederick Fenter described Frontiers’ efforts to increase article discoverability and visibility in the global research community by using a scientific social network. Martin Hicks of Beilstein-Institut focused on the challenges in scholarly communication, such as data reproducibility and integrity, issues in the peer review system, and plagiarism.

Finally, the symposium concluded with a talk on how to engage with non-scientific audiences to fight chemophobia.

Elsa Alvaro, Symposium Reporter

Please join us again for the CINF symposia in Denver, March 22-26, 2015!


A list of the CINF symposia planned for Denver is at: http://www.acs.org/content/acs/en/meetings/abstract-submissions/cinf.html
Herman Skolnik Award Symposium 2014
Honoring Engelbert Zass

Introduction

Throughout his career Dr. Engelbert Zass (“Bert”), head of the Chemistry Biology Information Centre at ETH Zürich (retired), has been a bridge builder and mediator between database producers, vendors, publishers, librarians, and end users in chemistry, contributing to advancing chemical information as a whole. Specializing in chemical information after receiving his Ph.D. in organic chemistry, Dr. Zass has more than 30 years of experience in searching, operating and designing chemistry databases, as well as in the support, training, and education of users of chemical information. He has given numerous lectures and courses in Europe and the United States, is author of more than 60 papers on chemical information, and served on several publisher advisory boards. From 1999 till 2004, he was a partner in the German Federal Ministry of Education and Research’s project “Vernetztes Studium – Chemie,” where he was engaged in the design of multimedia educational material for chemical information. Through his leadership, vision, and collaborative efforts with his staff, ETH Zürich developed a model 21st century library. Dr. Zass did his undergraduate studies in chemistry at Universität zu Köln, followed by a Master’s degree (Diplom) in Chemistry with Prof. E. Vogel. He went on to complete his Ph.D. (Dr. sc. nat.) studies with Prof. A. Eschenmoser at ETH Zürich. He then became a lecturer and senior scientist at ETH, later serving as Head of the expanded ETH Chemistry Biology Pharmacy Information Center until his retirement in 2012.

Evolution and transformation of journals in a digital environment

Grace Baysinger of Stanford University opened the proceedings with a talk about electronic journals. The number of electronic journals continues to increase: CrossRef (http://www.crossref.org/01company/crossref_indicators.html) covers over 35,000 and the Directory of Open Access Journals (http://doaj.org/) lists about 9,700. Chemists make extensive use of journal articles. Most publishers now offer them electronic manuscript submission systems and authoring tools. The Royal Society of Chemistry (http://www.rsc.org/Publishing/Journals/guidelines/AuthorGuidelines/AuthoringTools/), for example, offers author templates, an experimental data checker, and a Crystallographic Information File data importer.

We need more automated data checking tools, not just to aid authors, but also to help prevent fraud. It is important that readers should be able to reproduce the work reported in an article; reproducibility depends partly on the availability of supporting information. Open source software and lower computing costs make it easier nowadays to re-use data. NISO and NFAIS have published Recommended Practices for Online Supplemental Journal Article Materials (http://www.niso.org/workrooms/supplemental). CrossCheck (http://www.crossref.org/crosscheck/index.html) prevents plagiarism; CrossMark (http://www.crossref.org/crossmark/) provides a standard way for readers to locate the authoritative version of a piece of content; FundRef (http://www.crossref.org/fundref/) provides a standard way to report funding sources, and ORCID (http://orcid.org/) provides a persistent digital identifier that distinguishes an author from every other researcher.

Many people think that traditional peer review is “broken” (http://www.nature.com/nature/peerreview/debate/) because it causes delays, and reviewers are overloaded. Alternatives are pre-publication review as carried out by arXiv.org (http://arxiv.org); post-
publication review as in Faculty of 1000 (http://f1000.com/); and open two-stage peer review as used by Atmospheric Chemistry & Physics (http://www.atmospheric-chemistry-and-physics.net/review/review_process_and_interactive_public_discussion.html).

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Collection management is different in the era of the electronic library. Expenditure reports have to be produced; electronic resource management systems are needed for storing licenses; and authentication and security must be handled correctly. Catalog records for bibliographic data and knowledge bases for online holdings must be maintained. COUNTER (http://www.projectcounter.org/about.html) and SFX reports (http://www.exlibrisgroup.com/category/SFXOverview) measure electronic usage. Print collections get sent to storage and archiving of print may be shared. Online access may be perpetual or there may be archival access to an online version. Repositories for data have been established. Pricing is a major issue. Chemistry journals reportedly have the highest average cost (http://lj.libraryjournal.com/2014/04/publishing/steps-down-the-evolutionary-road-periodicals-price-survey-2014/#) of all subject areas: $4,215. A recent article has drawn attention to variations in pricing across institutions and a lack of transparency. All sorts of metadata issues may arise. There can be multiple titles in one catalog record for the print version of a journal. Only the latest title may be on the publisher site, or in the open URL knowledgebase, but the link and content may include older titles. Digitization and metadata for a journal may be incomplete. Multiple versions or copies of the same article may be on different sites. Problem-solving is more difficult now that print copies from libraries are in storage or withdrawn. NISO has published Recommended Practices for the Presentation and Identification of E-Journals (http://www.niso.org/workrooms/piej).

Archival material can be accessed through the Wayback machine (http://archive.org/web/), Portico (http://www.portico.org/digital-preservation/), Hathi Trust (http://www.hathitrust.org/help_general), and Lots of Copies Keep Stuff Safe (LOCKSS, http://www.lockss.org/) and Controlled LOCKSS (CLOCKSS, http://www.clockss.org/clockss/Home), but there are still problems with "bit rot" and multimedia content. LOCKSS and CLOCKSS are the only services that check for bit rot. Data are being stored in repositories and databases, and on Amazon cloud.

Mobile access is another big theme. Enhanced journal article services are now being added by publishers: see, for example, the tools supplied by ACS (http://pubs.acs.org/doi/abs/10.1021/cb500271c) and Wiley (http://onlinelibrary.wiley.com/doi/10.1002/ajoc.201402054/full). The University of California Irvine has an online guide to research impacts using metrics (http://libguides.lib.uci.edu/researchimpact-metrics). Article level metrics are increasingly becoming an alternative method of measuring the impact of scholarly and other output: Altmetric (http://www.altmetric.com/) is an example.

There are many resources for discovery and delivery including open URL knowledge bases, Portico (http://www.portico.org/digital-preservation/), databases, federated sites and tools (e.g., xSearch at Stanford, https://xsearch.stanford.edu/search/), alerts and RSS feeds, data mining and visualization, XML parsing of content, linked data and taxonomies, and machine-to-machine retrieval via APIs and Web Services (e.g., Stanford Profiles (https://profiles.stanford.edu/), a LinkedIn-type service for Stanford faculty).
End user behavior

Research publications are ultimately intended to be read by scientists. What do they want and need in a publication? How do they gather their information and decide what to read? When and how much do they read? User studies of various kinds have been done to try and find answers to these questions. Andrea Twiss-Brooks of the University of Chicago Library reported on recent studies in which she has been involved.

User studies carried out in around 2005, many conducted by Tenopir and King, showed that users browse for current articles and current awareness, but search databases or follow citations for older articles. They rely on the library copy for all but a few core titles, and authoritative and trusted sources are preferred. They need an efficient means of accessing literature: time management is a priority. Reading supports primary research, background research, teaching, and writing.2

User behavior research may be basic or applied, and methods may be quantitative or qualitative. Quantitative methods include surveys (using the Likert Scale, for example, a psychometric scale often used with questionnaires), return on investment metrics, citation metrics, altmetrics, and server log analysis. These methods answer the “how much?” “what?” and “when?” type of question. They are easier to manage and design (sometimes), empirical, and perhaps extensible. Standardized statistical approaches can be used.

Qualitative methods include focus groups, interviews, open-ended comments on surveys, and applied ethnographic techniques which may include research diaries, mapping the diaries with interviews, and observation. Qualitative methods often require more oversight by Institutional Review Boards (IRBs). They produce information only on the cases studied: generalization is more difficult. They give insight into “how?”, “why?” and “who?” These questions can often not be answered by quantitative methods, but analysis of qualitative results can be more challenging and is usually not statistical.

Nancy Fried Foster and Susan Gibbons have used anthropological and ethnographic methods to examine how undergraduate students at the University of Rochester write their research papers. Students (with informed consent) were watched, and they kept diaries. The results were published in Studying Students: the Undergraduate Research Project at the University of Rochester (http://www.ala.org/acrl/sites/ala.org.acrl/files/content/publications/booksanddigitalresources/digital/Foster-Gibbons_cmpd.pdf).

Early in 2012, David Bietila and Gina Petersen at the University of Chicago conducted a qualitative study of the research process of eight graduate students in the humanities and social sciences. This study aimed to model the research process, enhance the understanding of the relationships between information tools and services, and identify gaps between participant behavior and librarian expectations. The study’s data collection comprised three components: research logs, semi-structured interviews, and commentary by subject librarians on student research practices. The findings indicated that source discovery was not a primary concern for participants, but that developing a feasible, clear, and relevant topic was a much greater obstacle for most participants. Bietila and Petersen spoke about this in “Guiding Interface Design with Ethnographic Methods” at the American Library Association Annual Meeting in 2013.

Some examples of research log questions were:

- What were you trying to accomplish during this research session?
- At what time did you conduct this research session?
- Where were you when conducting this research session?
What tools did you use to help conduct your research?

Examples of interview questions were:

- What do you anticipate will be the most difficult part of the research?
- How do you evaluate sources?
- How have you converted your topic into a searchable phrase or keywords?

Graduate students tended to use the same resources, for example, JSTOR. They did a broad search and read a few articles. They used a non-linear, non-structured process; they did not have a set process for doing things. The librarian would always have done the job differently. A report on the study has been published (http://www.lib.uchicago.edu/gradstudy).

A second project, “A Day in the Life,” is ongoing. This mapping project is applying ethnographic methods to clinical health information research. It is a low-cost, six-institution study investigating how third-year medical students seek and use information in the course of their daily activities. The students mark their movements on a map for one full day. Each participant is then interviewed (and rewarded with a $100 gift card). Interviews are audio recorded and transcribed. The transcripts are coded and analyzed in order to identify possible service, facility, resource and other improvements.

Nancy Fried Foster, who was involved in the University of Rochester work, is the analyst and consultant. The medical students have a much more focused life than the University of Rochester students did: they went to the clinic and stayed there. The interviewers carried out “interested, neutral listening.” They were taught how to code the transcripts in a two-day workshop. Preliminary results suggest that “putting on the white coat” is significant, and time management matters. When selecting the best information tool, print books are more important than predicted. Andrea has learned some other lessons concerning timeframes, the challenges of multi-institutional studies, the funding and IRB process, and achieving consistency in methods in study design. The importance of the team leader for each institution, and the value of the consultant are significant success factors.

Panel discussion on information literacy

Two speakers were unable to attend at the last minute so an impromptu panel discussion was arranged. While impromptu, this discussion sparked a lively dialogue between panel members and attendees. The panelists were Engelbert Zass, Grace Baysinger, Andrea Twiss-Brooks and Donna Wrublewski (of Caltech).

Bert has been running courses at ETH Zürich and at the Universities of Bern and Innsbruck, teaching chemical information since 1981. Nowadays, he said, the providers do a much better job of training, but it is source-oriented; Bert does problem-oriented training. He reported that registration for SciFinder is not liked; at Innsbruck students found it even difficult. In order to register as SciFinder users, students have to find a link on their University’s website, and from there connect to the specific CAS connection page; for SciFinder, there is no direct registration from the general database start page as in Web of Knowledge, Scopus, or Reaxys. Trainees are better at searching nowadays (because of better user interfaces), but they find it harder to find the full text and original source if the link is broken: they often do not know how to use the library’s online public access catalog (OPAC). Many also have problems in defining a structure query.
Grace offers workshops, gives presentations to classes, and does a lot of one-on-one consultation to users. All of the major database vendors also provide short online tutorials that users can consult. The spectrum of expertise levels varies considerably. While some users are very “tech savvy,” they may have limited experience searching chemical information. Because Google provides a couple of highly relevant citations quickly and easily, multi-tasking users have developed “short attention span theater” and now expect to locate information without any training. Unfortunately, they do not know what they do not know. One colleague reported that some students hired to work in a corporate environment did not have the information skills needed for the job because they had relied too much on Google while in school. One area that Grace has been concentrating on is compiling information about laboratory safety resources as users may not be as familiar with them as they are for materials in other areas of chemistry. With so many materials now being purchased only in a digital format, it is critical for users to learn how to navigate in the OPAC rather than to rely on browsing print copies in the stacks. With student populations in universities now being more diverse, English may be a second language. Hands-on practice is essential in chemistry, not just a demo.

Donna was taught by a member of the audience as an undergraduate student; her academic advisers were not much help. Some people just go to the library to hide. When Donna arrived at the University of Florida she was able to think what would have made her thesis project less painful. She modularizes her information literacy courses. Controlled vocabulary is very important in chemistry. She teaches one useful strategy for each of Google, Wikipedia, the OPAC, and Web of Science. She uses a topic with which the user is familiar in order to start formulating a strategy. If you can find it on Amazon you can use an OPAC.

Andrea outlined some challenges faced at the University of Chicago. Two thirds of students are graduate students and one third is undergraduates. There are non-bibliographic information sources and tools used in science and medicine research that librarians may not be familiar with, nor have the training or knowledge to use. Students are being asked to use all sorts of new IT and analysis tools, for example, OpenBLAST, FlyBase, and other bioinformatics tools. The University’s Computer Science Instructional Laboratory tutors teach the use of computer programming tools. Librarians collaborate with the tutors to see what resources the students need and how best to refer the students needing expert training. The library tries to keep aware of where the expertise lies at the University. For example, 3D visualization is available at the Research Computing Center. In joint courses, the library provides the space, and the partners provide the expertise. The library also works with the IT group: the IT group can do problem-solving for mobile devices setup, and they will do things such as MatLab training, for example. The library also works with vendors for on-site and Webinar training, providing the room with computers, or the needed audio and video setups.

Questions were invited from the audience. One person said that the four panelists were all from big libraries; what about smaller schools? Bert replied that Bern and Innsbruck are much smaller than ETH Zürich. Even with a limited number of databases you can teach people to use what they have, but this demands creativity. The questioner felt that Europe is different. Grace said that at undergraduate institutions librarians usually spend more time teaching than doing collection development, but the number of resources being taught is smaller. Grace helped revise a document on information literacy skills that undergraduate chemistry students should achieve by the time they graduate (e.g., search by topic, author, and physical properties). This document included resources that could be used to learn that skill. Due to small budgets, at some skills an effort was made to include high-quality free resources and to put a dollar sign by resources that need to be purchased. Often, instruction that is integrated into a course and tied to an assignment that a student must complete is the most effective type of training at the undergraduate level. Starting her academic career at a junior college, Grace benefited by getting personalized help from her instructors and the librarians. Because so much stuff in chemistry can be related to ordinary life, it provides an
opportunity to introduce undergraduates to chemical information tools and to increase their interest in chemistry as a discipline.

Another person asked if it is appropriate to use Google. Yes, said Donna, with some hesitation. Bert recommends using all sources. Yes, said Grace, if the risk is low. It should not be used for explosives, for example. The questioner pointed out that Google points you to a source. Could you run a course on Google? Andrea thought you probably could; searching is a general skill that everyone should have. Grace would prefer to teach Google Scholar rather than Google for finding information. When Grace attended the Biennial Conference on Chemical Education (BCCE) in 2012, she heard a presentation by a chemistry professor who is using Wikipedia to help teach students better writing skills. First the students evaluate an article present in Wikipedia and then they have to write an article for Wikipedia. With Google you can get 1 million answers in under a minute, but it can take hours to evaluate the hits if you are trying to do a more comprehensive search. Donna pointed out that Google has offered courses, but not in chemistry. A librarian in the audience has taught a laboratory class for non-chemistry majors. She used Wikipedia and got the message across about the pros and cons. Faculty and students do not think they need teaching. There are cultural differences too: students need to get something useful that they can use in their own projects.

Donna reported the same problem in teaching ethics and communication and safety. Faculty do not have time to care. Grace said that the Stanford Chemistry Department has laboratory safety coordinators for each laboratory group, who are semi-expert. She has resisted this model for chemical information as everyone should learn how to use information, but maybe an information coordinator in the laboratory would be helpful. Bert said that in “the STN days” ETH had this concept in order to save money. When Beilstein CrossFire came along, the information coordinators were known and could be useful contact persons.

Another librarian in the audience said that the answer is in the kind of question you ask on Google. In the print days you asked the librarian if you could not find something in a book. In the electronic era you do find something so you may not ask the librarian. Google is superlative at the “good enough” answer, but it fails on an exhaustive search. Yet another librarian said that he introduces Web of Science. Students do not use the right fields. He uses queries such a “XYZ was published in Tetrahedron; how often has it been cited.”

A German attendee pointed out that courses of this sort are not usually taught in Germany. Andrea said that, in theory, information literacy has to be taught in the United States. The German attendee said that the course could take two hours out of a laboratory class. Grace noted that if it becomes a library class rather than a chemistry class, the faculty member may object. For example, faculty may want the students to analyze peaks in their spectra manually, rather than do a spectral peak search in a database. Doing this may be harder and take longer when trying to identify an unknown, but the students understand chemistry better if they have done the analysis manually. Donna said that learning how to use SciFinder should not be made difficult.

Grace added that in the days of print, people used to be able to browse the stacks; they have to use the OPAC now. Bert feels that it is important to show people how to find a good book or review. You have to show them an example. Grace said that some people know how to use RSS feeds, but others do not know what tools are available for keeping current.
Chemical publications revisited

Guido F. Herrmann of Georg Thieme Verlag also addressed the topic of chemical publications, but concentrated on the connections between full-text information and information embedded in the chemical structures and reactions. Thieme (http://www.thieme.com/) is a medium-sized publisher that has had an internationally strong position in chemistry (https://www.thieme.de/en/thieme-chemistry/home-51399.htm) since 1886. It produces journals, textbooks, monographs, reference works, dictionaries, databases, continuous education products and interactive online libraries, in multiple formats. These basic categories have been very robust and stable for more than a hundred years. In contrast the published formats (digital versus print), the user expectations, the production processes, and the distribution channels have seen significant change over the last decade.

According to the November 2012 STM report An overview of scientific and scholarly journal publishing (http://www.stm-assoc.org/2012_12_11_STM_Report_2012.pdf) “the number of articles published each year, and the number of journals, have both grown steadily for over two centuries, by about 3% and 3.5% per year respectively. The reason is the equally persistent growth in the number of researchers, which has also grown at about 3% per year.” A major change, a veritable revolution, has been the move from print to electronic distribution, and Thieme is still managing an ongoing change process. All Thieme’s chemistry publications now have digital versions, including backfiles from 1909 onwards.

The basic role of a publisher has remained, but the actual operations and production processes have changed drastically. The STM Tech Trends 2013 poster (http://www.stm-assoc.org/future-lab-trend-watch-2013/) illustrates many things that are starting to happen: where should a medium-sized publisher focus? Can a publisher help in converting scientific information into applied knowledge? One goal is not just to produce information, but to create value. In May 2008, a Research Information Network report (http://www.rin.ac.uk/system/files/attachments/Activites-costs-flows-report.pdf) estimated that “the global cost each year of undertaking and communicating the results of research reported in journal articles is £175bn, made up of £116bn for the costs of the research itself; £25bn for publication, distribution and access to the articles; and £34bn for reading them.” Publishers could add value by reducing the cost of reading, that is, by providing researchers with relevant information more effectively.

Guido gave two examples. The first concerned primary data. Guido estimates that there are 500,000 to 1 million datasets a year in organic chemistry. To preserve them, and make them discoverable and re-usable, requires servers and data centers, metadata, and digital object identifiers (DOIs). FIZ Karlsruhe (http://www.fiz-karlsruhe.de/home.html?&no_cache=1&L=1) houses the Thieme data, and Technische Informationsbibliothek (TIB, the German National Library of Science and Technology (http://www.tib-hannover.de/en/) assigns DOIs to them, stores the metadata and keeps them searchable. TIB is the managing agent of the DataCite organization (http://www.datacite.org/). At the same time as an article is published, the primary data are published as an independent entity: the article quotes the research data as reference items with the assigned DOI.

Authors of articles in the Thieme journals SYNLETT and SYNTHESIS are now being invited to submit their datasets for publication alongside their articles. The primary data have their own DOI, different from the one of the paper, and can thus be cited independently. Spectra, for example, are published not as PDFs or JPEGs, but as raw, interactive data, which can be downloaded and analyzed. Benefits are citability and high visibility of research data, easy re-use and verification of the datasets, avoidance of duplication, and motivation for new research. Unfortunately, authors are, thus far, not enthusiastic about supplying their data, and reviewers claim they have no time to check the data.
Guido’s second example concerned full text, structures and reactions. Science of Synthesis (https://science-of-synthesis.thieme.com/app/home) is the successor to Houben-Weyl, the archive of which contains approximately 146,000 experimental procedures, 580,000 structures and 700,000 references, in 160 volumes. Science of Synthesis (from year 2000 onwards) contains approximately 50,000 experimental procedures, 270,000 reactions, and 1,250,000 structures in 48 volumes. Science of Synthesis Updates (since 2010) contains a further 18,000 experimental procedures and 40,000 reactions in 17 Volumes. Science of Synthesis Reference Library (since 2010) contains 15,000 experimental procedures and 40,000 reactions in 13 Volumes. New material is uploaded several times a year.

Science of Synthesis 4.0 has a new production system this year, developed in collaboration with InfoChem (http://www.infochem.de). Previously, all reaction schemes were completely redrawn and indexing was done manually. Now authors’ schemes are used (with modification), the schemes are checked and modified by a scientific editor, and the indexing is mostly automated. In the days of manual indexing, each structure was taken from a scheme and loaded into a database; starting materials, products, reagents, solvents, temperature and yield were defined by an indexer; each individual structure and reaction was extracted from tables and scheme tables; and it took about three months in all to index a Science of Synthesis volume. Now Thieme, in a continuing collaboration with InfoChem, has developed an automated indexing system: structures and reactions are automatically indexed using InfoChem’s SchemeAnalyzer software, which is 85% successful in extracting structures and single-step reactions directly from complex schemes in ChemDraw files. Another new development is the implementation of a MarkLogic NoSQL database (http://www.marklogic.com/what-is-marklogic/) for a new graphical user interface, and full-text and data search. Work is ongoing further to improve the link between the InfoChem system (i.e., chemical information) and the MarkLogic system (i.e., full-text information). The final system will give even better value to the user.

CAS keeps pace with the worldwide growth in disclosed chemistry

Chemical Abstracts Service (CAS) has always been a leader in providing scientists with access to chemical information. Matt Toussant of CAS described how CAS has adapted to the phenomenal growth in chemical information being published today. The ACS is committed to “improving people’s lives through the transforming power of chemistry.” Its mission is “to advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people.” The mission of CAS is “to provide the world’s best digital research environment to search, retrieve, analyze, and link chemical information.” Chemistry is the central science.

Matt showed a timeline of some influential events in publishing. Johannes Gutenberg invented the printing press in about 1450. The Internet started with the time-sharing of computers in the early 1960s at U.S. universities and with the Advanced Research Projects Agency Network (ARPANET), developed after the launch of Sputnik in 1957. Ebooks are now an alternative to printed books. Galileo’s heliocentric dialogue was published in Latin by Elzevir. Robert Boyle’s five-person dialogue The Sceptical Chymist was published in 1661. Books were printed in small numbers in those days; nowadays books are widely available.

The history of scientific journals dates from 1665, when the French Journal des sçavans and the English Philosophical Transactions of the Royal Society first began systematically publishing research results. The number of serials (http://www.stm-assoc.org/2012_12_11_STM_Report_2012.pdf) has grown every year since then. Eventually abstracting and indexing services such as Chemisches Zentralblatt (born in 1830) were needed to help readers keep pace with the literature. Chemical Abstracts (CA) began in 1907. Later, CAS extended its reach into the patent world. In 1641, Samuel
Winslow was granted the first patent in North America for a new process for making salt. The first U.S. patent was granted in 1790. The first patent in *Chemical Abstracts* dates back to 1808 and concerns an alcohol still.

CAS has covered several serials for more than 100 years, for example, *Annalen der Chemie und Pharmacie* (later *Justus Liebig's Annalen der Chemie und Pharmacie*, now part of the *European Journal of Organic Chemistry*) which began in 1840. CAS has covered 50,000 journal titles over the years; it now covers 10,000. It has more than 100 years’ experience of analyzing and organizing disclosed chemistry from around the world. The work is no longer done manually in a library at Ohio State University; nowadays computerized data entry and sophisticated tools are used. Chemist labor around the world, and “postal support” to analyze chemical publications, ended in 1994 because it was too slow. At its peak in 1967, this process involved nearly 3,500 people. A newsletter called *The Little CA*, published up to four times a year, kept the “volunteers” informed. E. J. Crane (editor of *CA* from 1915 to 1958) was the main author. The volunteers worked all over the world: Czechoslovakia, Poland and the United States were well-represented, but the largest number was that of Japanese chemists. Neutral parties helped during the war years. Much analysis is now outsourced to India, Japan and China.

The history of CAS REGISTRY goes back to a concept of Malcom Dyson’s in the 1950s. The original database was a file of fluorine compounds using the Dyson-IUPAC notation on edge-notched cards. In the 1960s, Harry Morgan of CAS, building on the work of Donald Gluck at DuPont, published an algorithm that converted structure diagrams into unique tabular forms. This handled aromatic and tautomer bond representations and established the basis for REGISTRY. The building of REGISTRY began in 1964.

The CAS indexer analyses the whole document, creates a CAS REGISTRY record and interprets when compounds are described in terms other than singular structures or names. A typical chemistry patent (a PCT application for “A new antibacterial,” with 250 pages and 24 claims) took 15 days to index completely, with 917 compounds, 576 new compounds, 613 single-step reactions, 5,394 multistep reactions, 1,029 reaction participants, and one MARPAT Markush structure with 2,119 substituent definitions. CAS specialists in many fields of chemistry interpret author terminology to register compounds. Spectra, numeric properties, tags, and published sources are recorded. CAS databases continue to show strong growth. In particular the number of patents has greatly increased recently (9.2% growth in 2012); much of the increase is due to China, Korea and Japan. About half of small molecule registrations are compounds from patents. Sixty-three patent authorities are now covered, and it usually takes less than 27 days from receipt for a patent to appear in *CA*. In non-patent information, Matt drew attention to growth in Asia. Nowadays, 69% of items indexed by CAS are in English, 13% in Chinese. More than 89 million CAS Registry Numbers have been issued; 29 million registered substances have been indexed in the last 5 years alone. The number of prophetic substances and Markush structures is up more than 10%.

Apart from journals and patents, CAS also covers dissertations, meeting abstracts, and conference proceedings, more than 1,000 ahead of print journals, valuable Web sources, commercial chemical suppliers and regulatory inventories. Attendance at national meetings by larger societies does not really seem to be decreasing. “Ahead of print” appearance of journal articles, rapid publication, and “letters” journals are other trends. Speed of publication is critical. The proportion of ACS articles with supporting information rose from 60% in 2012 to 70% in 2014; supporting information is mostly in the form of PDF files, but there are also Crystallographic Information Files.

Matt ended with some predictions. Numbers of all forms of publications will continue to increase annually by 3% to 5%; Web-based “As Soon As Publishable” will dominate. Supporting information
will broaden. Open access will play a significant role. Asia will be the origin of much new science. Disclosures originating from commercial sources will increase as new substances are being created in laboratories around the world. The pace of growth in patent applications will slow, but patents will remain a main vehicle for the monetization of science. Finally, meetings with a geography requirement will lessen further, as technology makes global connections easier and more efficient.

**InChI and the information chain**

Steve Heller of the National Institute of Standards and Technology (NIST) gave an overview of the IUPAC International Chemical Identifier (InChI, [http://www.iupac.org/inchi](http://www.iupac.org/inchi)). InChI is a non-proprietary, freely available, machine-readable string of symbols that enables a computer to represent a compound in a completely unequivocal manner. InChIs are produced by computer from structures drawn on screen with existing structure drawing software, and the original structure can be regenerated from an InChI with the same software.

Like bar codes, and QR codes, InChIs are not designed to be read by humans. InChI should be thought of as “plumbing,” a modern enabling technology. It is not something the average chemist needs to know about: researchers merely use it to find and link information on the Web. There is too much information on the Web and it lacks integration and connection; InChI is an infrastructure foundation that allows for linking, and hence for higher productivity. It is not a replacement for any existing internal structure representations; it is in addition to what is used internally. There are four amusing videos on the Web that explain InChI simply:

- *What on Earth is InChI?* ([http://www.youtube.com/watch?v=rAnJ5toz26c](http://www.youtube.com/watch?v=rAnJ5toz26c)),
- *The Birth of the InChI* ([http://www.youtube.com/watch?v=X9c0PHXPfso](http://www.youtube.com/watch?v=X9c0PHXPfso)),
- *The Googlable InChIKey* ([http://www.youtube.com/watch?v=UxSNtvs8Rjw](http://www.youtube.com/watch?v=UxSNtvs8Rjw)), and
- *InChI and the Islands* ([http://www.youtube.com/watch?v=qrCqJ0o4jGs](http://www.youtube.com/watch?v=qrCqJ0o4jGs)).

Some people question why InChI should be used instead of SMILES. SMILES is a popular line notation but it is not a published standard. Each vendor has a different implementation of SMILES, so strings cannot reliably be compared. SMILES has no structure normalization, so different structural representations yield different SMILES strings: a subscriber to chminf-l has reported finding 172 different SMILES representations for caffeine on the Web. InChI is easy to generate using existing software, expressive of structural information, unique and unambiguous, and amenable to searching for structures using Internet search engines (using a hash key).

The InChI standard was developed by consensus, by a technically competent team, with political and technical cooperation. The work involved precompetitive collaboration among publishers, database producers, and software vendors. InChI is not in competition with commercial products, it has no “mission creep,” and it is endorsed by IUPAC. The standard has been widely adopted: there are, for example, tens of millions of InChIs in each of PubChem, ChemSpider and Reaxys, and an InChI can be input to SciFinder to search the 89 million compounds in CAS REGISTRY.

If the work of the InChI project were to endure, it needed to be turned over to an entity that would ensure its ongoing activities, and be acceptable to the community. A not-for-profit organization was best; hence the decision to create and incorporate the InChI Trust ([http://www.inchi-trust.org](http://www.inchi-trust.org)) as a UK charity. The Trust has about 60 Members, Associate Members, and (non-paying) Supporters. The InChI project has experienced remarkable cooperation and support. It is a truly international project with programming in Moscow, computers in the cloud, incorporation in the United Kingdom, and a project director in the United States. Collaborators from over a dozen countries, from academia, the
pharmaceutical industry, publishers, and the chemical information industry, have all offered senior scientific staff to develop the InChI standard.

Organizations need a structure representation for their content (databases, journals, chemicals for sale, etc.), so that it can be linked to and combined with other content on the Internet. InChI provides an excellent return on investment and increases productivity. It is a freely available, open source algorithm that anyone, anywhere can freely use, and it is certainly widely used: its success is proved by un-coerced adoption. InChI’s combination of the Internet, open source software, crowdsourcing, graph theory, existing representation algorithms, digitized data available on the Web, and search engines has created a very valuable tool. This is taking advantage of “the second machine age,”6 which includes “recombinant innovation,” or mashups.

InChI is a “layered” line notation, currently with the following layers:

- Formula
- Connectivity (no formal bond orders)
  - disconnected metals
  - connected metals
- Isotopes
- Stereochemistry
  - double bond (Z/E)
  - tetrahedral (sp3)
- Tautomers (on or off).

Charges are added to the end of the string. Layers are separated by slash marks. Opening characters before the formula denote the version of the algorithm used. An example is alpha-D-glucose:

\[
\text{InChI}=1S/C6H12O6/c7-1-2-3(8)4(9)5(10)6(11)12-2/h2-11H,1H2/t2-,3-,4+,5-,6?/m1/s1
\]

The InChI algorithm normalizes chemical representation, and includes a “standardized” InChI, and a “hashed” form called the InChIKey. The key facilitates Web searching, previously complicated by unpredictable breaking of InChI character strings by search engines. The “standard InChI” and InChIKey for caffeine are shown below.

\[
\text{InChI}=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3
\]
\[
\text{InChIKey}=RYYVLZVUVJJVGH-UHFFFAOYSA-N
\]
The first block of 14 letters of the InChIKey (RYYVLZVUVIJVGH) encodes the molecular skeleton (the connectivity). The first eight letters of the second block (UHFFFAOY) encode stereochemistry and isotopes. After that, “S” indicates that the key was produced from standard InChI and “A” indicates that version 1 of InChI was used. The final character, “N,” means “neutral.” The first 14 characters of an InChIKey can be used to search for structures with the same skeleton (e.g., to find all stereoisomers).

The InChI certification suite is a software package designed to check that an installation of the InChI program has been performed correctly; it ensures that InChIs have been generated properly and consistently. Currently, InChI handles straightforward organic molecules; it is being extended to handle more complex entities such as organometallics, Markush structures, macromolecules, and reactions.

Virtual communities and beyond

Wendy Warr, of Wendy Warr & Associates (the author of this CIB article), looked at the evolution of virtual communities and publishing platforms. As research has become increasingly collaborative, possibilities for communication and collaboration on the Web have also increased. Virtual communities in science such as EiVillage and BioMedNet began to spring up in the 1990s. The earliest virtual community in chemistry, ChemWeb.com,7 was announced in August 1996 by MDL and Current Science Group, and launched in April 1997. It was acquired by Elsevier in October 1997. Elsevier closed all its “portals” in the middle of 2003, and ChemWeb.com was sold to ChemIndustry in April 2004.

ChemWeb.com was a pioneer in virtual conferences: the first was held in December 1997. The technology (interactive chat alongside PowerPoint slides and audio) was hardly ready to support such innovations at that time. Many chemists were unwilling to register themselves into a virtual community in the 1990s, but by 2002, ChemWeb.com had 300,000 members, and it offered 350 journals, 25 databases, structure searching, a careers center, a conference center, a bookstore, a magazine (The Alchemist), 11 forums, and a preprint server, the Chemistry Preprint Server (CPS, http://www.sciencedirect.com/preprintarchive).

The CPS was launched as an experiment in 2000. By Elsevier’s own criteria it was a partial success: the number of readers and their geographic spread were excellent; the number of preprints (466) was encouraging, but rather less than had been hoped for; and, unfortunately, it was difficult to ascertain the number of preprints going on to traditional publication. The CPS was terminated in 2002. An evaluation has been published.8

Chemistry as a discipline has been slow in adopting open access, but some journals merit a mention: Chemistry Central Journal, Journal of Cheminformatics, the Beilstein Journal of Organic Chemistry, Frontiers in Chemistry, Chemical Science, and ACS Central Science. ChemSpider (http://www.chemspider.com/), in particular, is worthy of note. Most of the publishing services discussed in the rest of this talk concern biology, medicine and biomedical sciences rather than chemistry.

In 2004, the year that ChemWeb.com changed hands, the term “Web 2.0” was first coined by O’Reilly. Not everyone would agree on the definition, or usefulness, of the term, but the era of wikis, blogs, feeds, podcasts, webinars, social networks, social bookmarking, and virtual worlds had begun.9 Facebook had 66 million users in March 2008: compare that with ChemWeb’s 300,000 in 2004.
People are no longer afraid of signing up to virtual communities. The traditional peer review process can now be challenged.

Peerage of Science (https://www.peerageofscience.org/), for example, promotes one peer review process for multiple journals, in ecology, and evolutionary and conservation biology. It is run by a for-profit organization, funded by publishers etc. The reviews themselves are peer-reviewed, but there is no journal editor in control of the peer review process. As of July 2014, 176 manuscripts have received 381 peer reviews, and there have been 942 peer review evaluations. Rubriq (http://www.rubriq.com/) also supports one peer review process for multiple journals. It offers independent, double-blind peer review and manuscript submission, recommends a suitable journal, and provides a score-card for reviews. The reviewer is rewarded financially, while the author pays for the R-score etc. Axios Review (http://axiosreview.org/) is another independent review service in ecology and evolutionary biology. The author aims at a top choice journal and “plays safe with others.” (Few manuscripts completely fail to be published, rather they are resubmitted, after rejection by one journal, to a less prestigious journal, in the so-called “journal cascade.”) eLife, BioMedCentral, PLoS and EMBO have started a peer review consortium in which papers are redirected with reviewer reports. Reviewers are anonymous to the author, but anonymity is optional for the journal cascade editor. SciRev (https://scirev.sc/) claims to be “speeding up scientific knowledge:” authors rate journals on efficiency and seek an efficient journal. An editor can compare his or her own journal with competitors.

So-called “mega-journals” (PLoS ONE, PeerJ, and eLife) are another trend. eLife arose from the San Francisco Declaration on Research Assessment (DORA, http://am.ascb.org/dora/). It is opposed to journal Impact Factors and runs a consolidated, pre-publication peer review service. Researchers can read and publish in eLife for free; the journal is supported by the Howard Hughes Medical Institute, the Max Planck institutes, and the Wellcome Trust. As of July 2014, it had published 488 articles, 85 of them in biochemistry. PeerJ is a peer-reviewed journal and preprint server in biological and medical sciences. It offers cheap, lifetime accounts (pre-paid). An editor handles pre-publication peer review. Some reviews (about 40%) are not anonymous. It links to Publons (vide infra). As of July 2014, it had published 476 articles and 433 preprints.

Frontiers (http://www.frontiersin.org/) was launched in 2007 by scientists from the Swiss Federal Institute of Technology, Lausanne, with a major investment by Nature Publishing Group. Its journals are largely in medicine etc., but also in chemistry, earth science, ecology and evolution. It offers open peer review in two phases (independent and interactive); anonymity is not allowed. Analytics automatically track views and downloads. The Frontiers evaluation system allows an entire community to score a paper. Frontiers has published 20,000 articles in 45 community-driven journals.

The business model is author-pays. The community also shares jobs postings. Other communities or social networks include Academia.edu (http://www.academia.edu/) and ResearchGate (http://www.researchgate.net/), where millions of researchers share papers, see analytics, and follow other people. The data repository Figshare (http://figshare.com/) has collaborative space in the cloud.

A number of centralized commenting platforms have sprung up. PubMed Commons (http://www.ncbi.nlm.nih.gov/pubmedcommons/) enables authors to share opinions and information about scientific publications in PubMed. Publons (https://publons.com/) collects peer review information from reviewers and publishers, produces reviewer profiles with publisher-verified peer reviews, and handles pre- and post-publication peer review. Authors (and a few peers) are notified of comments, and reviewers get credit in the form of DOIs. As of July 2014, 1,954 reviewers had produced 4,247 reviews. The service is free to academics. PubPeer (https://pubpeer.com/) offers anonymous post-publication peer review. Users can comment on any scientific article with a DOI, or
on an arXiv preprint, adding comments to a centralized database. Authors and other interested parties are alerted to comments. Journal Lab (http://www.journallab.org/) handles open summaries and peer review of PubMed papers, but anonymity is optional. It also offers journal clubs and discussions.

A few “publishing platforms” such as Faculty of 1000 (http://f1000.com/), ScienceOpen (https://www.scienceopen.com/) and The Winnower (https://thewinnower.com/) offer a wider range of services. Faculty of 1000 has F1000Prime (http://f1000.com/prime) literature filtering, and F1000Research (http://f1000research.com/), an open access journal and journal club, with open post-publication peer review. It has published 522 articles. F1000Posters (http://f1000.com/posters) was launched recently.

ScienceOpen is an open access, research and publishing network, launched on May 29, 2014. It features almost 1.3 million articles from PubMed Central and arXiv, by 2 million networked authors. It will publish all sorts of article types in the sciences, humanities, and social sciences. It offers collaborative pre-publication workspaces where authors can manage draft versions and share files, and easily collaborate on a paper. Authors get almost immediate publication with a DOI. Reviewers get DOIs for their open, post-publication peer reviews. Article metrics are powered by Altmetric. Authors benefit from automatic proofs, easy corrections, and versioning. User roles are allocated based on ORCID publication history. Public and private groups can be constructed.

In the world of open access, open data and open science what might happen next? It certainly seems likely that there will be consolidation (or closure) among the services mentioned above. Does Science Open have anything to learn from ChemWeb.com? ChemWeb was ahead of its time. If Elsevier had hung on to ChemWeb for just a short time longer, it would have had a ready-built community for Article of the Future and its other ventures. More than a decade after the Chemistry Preprint Server closed, chemistry still has a different culture from other disciplines, but a number of members of ScienceOpen’s scientific advisory board were in the audience, wishing the new venture well.

Reaxys: a digital transformation

Sebastian Radestock of Elsevier Information Systems gave this talk, replacing David Evans of Reed Elsevier Properties, who was indisposed. Sebastian talked about the long road leading to the current version of Reaxys (http://www.elsevier.com/online-tools/reaxys). Reaxys has its origins in the preeminent Gmelin and Beilstein Handbooks, begun by Prof. Leopold Gmelin in 1817 and Prof. Friedrich K. Beilstein in 1881. In the 1980s the focus was on database development: SANDRA (a structure-based tool to locate references in the Beilstein Handbook), and the Gmelin Formula Index were released in 1987-1988, and the Gmelin and Beilstein databases went online on STN and Dialog in 1989-1990.

Since then, the development focus has been the user. CrossFire was launched and improved between 1993 and 1995, and the printed Handbooks were discontinued in 1997-1998. The Patent Chemistry Database was launched in 2005. In 2009, Reaxys was launched, based on Gmelin, Beilstein, and the Patent Chemistry Database. In 2013, Reaxys was completely overhauled and its scope was expanded. In 2014, it was upgraded with re-indexing and concept search.

The 1989 version of Beilstein on STN was text-based; knowledge of the database structure and STN commands was needed; and not all query forms or results were readily accessible. CrossFire Commander in 1996 was a graphical, client-server based system. Access was improved with input forms, and structure and reaction searches could be combined with factual queries, but displays were rather cluttered. The 2014 version of Reaxys has a subject-oriented, customizable, Web-based user
interface; concept search is enabled; all types of chemical information needs are supported; and there is one-click access to advanced-query forms for multiple source databases.

The CrossFire database structure had three different, tightly connected contexts: substances and properties, reactions and reaction details, and citations and abstracts. This concept is still valid today: Reaxys is a bibliographic database with more than 46 million records from 16,000 journal titles; it is a substance database with more than 57 million unique substances and more than 500 million experimental facts; and it is a reaction database with more than 36 million single- and multi-step reactions. The database structure is built around a sustainable chemical substance model for single compounds, component compounds, and Markush compounds.

Chemists like to do graphical structure searching, but Elsevier wondered if they would also like to start searching for a topic by typing text. The company therefore surveyed 700 chemists with a wide range of job roles, years of experience, and worldwide locations. The chemists were from many different areas of interest (14% were in materials chemistry, 9% in organic chemistry, and 4% in electrochemistry, for example), and all sorts of organizations in many sectors.

The survey revealed a definite need for keyword search capabilities. On average, chemists search for chemistry-related information five times a week. Researchers in organic, inorganic, medicinal and organometallic chemistry are the most intensive searchers. Some 70% of the chemists are keyword searchers (in that they spend more than 60% of their time searching for keywords); 10% are structure searchers; 20% search for both keywords and structures. Structure search is highest among organic and inorganic chemists.

The searching pattern for both structure search and keyword search is similar. The top four use cases are:

- find reviews, introductory articles and other starting points for research
- find the very latest information on a certain topic
- search and retrieve substance properties, and
- compile a comprehensive survey of the published literature.

Keyword searchers more often search for reviews and introductory articles, properties, and comprehensive surveys of the published literature. There are some use cases which are ideally supported by structure searching.

Based on these results, Elsevier developed Ask Reaxys to be more than just a text search. Text input is analyzed to identify all possible queries; all queries are assigned a probability factor; and the query exceeding a certain probability factor threshold is automatically selected, or the user is prompted to select a query manually from the list of possible queries. Each word, or group of words, can be classified as bibliography, compound, concept, date, or keyword, or it can be ignored. An example is “electrical conductance of titanium.” This query could be “electrical conductance” as a concept and “titanium” as a compound; or it could be “electrical conductance” and “titanium” as keywords with “of” ignored. The former option is translated into a combined structure and factual query, and this is executed in the substances context (on a substances tab in the Reaxys interface). The latter is translated into a pure keyword query, which is executed against all text fields in the citations context. To improve the relevancy of the results, all citations and abstracts have been indexed, and enriched with additional Elsevier keywords.
For text input analysis, the input string is tokenized and each token is annotated using

- a proprietary tool for chemical entity recognition
- a regular expression for third party registry numbers and InChIKeys
- a list of author names
- a regular expression for dates
- a list of words that can be ignored, and
- a large chemistry taxonomy.

Text input analysis also involves annotation clean-up. Query translation takes the annotated text input and returns an advanced database query string.

ReaxysTree, a new chemical taxonomy, has been developed. Tree development started with looking at the Reaxys data structure (the field codes) and the database content. The tree was further extended using keywords from more than 46 million records from 16,000 journal titles. Synonyms and spelling variants were also added to each term. ReaxysTree contains more than 15,000 concepts with more than 40,000 synonyms. It is poly-hierarchically structured and organized in several chemistry-related facets. There are broad and narrow terms, each with a unique label ID, language, date, source, type, case sensitivity, etc. Elsevier’s taxonomy construction rules were followed. ReaxysTree is used for indexing the content in a continuous process of application and learning. After automatic indexing has been carried out, statistical analysis reveals new synonyms and additional terms, which are subjected to editorial work, and then fed back into ReaxysTree before further automatic indexing. The Ask Reaxys keyword search functionality is now prominently available at the top of the Reaxys query page (with a Google-like appearance). ReaxysTree can also directly be accessed, searched and browsed.

Award address

Finally, Bert gave his own presentation. In the last century, publications about total syntheses in journals would usually have full experimental details. A remarkable exception was the total synthesis of vitamin B12, considered a landmark in organic synthesis, involving the research groups of Robert Burns Woodward at Harvard, and Albert Eschenmoser at ETH Zürich. The synthetic target was actually cobyric acid, because this compound had already been converted to Vitamin B12.\(^\text{12}\) Hence total synthesis of cobyric acid would amount to a formal synthesis of Vitamin B12.
There are two variants of the total synthesis, differing in their overall strategy of creating the corrin system (in red in the vitamin structure below).
The variant collaboratively pursued closes the macrocyclic corrin ring between rings A and B (the “A/B variant”), while the synthesis accomplished at ETH achieves the corrin ring closure between rings A and D by a photochemical process (the “A/D variant”); the final steps toward cobyric acid were jointly carried out at Harvard and ETH, using material from the respective variants. Woodward reported on the A/B variant in lectures published in 1968, 1971, and 1973, culminating in the announcement of the total synthesis of the vitamin in his lecture at the IUPAC Conference in New Delhi, in July 1972. Eschenmoser discussed the ETH contributions to the A/B variant in his Centenary Lecture, published in 1970, and presented the approach to the photochemical A/D variant of the B12 synthesis at the 23rd IUPAC Congress in Boston, published in 1971 (http://e-collection.library.ethz.ch/eserv/eth:8691/eth-8691-01.pdf). A full report on the photochemical variant is given in a Science article which is an extended English translation of an article based on a lecture by Eschenmoser.

Seventy-seven postdoctoral students, but no Ph.D. students, worked on the project at Harvard between August 1961 and December 1975. Twelve Ph.D. students and 14 postdoctoral students worked on the project at ETH between September 1960 and August 1974. Research records consist of 67 postdoctoral reports (not publicly accessible) and 48 individual experimental procedures at Harvard, and 12 Ph.D. theses (publicly accessible) one diploma thesis (not publicly accessible) and 6 postdoctoral reports (not publicly accessible) at ETH. Unfortunately theses are not indexed in Chemical Abstracts and most European theses are not even covered by Chemical Abstracts or Dissertation Abstracts.

Bert found that a SciFinder search for “total synthesis of vitamin B12 (total synthesis of cobyric acid)” does not retrieve the significant publications by Woodward and Eschenmoser, although they can be found in Google. Web of Science finds Eschenmoser’s paper in Science and is the only database to find two papers in Chimia. (These references are just one short abstract about two talks given at a Swiss Chemical Society Meeting, so it is perhaps not surprising that they are not found in SciFinder.) Scopus finds Eschenmoser’s paper in Science, a paper in Japanese that is not found by SciFinder, although it is in Chemical Abstracts, and a paper by Wintner with recollections of ETH. Note the absence of papers by Woodward. Woodward’s 1972 lecture is found in Scopus and SciFinder if you include a space between “B” and “12.”

In summary, the primary publication record is incomplete: Harvard has no experimental details and ETH has them only in theses. In the secondary literature, too many publications are missed altogether and those that are covered are hard to retrieve. The tertiary publication record (plus the Web and Wikipedia) is often incomplete, and the change of paradigm exemplified by the two variants of the total synthesis is not recognizable.

In a lecture given at Wesleyan University on September 29, 1972, Woodward gives the only complete list of both Harvard and ETH co-workers ever made public so far; 50 Harvard postdoctoral students are not mentioned in other lectures published by Woodward. Only the Harvard-ETH A/B route is mentioned in this 1972 lecture; the A/D alternative is not. The tapes and slides of this lecture are no longer available, but Bert has a shorthand transcript by Eschenmoser’s secretary, Miss H. Gächter (now Frau Zass).

The ETH publication project started by Eschenmoser and the Zasses in 1979 is without precedent. It seeks to produce a high quality, fully documented record of 2,123 man-months of work, 3,732 pages of postdoctoral reports and procedures, and 1,889 pages of Ph.D. theses. Bert started by applying for all the Harvard records and recording individual reaction steps; 75 out of 77 postdoctoral students are now covered; two Russians are not included, for lack of information. Bert showed pages and pages of reports, listings, strategies, and handwritten records. Attribution is given to scientists for the specific
work they did, with detailed comments; everyone’s work should be acknowledged. The summaries for 238 compounds, with nomenclature and spectra, were at first recorded on edge-notched cards, in different colors to distinguish Harvard and ETH. Reaction pathways and flow charts for synthesis pathways and reaction details were drawn up. Compound-centered manuscripts and modular, standalone, experimental descriptions were produced. Literature references were listed and standards were drawn up for the data, solvents, reagents etc. All this work was patiently typed by Frau Zass and then retyped when corrections were needed.

Between 1979 and 1986, 599 handwritten pages were typed on a Remington typewriter and later retyped into Macintosh Word; 210 pages were processed on an Olivetti ETV 300 and later converted into Macintosh Word. From 1984 a computer graphics program was used. By 1983 the Harvard ring A/D work was finished; ETH rings B/C and D were finished in 1986. Bert had other work to do for ETH at this time, including most non-routine online searches, but the project was resumed in January 1990. The Olivetti work was converted in 1990. Corrections to the A/D seco-corrin records were completed by June 1991, and retyping of the Remington material was finished in February 1992. In 2006, work began to add theses to the ETH collection. By February 2009, the Macintosh Word 5.1 files were converted to Windows 97-2003. Unfortunately for the project, Bert and Eschenmoser had an enormous number of other commitments between 1984 and 2012, and the final steps carried out at Harvard and ETH are still missing. Bert is now resuming work on the project (in 1979, his first cheminformatics project) and he intends to finish it as a tribute to all the chemists involved, and in particular to Albert Eschenmoser.

Conclusion

The symposium was ably chaired by Andrea Twiss-Brooks. After Bert’s award address, Judith Currano, chair of the ACS Division of Chemical Information, formally presented the Herman Skolnik Award:

![Image of Bert Eschenmoser and Andrea Twiss-Brooks receiving the Herman Skolnik Award](image-url)
References


Wendy Warr, Symposium Presenter and Reporter
“During almost 50 years of service to the chemical information profession, Dana Roth has clearly demonstrated the need for chemistry librarians and information professionals to work closely with researchers and publishers. In honor of his achievements, we present a day of accepted and invited presentations, highlighting the many ways that chemistry librarians and information professionals are working closely with publishers and researchers.” (Call for papers)

This symposium was organized by Judith Currano (University of Pennsylvania) and Ted Baldwin (University of Cincinnati) to honor Dana Roth in the best way possible. His dedication to building relationships among all the players in the chemical information “ecosystem” was emulated in all presentations. Talks from librarians described their relationships with their campuses, publishers and other information providers, and the broader community of librarians and information professionals. From the information provider side, we heard about improvements and growth that were directly influenced by valued interactions with the library community.

As the slides for all talks will be made available, the summary provided below is primarily from my own notes and thoughts, and does not exactly follow the order of the presentations – please consult the program listing for those details and abstracts (http://bulletin.acscinf.org/node/621#W1a). Any mischaracterizations and omissions are solely errors on my part.

Understanding one’s campus is arguably the most important information a librarian can have. In recent years, campus libraries have borne the brunt of both reorganizations and budget cuts. Susanne Redalje (University of Washington) gave a poignant update on the closure of the campus’s Chemistry Library five years ago. One important note was that with the loss of physical space also came the loss of both virtual space and organizational structure, both major hindrances to effective outreach. She stressed the importance of a physical presence in an increasingly virtual world, and how that presence involves more the librarian and the services than the actual physical place.

However, campus feedback indicated that the library was missed, and there was a distinct lack of understanding as to why it was closed. In turn, this emphasizes that direct engagement and communication with users, and especially with administration, is critical to successful outreach. This includes staying abreast of campus developments such as new research centers or initiatives, hosting on-campus events (such as ACS On Campus), surveys on services, and direct email notifications to patrons whenever possible. Finally, organizing on-campus services, as well as networking with the larger science librarian community through events such as the Science Librarian Boot Camps, has provided a structure and a “way forward” for improving and innovating services.
Ted Baldwin described several projects underway at the University of Cincinnati in response to input on meeting the needs of researchers. The Science Libraries are being reorganized to provide additional collaborative and study space, as well as a Research Commons with features including a data visualization studio and GIS capabilities. This involved significant relocation of print materials, which was done with “lots of consultation” with the affected researchers, emphasizing again the importance of clearly communicating changes. Another innovation is the creation of the “science informationist” position, working with everything from data management to digital repositories to best practices. Finally, fall 2014 will see collaborations with faculty “early adopters” of the campus digital repository and open journal systems, emphasizing the focus on responding to researchers, giving them what they need.

Understanding what your campus is doing is vital to both informing the services you provide and lobbying effectively for services that you need from information providers and publishers. Grace Baysinger (Stanford University) talked about the various needs of a campus, both in terms of education and research, and the importance of partnering with information providers to meet these needs. Campus visits, one-on-one meetings, and focus groups are just some of the ways to give feedback to providers, and one should take advantage of any opportunity presented. This will in turn improve offerings and services, including everything from content to metadata to training materials. Engaging with providers and offering substantive feedback is a highly effective method to truly “partner” with providers and serve your campus users.

From the provider viewpoint, two longtime stalwarts in the chemical information field, CAS and ACS Publications, provided insight into their development and relationship with librarians, pointing to Dana Roth as an influential partner and how librarians in general provide valued feedback. Steve Hansen from ACS Publications, speaking in place of Sara Rouhi, echoed Grace’s sentiments, this time from the publisher side. He described ACS’ efforts to engage librarians in discussions and summits to address issues ranging from pricing to Open Access to metrics. As a nice side note, Steve mentioned a story that Sara had told him that visiting Caltech was one of her first trips as an ACS Publications representative, and she spoke warmly of Dana’s kindness and hospitality.

Roger Schenck (Manager, CAS Content Promotions) told a brief history of CAS, including the evolution of the CAS REGISTRY, arguably CAS’s most “far-reaching development.” He emphasized that the adoption by libraries and engagement of users with its services, SciFinder Key Contacts in particular, have been instrumental to CAS’ growth and success. As a Key Contact, Dana has provided feedback throughout the years to improve and expand CAS’ services, including its databases and interfaces. Roger closed with some of Dana’s most notable contributions to the “chemical information enterprise,” including co-editing the volume “Chemical Information for Chemists” with Judith Currano and his significant activity on the CHMINF-L mailing list. Roger counted over 700 messages (and rising) sent by Dana since its inception in 1991: yet another statement of his service to his fellow information specialists and his contribution to the field as a whole.

Returning to the academic realm, my presentation touched on a number of topics to show how Dana’s vision for service and librarianship at Caltech is being continued and expanded upon by his current colleagues. Among some of the projects described were innovations in awareness, the continuing relationship with Thomson Reuters by providing extensive feedback on Web of Science, and the growth of Caltech’s Institutional Repository, CODA (Collection of Open Digital Archives). Although the methods and technological tools available to libraries have changed throughout the years, we are still fundamentally doing the same things we always have been doing: serving the information and research needs of our patrons.
Taking both campus awareness and provider collaboration to a new level for patron service, Leah McEwen (Cornell University) gave an update on a data management project. There are many, many issues involved, including what to keep, how to document and annotate it, and how to store it, among others. Her collaboration with researchers at the Royal Society of Chemistry and the University of Southampton saw her embed with and observe chemical researchers on her campus. “People are already doing data management as part of their research,” she noted, “but a significant issue is a lack of standards and/or best practices particular to chemistry,” something her project hopes to help resolve. One goal will be to evaluate how an electronic laboratory notebook can be useful to streamline information needs, including linking to repository data as well as chemical safety considerations.

The presentations so far had touched upon interactions with campuses and companies, but what about our colleagues? How do librarians learn about these tools, and learn about how to communicate with their researchers? Because chemistry essentially has its own language, it may be hard for librarians without a background in chemistry to talk to researchers and understand research questions being asked. Judith Currano described the evolution of “Chemistry for the Non-Chemist Librarian,” a continuing education course offered through the Chemistry Division of the Special Libraries Association (SLA). Dana was an inaugural instructor of the course in 1999, along with Bartow Culp. At the time, the course was called “Chemistry and Chemical Librarianship for Non-Chemists,” and gradually expanded in scope after Judith and Sue Cardinal (University of Rochester) joined the instruction team. In addition to overviews of the main areas of chemistry, it covers information sources and tips for framing research questions and how to find out what your patron is really asking. One common thread was that the time slot of four hours is simply “not enough time” to explore the relevant topics. The course continues its success and influence, and was offered in 2013 outside of SLA for the first time.

Finally, Dana himself said a few words in gratitude to Judith and Ted for organizing such a wonderful slate of talks. He also thanked Caltech for being such a unique institution that allowed for much of his influential work to happen. Because of its small size and sharp focus, meeting the community’s needs still allowed for time and inspiration to pursue projects for improving service not only to the Caltech campus, but also to the profession as a whole. And this unwavering dedication to service, local and global, to students, librarians, and publishers, is what makes Dana such an extraordinary librarian and luminary to others in this field.

“Caltech Chemistry Librarian Discovers Equation for a Satisfying Career” Caltech News, 05/26/2011 http://www.caltech.edu/content/caltech-chemistry-librarian-discovers-equation-satisfying-career

Papers in Caltech CODA by Dana: http://authors.library.caltech.edu/view/person-az/Roth-D-L.html

Dana Roth’s Caltech Library Profile: http://libguides.caltech.edu/profile.php?uid=7047

Chemical Information Sources Wikibook: http://en.wikibooks.org/wiki/Chemical_Information_Sources

Chemical Information for Chemists: http://dx.doi.org/10.1039/9781782620655

Donna Wrublewski, Symposium Presenter and Reporter
Exploring the Application of New Technologies in Chemical Research and Education

This session was somewhat unusual in the CINF program, with a focus on devices offering new mechanisms for processing and collecting of chemical or scientific information. Sean Ekins from Collaborative Drug Discovery led off with a description of an iPad-based tool for analyzing TB data, using Bayesian statistical analysis to rank active molecules and probable targets for TB prediction and visualization. The resulting app can handle approximately 800 compounds and associated targets. While the app represents a niche use of informatics, it demonstrates that other datasets could also be “appified” to make data visualization and prediction tools available to a broad audience.

Rajeev Hotchandani from Scilligence discussed the use of a touch-optimized Electronic Lab Notebook (ELN). ELNs have been largely unused in academic environments, but this is beginning to change. Since Scilligence’s app is JavaScript-based, and because it makes use of the cloud, there is a very small footprint on the client. The app also integrates with Scilligence’s registration system, so entry of substances, and even ordering of chemicals, is seamless.

Vin Scalfani from the University of Alabama described the use of 3D printers to print crystal structures. While 3D printers have been around for many years, the appearance of inexpensive printers in the last couple of years has enabled the technology to be used in academic labs. Scalfani described several software packages that could be used to convert CIF files into the .stl format recognized on 3D printers. The process uses Jmol to convert the CIF files into VRML, and then AccuTrans 3D to convert VRML to .stl, and Netfabb to repair the .stl file. In order to make 3D files more readily-available to users, Scalfani enlisted Bob Hanson at St. Olaf College to create a custom version of Jmol to automatically handle counterions and solvents, and to pack the crystal lattice, allowing the software to run in batch mode. Scalfani has created over 30,000 3D files and stored them in a crystal data repository hosted by the Royal Society of Chemistry. Scalfani also referred to a 3D print exchange hosted by NIH. (Photo credit: http://chemistry.ua.edu/3-d-printing-of-molecular-models/).

Jeffrey Lancaster, Emerging Technology Director at Columbia University, described his approach at Columbia to envision the library as a neutral space where access to devices, software, and even software training modules, complement the traditional access to content. Lancaster noted that while installing 3D printing into the library was a highly visible technology, “3D printing is not about the printing.” Instead, while people are interested in the printing technology itself, once the novelty of the technology has passed, the real question becomes how the printer can be used to do something to help the researcher. In some cases, there may be nothing. In other cases, with the help of the expert, the researcher may find something useful that would justify purchase of a device to use in his or her own lab.

Julea Vlassakis, a graduate student at UC Berkeley and UC San Francisco, is part of an innovative group of graduate students who launched the website http://www.teklalabs.org/. The purpose of the website is to share designs for laboratory equipment that can be created by the end user on either an additive device (such as a 3D printer) or a subtractive device (such as a laser cutter), resulting in devices that are far less-expensive to purchase and maintain than vendor equipment. The designs are peer reviewed and must be research grade. Safety is also a concern. Developing countries often
receive used equipment from the developed world, and too often the equipment is impossible to maintain.

Teklalabs experience is that there are many willing “makers” in the world, and they are happy to share their experience and ideas, especially when there is a contest involved. From a 3D printing design competition in 2012 with 17 designs, a PrintMyLab competition in 2014 attracted 174 designs. The BuildMyLab 2 contest is scheduled for 2015. Teklalabs cosponsored a Diagnostics by Design Hackathon, which brought together 30 experts in global health, engineering, and computer science to build a prototype to address a global health need. The winning team produced a bug zapper that counted mosquitoes for malaria monitoring.

Steve Feng, from UC Los Angeles, described several projects that involved creation of 3D printed attachments to smartphones in order to create portable instruments. His latest development involved a technique using Google Glass to record and analyze results from home HIV test kits, which are often misread by consumers. The technique involved capturing a picture of the test kit using Google Glass, applying an algorithmic enhancement of the low quality Glass image, and then determining whether the result was positive or negative. Results were promising, and similar test procedures are under development for other visual test kits as well. While this experimental setup and workflow point out some of the limitations of Glass, it demonstrates the potential for more robust Glass-like devices. (Photo credit: http://www.universityofcalifornia.edu/news/google-glass-app-performs-instant-diagnostic-tests).

Manu Prakash, Stanford University, with a vision to equip labs and citizens in remote and poverty-stricken areas with tools to understand their environments better, described his approach to what he has called “frugal science.” He has created a microscope, the Foldscope, out of a single sheet of paper with a lens made in his lab. For under a dollar, a working microscope enables parents and children to see the difference between washed and unwashed hands, impure drinking water, and swimming areas. With this knowledge, the adults and children might be more motivated to acquire healthy practices. Equipping hospital labs is also a challenge, but Prakash is now focusing on the development of punch-card chemistry to assist in medical and environmental analysis. In the technique, a music box mechanism, normally used to play music, is instead used to inject droplets into microfluidic channels based on the program in the punch-card. In almost any CINF program, someone will allude to the historic use of punch-cards as a precursor to the digitized and automated databases we use today. The concept of punch-card chemistry brings that legacy medium back to practical use. Following the symposium, Prakash demonstrated the Foldscope.

I don’t remember ever hearing the word “inspiring” used to describe our CINF sessions, but that was the word used by a couple of those attending. Thanks to all of the speakers for a great symposium.

David Martinsen, Symposium Organizer
The IUPAC Solubility Data Series: 100 volumes of Solubility Data Online

During the IUPAC 47th General Assembly, which occurred in 2013 in Istanbul, it was proposed that members of the Subcommittee on Solubility and Equilibrium Data (SSED) of the IUPAC Analytical Chemistry Division participate in the 2014 Fall American Chemical Society National Meeting in San Francisco as a venue to celebrate the publication in early 2014 of the 100th volume of the IUPAC-NIST Solubility Data Series. The Solubility Data Series (SDS, http://www.iupac.org/index.php?id=593) has been providing comprehensive compilations and (whenever possible) critical reviews of published data. This has been a major vehicle for helping IUPAC fulfill one of its long-range goals: international standardization of physical constants. The symposium was hosted by the Division of Chemical Information and cosponsored by the Divisions of Analytical Chemistry and History of Chemistry. The presentations were organized so as to highlight the practical importance and present relevance of the work being done inside the SSED framework on solubility data and stability constants.

Mark Salomon, the present editor-in-chief of the IUPAC-NIST Solubility Data Series, made a brief reference to the history of the project that can be traced back to 1972 when A. S. (Stevan) Kertes proposed to the then Commission V.6 a project on collecting and evaluating solubility data. Publication began in 1979 with the first volume on the solubility of helium and neon in liquids. Since then 102 volumes have been published. Besides the historical aspects, Salomon also outlined the process of data compilation and evaluation. In the compilation process all the available literature sources of data for a specific solute/solvent system have to be considered, even the very old ones. For example, solubilities published in the 19th century often compare favorably with values measured recently. Thus, solubilities of NaCl in H₂O published in 1885 were found to be comparable to the best modern results. Sometimes such old values constitute the only source of data available. For each published paper Compilation (data) sheets are built providing information on materials, experimental methods and errors. Where sufficient literature data exist, contributors to the SDS provide a critical evaluation of the data to determine their merits. Data can be classified as Recommended when good agreement between independent authors exists, Tentative when sufficient literature comparisons cannot be made, but the data appear to be reasonable, or Rejected when qualitative or incorrect. The format of a typical Compilation sheet was presented as well as the general format for critical evaluations.

Allan Harvey, the co-editor-in-chief of the Journal of Physical and Chemical Reference Data (JPCRD, http://scitation.aip.org/content/aip/journal/jpcrd) where the IUPAC-NIST Solubility Data Series has been published since volume 66 in 1998, made the bridge between NIST Standard Reference Data and the Solubility Data Series. The publication of SDS as articles in the JPCRD substituted their earlier publication as monographs by Pergamon Press (volumes 1 to 53) and Oxford University Press (volumes 54 to 65). In their communication, Harvey and D. R. Burgess analyzed the fruitful cooperation between NIST and IUPAC from the perspective of the journal and in the context of NIST’s mission. Efforts are being made to make the data published in the journal more accessible and useful in the future. An effort to make the contents of the pre-1998 volumes available on the Web in a format that will be more easily searchable by researchers was described.

Stuart Chalk (University of North Florida) spoke next about the application of the “REST API for the IUPAC Solubility Data Series: a ‘Skunkworks’ project.” The focus of his presentation was to show a way to make the data published by NIST available in a more web-enabled format. Chalk presented an outlined project to scrape data and metadata from pages of the IUPAC Solubility Data Series.
Glenn Hefter (Murdoch University, Australia) spoke about the work being done in IUPAC on the critical evaluation of stability (formation) constants of metal-ion complexes with inorganic and organic ligands in aqueous solution. He traced the history of projects in this area back to the 1950s with the creation of the IUPAC Commission V.6 on Equilibrium Data. The present SSED of the IUPAC Analytical Chemistry Division was formed in 2000 when V.6 was re-combined with Commission V.8 on Solubility Data. Stability constants are important for modeling chemical speciation in areas as diverse as medicine, engineering, process control, extractive metallurgy, environmental management, and so on. In his talk Hefter provided an overview of the many contributions that have been made by the IUPAC group to the important task of compiling and critically evaluating the plethora of available stability constant and related thermodynamic data, which are widely dispersed across the scientific literature.

Johan Jacquemin (Queen’s University Belfast, UK) and William E. Acree (University of North Texas, USA) spoke about specific aspects related to the IUPAC projects they chair, “Progresses and prospects in the database on ionic liquids solubulities in molecular solvents” and “Models to evaluate experimental solubility data for crystalline nonelectrolyte solutes in organic mono-solvents and solvent mixtures,” respectively.

Clara Magalhães (University of Aveiro, Portugal) and Earle Waghorne (University College Dublin, Ireland) spoke about the need for reliable data that can help in the creation of new paradigms about the present impact of carbon dioxide in global warming, environment remediation technologies, and the effects of solvents on the thermodynamics of electrolyte and non-electrolyte solubilities, respectively.

Clara Magalhães, Symposium Organizer

The following is an overview of the IUPAC Subcommittee on Solubility and Equilibrium Data (SSED), a handout was made available at the CINF Symposium in San Francisco, and also kindly provided to Chemical Information Bulletin by Clara Magalhães, Chairman of the IUPAC SSED.
The IUPAC Subcommittee on Solubility and Equilibrium Data (SSED)

Who are we?

Membership of the SSED is open to all scientists who wish to contribute. The current membership includes contributors from 21 countries spread over 4 continents.

Roles

The main roles of the SSED are the comprehensive compilation and critical evaluation of selected thermodynamic data, specifically:

- solubilities of gases, liquids and solids in liquids and solids, and
- stability constants for homogeneous reactions.

Topics

Topics range from those of pure scientific interest through to those of pressing environmental, medical and technological importance.

Examples of current projects:

- Solubility of non-steroidal anti-inflammatory drugs in both neat organic solvents and organic solvent mixtures
- Mutual solubility of rare earth metal (Sc, Y, Lanthanoides) bromides in molten alkali bromides
- Database on solubility and liquid-liquid equilibria of binary mixtures of ionic liquids and molecular solvents
- Critical evaluation of thermodynamic data of sulfate complexes in solution.

If you are interested in joining the existing project or proposing a new one, please contact us. Your expertise will be valued.

How to contribute?

New contributions are made through proposals addressed to the chairman of the SSED (Prof. M.C. Magalhães, mclara@ua.pt). We welcome proposals and suggestions for work on new projects from chemists everywhere.

Awards

Franzosini Award

The Solubility Data Commission, now the SSED, established the Franzosini Award to assist promising young contributors to the Solubility Data Project to attend SSED meetings and conferences. Since 1988, when the award was established, through 2014, the prize has been awarded to 20 recipients from 14 countries.
Outputs

**Publication of stability constants** (critically evaluated data) currently occurs as papers in *the IUPAC Journal Pure and Applied Chemistry* (impact factor in 2013 of 3.1).

Most recent publication:

**Publication of solubility data** (critically evaluated) currently occurs as papers in *Journal of Physical and Chemical Reference Data* (impact factor in 2013 of 3.2).

Currently 102 volumes (containing over 30 000 pages) have been published, others are in the pipeline. Editor-in-Chief of the *Solubility Data Series*: Dr. M. Salomon ([marksalomon@comcast.net](mailto:marksalomon@comcast.net)).

Most recent publication:

**Electronic databases** in stability constants and ionic liquids have been or are being developed.

**Books**


**Conferences**

The SSED organizes the *International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP)*, which has been held every two years for over 30 years. The next symposium is planned for 2016, in Switzerland.

**Additional information**

For more information consult the IUPAC web page: [http://www.iupac.org/nc/home/about/members-and-committees/divisions.html](http://www.iupac.org/nc/home/about/members-and-committees/divisions.html), and choose “Analytical Chemistry Division” and then “Subcommittee on Solubility and Equilibrium Data,” or contact Chairman Prof. M.C. Magalhães ([mclara@ua.pt](mailto:mclara@ua.pt)), or Secretary Prof. E. Waghorne, ([earle.waghorne@ucd.ie](mailto:earle.waghorne@ucd.ie)).
Multidisciplinary Program Planning Group

The theme of the 248th ACS National Meeting in San Francisco, August 10-14, 2014 was “Chemistry and Global Stewardship.” Our CINF division participated with a theme-related full-day symposium: “Nature’s Second Act: Revisiting Natural Products.”

The formal Multidisciplinary Program Planning Group (MPPG) meeting was held late Saturday afternoon, August 9, at the Hilton San Francisco Union Square. Lisa Houston welcomed all MPPG participants; division representatives introduced themselves; Richard Love was recognized for his years of service to MPPG as Staff Liaison; and the Dallas General Meeting minutes were reviewed and approved. Dan Daly was elected 2016 MPPG Chair and Christine McInnis was elected 2015-2017 MPPG at-Large Representative. Thematic program chairs gave their reports.

Robin Rogers from the University of Alabama, program chair for the San Francisco meeting, summarized the plenary speakers, and the subthemes of the San Francisco thematic program, and mentioned a few notable division events such as the 100th Anniversary of the ACS ENVR Division and its multiple symposia in San Francisco. He ended with a recommendation that future theme organizers be aware of subthemes and other competing programming.

Thematic program chair for the upcoming 2015 Spring National Meeting in Denver, Robert Weber from Pacific Northwest National Laboratory, updated MPPG on the Denver theme: Chemistry of Natural Resources. Plenary speakers have been chosen:

- Peter Kareiva, Santa Clara University and Chief Scientist for the Nature Conservancy
- Dr. Paul Bryan, formerly VP at Chevron and formerly manager of the biomass program at the US DOE
- Dr. Carolyn Koh, Department of Chemical Engineering at the Colorado School of Mines.

The Fred Kavli Innovations in Chemistry lecture will be given by Dr. Laura Kiessling from the University of Wisconsin-Madison. The Kavli Foundation Emerging Leader in Chemistry lecture has yet to be determined.

The theme for fall 2015, Boston, is Innovation from Discovery to Application. Thematic program chair, Rick Wagner from the University of Michigan, was not able to attend, but submitted his report. Plenary speakers will be:

- Paula Hammond, MIT
- Peter Schultz, Scripps Research Institute
- Karen Wooley, Texas A&M

The Fred Kavli Innovations in Chemistry lecture will be given by Dr. George Whitesides from Harvard. The Kavli Foundation Emerging Leader in Chemistry lecture has yet to be determined.

The theme for spring 2016, San Diego, is Computers in Chemistry. Thematic program chair, Kenneth Merz from Michigan State University, updated MPPG on progress so far. Modeling will be the broad theme of the meeting with subthemes on computer-aided drug design, big data, nanomaterials with a focus on energy and sustainability, and multiscale modeling.
The theme for fall 2016, Philadelphia, is *Chemistry of the People*. Thematic program chair, Rudy Baum, retired Editor-in-Chief of *C&EN*, is just getting started and asked that anyone interested in contributing or helping to organize get in touch with him.

Spring 2017, San Francisco
Theme: *Advanced Materials, Technologies, Systems and Processes*
Thematic Program Chair: TBD

Fall 2017, Washington, DC
Theme: *Chemistry’s Impact on the Global Economy*
Thematic Program Chair: TBD

The MPPG meeting ended with a general discussion and vote on themes for 2018 and beyond. The following were approved by the MPPG General Representatives and will be sent to the Divisions for confirmation.

Spring 2018, New Orleans
Theme: *Energy Solutions and the Environment* (To Be Confirmed)
Thematic Program Chair: TBD

Fall 2018, Boston
Theme: *Chemistry – From Bench to Market* (To Be Confirmed)
Thematic Program Chair: TBD

Spring 2019, Orlando
Theme: *Chemistry for New Frontiers* (To Be Confirmed)
Thematic Program Chair: TBD

*Roger Schenck, CINF Representative on MPPG*

Abstract submission for CINF symposia for Denver meeting deadline October 17, 2014
Editors’ Corner

This year, the ACS Division of Environmental Chemistry (ENVR) marks the 100th anniversary of its founding. The division traces its origin to the Division of Water, Sewage, and Sanitary Chemistry, which was founded in 1914. Its first chair was Edward Bartow, a professor of chemistry at Iowa State University who was instrumental in its formation. Edward Bartow would go on to become a lieutenant colonel in the U.S. Army during World War I, having been placed in charge of providing potable water to the American Expeditionary Forces. (Making his task more difficult, in Paris the water had to come from the then heavily-polluted Seine River). Later, he would serve as director of the American Institute of Chemical Engineers (AIChE) from 1923 to 1925 and as ACS president in 1936. To give some idea of what was on the frontier of water research in 1914, one of Edward Bartow's papers of that year, coauthored with Clarence Scholl, was titled "The comparative value of a calcium lime and a magnesium-calcium lime for water softening" (Ind. Eng. Chem. 1914, 6(3), 189-191).

As the 20th Century progressed, both chemical professionals and the public-at-large became more concerned about the wastes and emissions produced by the chemical industry. In 1959, the Division of Water, Sewage, and Sanitary Chemistry was changed to the Division of Water and Waste Chemistry to reflect this growing interest. The problem of air pollution and air quality was also a growing concern, hence a second name change in 1964 to the Division of Water, Air, and Waste Chemistry. (For reference: the Clean Air Act was passed in 1963, and the Clean Water Act in 1972). The Division of Environmental Chemistry got its current name in 1973. The division continues to be active: 6572 papers were presented at ACS national meetings between 2004 and 2013.

The ACS includes other governing bodies, in addition to ENVR, that are concerned with the environment. The Committee on Air Pollution was founded in 1952. It evolved into the Committee on Environmental Improvement (CEI), which was established in 1968. In 1969, the CEI published the report “Cleaning our environment: the chemical basis for action,” an update of this report was published in 1977. Today, the CEI awards the ACS ChemLuminary Award for Outstanding Sustainability Activities and the ACS-CEI Award for Incorporating Sustainability into Chemistry Education.

In 1967, ACS Publications launched Environmental Science & Technology, its first journal in the field of environmental chemistry. To this were added ACS Sustainable Chemistry & Engineering in 2013 and Environmental Science & Technology Letters in 2014. In addition, the Journal of Physical Chemistry A includes “atmospheric, environmental, and green chemistry” within its scope, and many other ACS journals publish articles pertaining to environmental chemistry, provided that they also meet the journal’s subject and quality requirements.

This year, the ACS Fall National Meeting and Exposition had an environmental chemistry theme - Chemistry and Global Stewardship - and the Division of Environmental Chemistry sponsored or co-sponsored 47 symposia in the meeting’s technical program.
The accompanying chart displays trends in publication in environmental chemistry. It graphs the number of Chemical Abstracts bibliographic records assigned to section codes 59 (air pollution and industrial hygiene), 60 (waste treatment and disposal), and 61 (water), both in terms of absolute number (blue bars) and in terms of percentage of total Chemical Abstracts records for that publication year (red curve). One can see a trend of increasing percentages up to a peak at 1998, after which the percentages level off a bit. In terms of absolute numbers, publications in the field continue to increase: the drop-off for 2014 is due to the fact that the year is not over yet (the data are as of August 20, 2014). By either measure, environmental chemistry remains an active field.

![CAS Records in sections 59-61](chart.png)

We wish to thank Matt Garver (CAS), Jillian Goldfarb (ENVR), Rhonda Ross (CAS), and Roger Schenck (CAS) for their help in compiling data used in this article.

*David Shobe, Assistant Editor, Chemical Information Bulletin*
Book Reviews


I’m sure that other scientists are like me, when watching a movie or TV show where science is involved, wondering or even critiquing the science, evaluating its accuracy or even plausibility. This book is the most recent of several describing the relationship of scientist consultants and the producers, directors, and staff of movies and TV shows. A previous example, Lab Coats in Hollywood¹, was reviewed by me in CHOICE (2012, 49-4353) and is cited several times in this book. For an ACS Symposium Series this book was actually inspired by two symposia presented as Presidential Events at the 2011 ACS National Meetings in Anaheim and Denver, and then expanded greatly with the number of authors. All of the co-editors (one of them the symposia organizer and a candidate for ACS office) also wrote chapters. Additional authors include other scientist advisors, communication academics, writers, directors, and scientist commentators.

Both the history and the evolution of movie themes and topics and the interaction between experts and artists are covered in the 25 chapters. Chapter one employs the unusual format of a dialogue between the director and a media writer concerning the movie, _Creation_, a unique biography of Charles Darwin. Both science topics _per se_ and science fiction are discussed and analyzed. In the latter genre, entire chapters cover _Star Trek, Breaking Bad, Eureka, Marvels Avengers_, and _The Big Bang Theory_. The tug of war between scientific accuracy and the need for creativity in entertainment and plot is treated in several chapters by contributors from both sides of the table. In the realm of science fiction, the current and future plausibility of science and technology presents its own struggle. One of the biggest dichotomies concerns alien invaders as described by S. Shostak of SETI Institute (why would they even come?).

Pervading themes also include the educational, inspirational, and even predictive aspects of movies. Both factual and fictional movies can be used in science education. Many scientists of a certain age claim inspiration for pursuing their careers because of movies and TV seen in their youth. R. Wessen of Jet Propulsion Laboratory describes the inspiration of the exploration of space via movies, especially the cooperative efforts of Wernher von Braun and Walt Disney. In general communications, the “CSI Effect” is described in several chapters, not only the resulting public demand for hastened and accurate jurisprudence and forensics, but also the great increase in demand by students for courses and programs in forensics. The evolution of the portrayal of scientists, especially as people, keeps evolving past stereotypes of the mad scientist.

I did find a couple of errors. Methylamine boils at -6.3 C, but in _Breaking Bad_, utilization of 30 gallon drums of the chemical (not gas tanks) are in key plots. The consultant, a physical organic chemist, does not note the discrepancy. In Chapter 3, on teaching writers science, the author, a physics and astronomy professor, refers to the “period table.”

This book should be of interest to those in science information and education, writers, both in entertainment and journalism, and the general public who enjoy watching TV and movies.


Bob Buntrock, Member, CINF Communications and Publications Committee
Ullmann's Encyclopedia Celebrates 100 Years

From the workings of the automated logwood chipper to predicting the future importance of oil shale, the 1914 First Edition of *Ullmann's Encyclopedia of Industrial Chemistry* set out to provide industrial chemists with the latest scientific research and practice. One hundred years on and now in its Seventh Edition, this now global reference work reveals just how far we have come.

For industrial chemists across the globe, *Ullmann’s Encyclopedia of Industrial Chemistry* has become a name synonymous with reliability, comprehensiveness and innovation. Starting out as a twelve-volume set available only in the German language, this leading global resource now consists of 40 volumes incorporating more than 30,000 pages. It draws on the knowledge of more than 3,000 authors from around the world, many of them from countries that did not even exist 100 years ago. Ullmann’s has truly come a long way since its conception in 1914.

Compiled by Professor Ullmann of Berlin University of Technology shortly before the outbreak of the First World War, and first published by the German publishing house Urban and Schwarzenberg, Ullmann’s quickly became the standard reference work in industrial chemistry. Translated into English by its new owner, Verlag Chemie (VCH) in the mid 1980’s, it went on to become the first Wiley-VCH major reference work to be made available via the Internet, now its primary home. Pioneering from the outset, the Ullmann’s will be among the first to use the newly developed Smart Article technology, allowing substances to be found, compared, and placed in relation to one another based on their chemical structure alone.

Aside from the vast amount of information available, what makes Ullmann’s Encyclopedia even more special is the way that the knowledge from earlier days is conserved alongside latest processes shaped by biotechnology and nanotechnology. Its breadth and depth of technical information have proven to be invaluable for plant operators and patent lawyers alike. Barbara Elvers, the current editor-in-chief, recalls one particular telling episode: “My most memorable experience as editor for *Ullmann’s* was a confession by a chemical engineer from a large German chemical company who told me that he had to build a new coal liquefaction plant with only the help of an old technician who used to work in such a plant. He consulted the 3rd edition of *Ullmann’s*, constructed the plant, and it worked from the start. What more does one have to say about *Ullmann’s*?”

For one hundred years, *Ullmann’s Encyclopedia of Industrial Chemistry* has proved an indispensable goldmine for anyone working in or studying industrial chemistry. One can only speculate what it will look like in a hundred more…

Found out more about 100 Years of Ullmann’s: 1914 to 2014

Read Fritz Ullmann’s Preface to the first edition

New: Ullmann’s free education site, *Ullmann’s Academy*, makes “hidden gems” freely available. About half of the current *Ullmann’s Academy* articles deal with chemical engineering topics, for example, process monitoring, process intensification, and miniaturization. In addition, there are articles on patents, cost estimation, life cycle assessment, risk assessment, and similar general issues that one encounters in the development and manufacture of chemical and pharmaceutical products. New topics will be added twice a year, so the new site has the potential to develop into a comprehensive collection for teaching and learning, or for simply refreshing your knowledge.
Snapshots from the first edition (1914 – 1923)

1. Batteries of chlor-alkali electrolysis cells for the production of hypochlorite bleach

2. Mobile hydrogen generator for use by the military

See more examples of Chemical Technology in the 1910s on ChemistryViews.

Frank Weinreich, Publisher, Ullmann’s Encyclopedia of Industrial Chemistry
Committee Reports

CINF Communications and Publications Committee

There has been much happening in the Communications and Publications Committee over recent months. One of the outputs of the Committee is the Chemical Information Bulletin. Published four times a year, the Bulletin includes news about the Division, information about CINF activities at the ACS National Meetings, as well as summaries of symposia, book reviews, interviews with leaders in the industry, and updates from our sponsors. The Bulletin now has an editorial team of four members: Vin Scalfini (University of Alabama) serving as Editor for the odd numbered issues with Teri Vogel (University of California, San Diego) as Assistant Editor, and Svetlana Korolev (University of Wisconsin-Milwaukee) as Editor of the even numbered issues with David Shobe (Patent Information Consultant) as Assistant Editor. Thanks to all of them for their efforts in producing this publication.

The CINF Website is undergoing a transition of sorts. It is with great thanks that we recognize Danielle Dennie, our departing webmaster. She oversaw the migration of the website to a Drupal environment, and has faithfully taken care of posting new content, maintaining the site, and interacting with all of our community with great efficiency and good will. Danielle has moved to the Computer Science, Electrical/Computer Engineering and Math Library at Concordia University in Montreal, and so is no longer involved in chemical information.

We welcome two individuals to our web environment. Patti McCall (University of Central Florida, photographed at right) is our new Webmaster. Patti is a Physical and Life Sciences Librarian with subject liaisons for biology, chemistry, environmental sciences, mathematics, statistics, and physics. Prior to coming to Central Florida, Patti was the Head of Public Services at Pratt Institute Library in Brooklyn, NY. Prior to that, she spent eight years as the Corporate Librarian at Albany Molecular Research, Inc. in Albany, NY. Patti may be unfamiliar to many of us, but looks forward to getting to know us through her position as Webmaster and attendance at future ACS meetings. Joining Patti is Erja Kajosalo (MIT) as Assistant Webmaster.

Finally, we hope you have had a chance to check out the CINF Webinar series this year. Belinda Hurley (Ohio State University) and Carmen Nitsche (CINforma Consulting) have developed an outstanding lineup for this year. Three webinars have already been presented, John Overington and Nicko Goncharoff on SureChem and ChEMBL, Howard Ratner on CHORUS, and Stephanie Dawson on ScienceOpen. The recordings are available on the CINF website under Meetings/Webinars. Information on upcoming webinars planned for October and December can be found at: http://www.acscinf.org/content/upcoming-cinf-webinars.

Thanks to a great team for support of the CINF Division through communications and publications.

David Martinsen, Chair, CINF Communications and Publications Committee
CINF Education Committee

The CINF Education Committee met on Saturday, August 9, 2014 from 1:00 pm-3:00 pm in the Marina Room of the Palace Hotel. Members attending included Grace Baysinger (Chair), Chuck Huber, Marion Peters, and Donna Wrubleski. Guests attending included Jeremy Garritano, Judith Currano, and Suzanne Redalje.

Membership: As three members’ terms will expire at the end of 2014, we are interested in recruiting replacements for them. If you are interested in joining this committee, please contact Grace Baysinger (graceb@stanford.edu).

Announcement: There will be a discussion forum on the CRC Handbook of Chemistry and Physics on Monday 12 pm -3 pm during the ACS Meeting in San Francisco. The discussion will involve both the hard copy and electronic versions of the Handbook. All are invited to attend and participate.

SOCED: A member of ACS Society Committee on Education (SOCED), Jeremy Garritano, gave an informal report from a SOCED meeting he had attended. The American Association of Chemistry Teachers (AACT), a new organization created to support K-12 teachers, became operational. The Science ABC’s book is now available digitally. Two new international student chapters have been formed, one in Germany and one in Singapore. As a follow up to the ACS Presidential Commission on Graduate Education in the Chemical Sciences, Jeremy briefly summarized results for a survey given to 3,000 graduate students.

Graduate Student Information Skills: In addition to comments already submitted, members were asked to send comments on this draft document to Grace by the end of October. If there are other CINF members who are interested in reviewing and commenting on this document, please contact Grace Baysinger (graceb@stanford.edu).

Short Journal Abbreviations: The need to be able to easily locate very short journal abbreviations used in the older literature was discussed. Options are being explored to for addressing this issue.

CINF Education Committee Programming: Ideas and possibilities were discussed for upcoming ACS National Meetings and for Biennial Conference on Chemical Education (BCCE) 2016, which will be held at the University of Northern Colorado.

Procedures Manual for the CINF Education Committee: The charge, objectives, and responsibilities for the CINF Education Committee were reviewed and revised. After any approvals that are needed by the Division, the revised document will be deposited into the CINF Procedures Manual and will be posted on the CINF Education Committee pages. A draft version of these changes is appended so that all CINF members can review them and provide comments.
Term of Office and Composition:

Chair:
The Committee Chair is appointed by the Division Chair for a term of three successive one-year terms. The Committee Chair may previously have served on the Committee, preferably as Assistant Chair, during the year immediately preceding his/her term.

Members:
Members are appointed by the Committee Chair for no more than three successive one-year terms with the approval of the Division Chair. Members should include representatives from a wide range of chemical information areas, such as chemistry faculty, academic librarians, industrial information specialists, government information specialists, and database producers and vendors. Attendance at ACS National Meetings is not required for committee members.

Objectives:
Help foster chemical information literacy and best practices among information professionals, information providers, and users.

Key Responsibilities:
Provide a liaison relationship with information producers and vendors. Help chemical information instructors improve the quality of information instruction.

Organize chemical information symposia or posters at the ACS National meetings. When possible, offer or participate in chemical information symposia, workshops, and posters at the Biennial Conference of Chemical Education (BCCE) and at ACS Regional Meetings.

Collaborate with other ACS Technical Divisions, Local Sections, and Committees.

Provide advice to the ACS Committee on Professional Training, ACS Society Committee on Education (SOCED), ACS Committee on Chemical Abstracts Service, and other ACS groups about chemical information literacy.

Maintain the Chemical Information Literacy page on the CINF website.

Meetings:
Meetings are held twice a year for two hours on the Saturday that immediately precedes the start of each ACS National Meeting. Virtual meetings, discussion by email, etc. are also held as needed.

Committee Pages:

ACS CINF > Committees > Education
ACS Network: CINF Education Committee Members (a private site for members; contains archive of Committee documents)

Grace Baysinger, Chair, CINF Education Committee
CINF membership increased dramatically by 39.1% to 1,316 between 2013 and 2014 with the net addition of 370 new members. Regular Student Members and Student Member Undergraduate categories together grew by 404 new members, which masked a 4.3% decline in Regular Members.

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CINF Membership Committee
Not all member records specify gender. Assuming a 50/50 split of those not specified, two thirds of CINF members are male and one third is female. While the overall split is not significantly different between 2013 and 2014, fewer members specified their gender in 2014.

2014

2013
A seismic shift in cross-divisional membership occurred between 2013 and 2014. The Industrial and Engineering Chemistry Division (IEC), Catalysis Science & Technology Division (CATL), and Cellulose and Renewable Materials Division (CELL) memberships all increased dramatically, overshadowing the Divisions that have historically been strong for cross-divisional overlap with CINF, namely, COMP, MEDI, and ORGN.

The new student members are responsible for the large increase in cross-membership with IEC, CATL, and CELL.
Geographically, the 80/20 rule applies to CINF membership, with 80% of the members having a primary address in the United States.

Gregory Banik, Chair, CINF Membership Committee
CINF Member Profile: Elsa Alvaro

A new feature, Member Profile, was introduced by Donna Wrublewski, Incoming Chair 2015 of the CINF Membership Committee, in the previous fall 2014 issue of *Chemical Information Bulletin* (http://bulletin.acscinf.org/node/648). Find out more about your CINF colleagues, what they find valuable about CINF, and even identify potential collaborators! If you're interested in being interviewed for an upcoming *CIB*, please e-mail Donna at dtwrub@caltech.edu.

Who are you?

Elsa Alvaro

What do you do?

I am the librarian for chemistry, physics, and astronomy at Northwestern University. I connect people with the information resources that they need and also manage Northwestern University Chemistry, Physics and Astronomy collections. I have an exciting job that allows me to work on many different things and constantly develop new skills. Right now, I am preparing the sessions that I'm going to teach during the fall quarter, working on an exhibit that I am co-curating about the intersection of art and science, and analyzing different sources of quantitative and qualitative data to see what we can learn about our users and their future needs.

Why are you in the chemical information field?

It's the perfect fit for combining a passion for information and a chemistry background. After I got my PhD in organic chemistry (Universidad Complutense de Madrid, Spain), I came to the United States to work as a postdoctoral researcher at the University of Illinois at Urbana-Champaign. My research focused on studying the mechanism of the palladium-catalyzed thiation of aryl halides. I loved it, especially the feeling of solving a challenging puzzle and the excitement of doing something new, but I realized that I also had an interest in what was going on in the information and scholarly communication worlds. So towards the end of my postdoc, I started taking courses as a community credit student at UIUC's Graduate School of Library and Information Science. I enjoyed it so much that I decided to go back to grad school and get a library science degree at Indiana University Bloomington. I was very lucky to have inspiring mentors who were supportive and encouraging: John Hartwig, my postdoc advisor, and Roger Beckman, chemistry librarian at IU Bloomington.

What makes CINF valuable to you?

CINF is a great group to be involved with and a true career enhancer. In CINF you find a mixture of librarians, publishers, developers, cheminformaticians, etc. that it is extremely hard to find anywhere else. I get to learn a lot from other people’s experiences and perspectives, and there is always something new and interesting going on. Of course, I also love coming to ACS Meetings and attending CINF Symposia. I am now a member of the CINF Program Committee.
The members of the Division of Chemical Information (CINF) will be interested in the following news from the ACS Council meeting held in San Francisco, August 23, 2014.

# Committee Election Results and Candidates for National Elections:

Please note that those elected to the following committees include three CINF officers:


N&E announced the candidates for the fall 2014 ACS national election as follows:

Candidates for President-Elect, 2015:
- Peter K. Dorhout, Dean of Arts & Sciences and Professor of Chemistry, Kansas State University, Manhattan, KS
- William A. Lester, Jr., Professor of the Graduate School, Department of Chemistry, University of California, Berkeley, CA
- Donna J. Nelson, Professor, Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK

Candidates for Directors-at-Large, 2015-2017:
- Dawn A. Brooks, Sr. Director, Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN
- William F. Carroll, Jr., Vice-President, Occidental Chemical Corporation, Dallas, TX
- Barbara A. Sawrey, Associate Vice Chancellor, Academic Affairs, and Dean of Undergraduate Education, University of California, San Diego, La Jolla, CA
- Ellen B. Stechel, Deputy Director, ASU-LightWorks, Tempe, AZ, Arizona State University

Candidates for District III Director, 2015-2017:
- Pat N. Confalone, Confalone Consulting, LLC, (Retired DuPont), Wilmington, DE
- Anne S. DeMasi, Hazard Communication Manager, Chemtura Corporation, Philadelphia, PA
Candidates for District VI Director, 2015-2017:

- Paul W. Jagodzinski, Dean, College of Engineering, Forestry & Natural Sciences, Northern Arizona University, Flagstaff, AZ
- Lee H. Latimer, Consultant, Oakland, CA

ACS and CINF members are urged to suggest names for ACS President, Board of Directors and elected committee positions: nomelect@acs.org

Selected Committee Reports:

Committees (ConC)
On the recommendation of ConC, Council voted to continue the Committee on Patents and Related Matters, subject to concurrence by the Board of Directors; and to continue the Committee on Technician Affairs.

Council Policy (CPC)
At the spring meeting in 2015, CPC will set the divisor for 2016 – 2019. The formula will be based on membership numbers as of December 31, 2014. Official notification of the Councilor divisor and the number of Councilors permitted for Local Sections or Divisions will be sent to Local Sections and Divisions no later than May 1, 2015, as it will affect elections conducted in 2015.

Budget and Finance (B&F)
B&F reviewed the Society’s 2014 probable year-end financial projection which calls for a Net Contribution from operations of $14.4 million, or $752,000 higher than the Approved Budget. Total revenues are projected at $497.2 million. This is $1.1 million or 0.2% unfavorable to the Approved Budget. The projected shortfall is primarily driven by lower-than-budgeted Electronic Services, Registration Fees, and Advertising revenues. Total expenses are projected at $482.8 million, which is $1.9 million or 0.4% favorable to the Approved Budget. This variance is the result of lower-than-budgeted expenses across multiple categories primarily in the Society’s information services divisions (CAS and Publications). The Probable 1 projection was developed using May 31 actual financial results. Based on more recent information through July, management believes this projection will be exceeded.
More details at the B&F website: http://www.acs.org/content/acs/en/about/governance/committees/budget.html

Education (SOCED)
SOCED received an update on the new American Association of Chemistry Teachers (AACT), which is now accepting members and will officially launch September 2, 2014. AACT member benefits include access to curricular resources, such as lesson plans and multimedia; professional development opportunities; a subscription to ChemMatters; and an online member network. Membership is available to any interested ACS member.
AACT website: http://teachchemistry.org/

Economic and Professional Affairs (CEPA)
CEPA announced that the unemployment rate for all ACS chemists has dropped from 3.5% in March 2013 to 2.9% as of March 2014, but the unemployment rate for new chemistry graduates as of August 2013 is considered to be an all-time high of 14.6%. The number is higher when we isolate bachelor’s level graduates, for whom the rate is 15.8%.
CEPA Career Navigator: www.acs.org/careernavigator
On the recommendation of CEPA, Council voted to approve the Professional Employment Guidelines.

Committee on Meetings and Expositions (M&E)
M&E reported that 11,847 papers were accepted for the 248th National Meeting in San Francisco. As of August 13, total attendance was 15,761. The last meeting in San Francisco was held in the spring of 2010 and attendance totaled 18,076. Attendance at this meeting broke down as follows:

- Regular: 9,840
- Students: 3,671
- Guests: 568
- Exhibitors: 1,131
- Exhibit-only: 551

Attendance at the fall National meetings since 2004 is as follows:

- 2004: Philadelphia, PA 14,025
- 2006: San Francisco, CA 15,714
- 2007: Boston, MA: 15,554
- 2008: Philadelphia, PA: 13,805
- 2010: Boston, MA: 14,151
- 2011: Denver, CO: 10,076
- 2012: Philadelphia, PA: 13,251
- 2013: Indianapolis, IN: 10,840
- 2014: San Francisco, CA: 15,761

The Exposition had 432 booths with 285 exhibiting companies. The Committee voted to recommend to the Board of Directors the following sites for National Meetings:

- Boston: fall 2024, 2029, 2031
- San Diego: spring 2025, 2031, and fall 2027
- New Orleans: spring 2027, 2032
- Chicago: fall 2022.


M&E has voted to strengthen the current recording policy at National Meetings by including enforcement language. Failure to follow the policy could result in disciplinary action up to and including expulsion from the meeting.

Divisional Activities (DAC)
The Multidisciplinary Program Planning Group is proposing the following 2018-2019 national meeting themes to the divisions for their consideration:

2018
- Spring: Energy Solutions and the Environment
- Fall: Chemistry – from Bench to Market
2019

- Spring: Chemistry for New Frontiers

Committee on Local Section Activities (LSAC)
National Chemistry Week will be held October 19-25 with the theme, “The Sweet Side of Chemistry: Candy.”

On the recommendation of LSAC, the Council voted to dissolve the Ocean County Local Section due to inactivity. The motion by to have the Ocean County Local Section territory annexed by the Philadelphia Local Section was withdrawn from further action.

Membership Affairs (MAC)
MAC reported that as of June 30, the total ACS membership was 158,869, a net increase of 512 since May of this year. The number of international members has grown this year by 312, to almost 25,000. The number of current, unpaid members declined in June and is 13% lower than June 2013. As of July 1, automatic renewal (on credit card) became available. The Committee also voted to extend its current test of an introductory membership offer to those who join the Society at non-ACS conferences and events to include the graduate students and potential Regular Members who attend ACS on Campus events worldwide each year.

International Activities (IAC)
On the recommendation of IAC, Council voted to approve the establishment of an International Chemical Sciences Chapter in South Africa. This action requires Board action, too.

Professional Training (CPT)
The Committee concluded discussion of the guidelines revision and voted provisional approval of the draft document. The draft will be distributed to department chairs of chemistry programs this fall. CPT also approved the final report of a survey on chemical information resources that will be published in the Committee newsletter and website.

Actions of the Board of Directors

The Board’s Executive Session

The Board’s Committees

The Board of Directors received reports from its Committees on Grants and Awards (G&A), Executive Compensation, and the Society Committee on Budget and Finance (B&F).

On the recommendation of the Committee on Grants and Awards, the Board voted to approve Society nominations for the 2015 Perkin Medal and the 2015 nominee for the National Science Board Public Service Award.

On the recommendation of the Committee on Budget and Finance, the Board voted to approve an advance member registration fee of $390 for national meetings held in 2015.

The Board received a briefing and approved several recommendations from its Committee on Executive Compensation. The compensation of the Society’s executive staff receives regular review from the Board.
The Executive Director/Chief Executive Officer’s Report

The Executive Director/CEO and her direct reports updated the Board on the following: a summary of a recent survey measuring ACS employee engagement; the ACS’s global presence and activities; a recommendation on allocating certain investment income from the ACS Endowment Fund to Project SEED; activities and plans of CAS (Chemical Abstracts Service) and the ACS Publications Division; and a report on “Challenges and Opportunities for ACS, 2015-2017.”

As a follow-up to the Publications report, the Board voted to appoint or reappoint several editors of Society publications.

The Board was also updated on the American Association of Chemistry Teachers (AACT), a new organization sponsored by the ACS that is officially launching in September. Membership is now open to anyone with an interest in chemistry education. The website is www.teachchemistry.org

Other Society Business

The Board also:

- Held a discussion on strategic questions related to how we can strengthen ACS’s service to chemistry communities and professionals worldwide.
- Received an update on the recruitment process for the Executive Director and CEO position. This position offers wonderful challenge and opportunity. We have retained Korn Ferry International, a large, globally known firm, to conduct the search, and the position is currently being advertised. We hope to complete the process in time to have a new Executive Director and CEO in place January 1, 2015.
- Received reports from the Presidential Succession on their current and planned activities for the remainder of 2014 and 2015.
- Approved, on the recommendation of its Committee on Professional and Member Relations, a resolution to recognize the contributions of the Organization for the Prohibition of Chemical Weapons (OPCW) in the peaceful application of the chemical sciences to improving people’s lives through the transforming power of chemistry and advancing its broader enterprise and its practitioners for the benefit of Earth and its people.
- Approved, on the recommendation of the Committee on Nomenclature, Terminology, and Symbols, a resolution welcoming the Consultative Committee for Amount of Substance: Metrology in Chemistry (CCQM) to co-locate its fall 2015 Committee meeting at the ACS Fall National Meeting in Boston, Massachusetts.

The Board’s Open Session

The Board held a well-attended open session which featured Sam Kean, author of The Disappearing Spoon and The Violinist’s Thumb, both of which were national bestsellers and named Amazon “Top 5” science books of the year. His newest book, The Tale of the Dueling Neurosurgeons, was recently released and is receiving high acclaim. Mr. Kean’s topic was “The Disappearing Spoon,” the wonders of the periodic table. Following the presentation, members of the presidential succession and the Executive Director and CEO offered brief reports on their activities. (The officers provided more extensive reports on their activities and/or future plans as part of their reports to the Council.)

Andrea Twiss-Brooks and Bonnie Lawlor, CINF Councilors
The Committee (CCAS) met in Executive Session on August 8, 2014, engaging with CAS management in a lively discussion on a number of recent developments that provide researchers with access to the most comprehensive, authoritative scientific content and enhance their workflows and productivity.

The CAS databases now contain more than 400 million cited references included for journals, conference proceedings and basic patents from the USPTO, EPO and German patent offices (1997 to the present).

One-click access to SciFinder is now available to customers from ChemDraw, providing scientists with a highly sought after shared research solution.

The new non-Java CAS structure editor continues to be updated and is approaching full functionality.

Ongoing content and functionality enhancements to new STN continue to drive increased engagement and usage.

Global patent coverage was expanded with the launch of full-text content from Korea, Australia and the United Kingdom.

New STN Global Value Pricing provides unlimited access for customers of all sizes at a fixed price while maximizing the value and power of STN.

CCAS continues its role as a conduit of information between Society members (and users of CAS services), the ACS Governing Board for Publishing and CAS management, providing CAS management with valuable and enthusiastic feedback on current and future initiatives throughout the discussions in San Francisco. For example, as a result of feedback, CAS will be conducting user research to understand the value of the CASSI Search Tool to help evaluate enhancement requests such as adding old, very short journal abbreviations.

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

Find out more at: http://www.cas.org/content/references/most-cited-references
Joint Board-Council Committee on Publications

The open session of the Joint Board-Council Committee on Publications (JBCCP) was held on August 8, 2014 in San Francisco, CA. The Division President, Brian Crawford, presented an overview of the ACS Publications Division’s operational highlights, new product introductions, recent editor appointments, technology-based initiatives, and open access developments including the “ACS is Open” strategic initiative. His presentation slides are available at: http://bulletin.acscinf.org/PDFs/JBCCP_080814.pdf.

Staff presented the final report for the strategic analysis of C&EN, a project initiated in September 2013. As a result of the analysis, C&EN launched a number of initiatives.

It was announced that three Editor Search Committees had recommended, and the ACS Board of Directors had approved, the following appointments:

- Professor Courtney C. Aldrich (University of Minnesota) to serve as the inaugural Editor of the new ACS journal, ACS Infectious Diseases, effective in 2015.
- Professor Paul J. Chirik (Princeton University) to serve as the Editor of Organometallics, effective in 2015.
- Professor David L. Kaplan (Tufts University) to serve as the inaugural Editor of the new journal, ACS Biomaterials Science & Engineering, effective in 2015.

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

ACS ChemWorx user base now >50,000; new 2.0 release imminent
Register free (even for non-ACS members) at www.acschemworx.org
ACS ChemWorx Introduced its English Editing Service in March 2014

Read more news of the ACS Publications in ACS Excellence, Fall 2014.
CINF Social Networking Events

The ACS Division of Chemical Information is very fortunate to receive generous financial support from our sponsors to maintain the high quality of the Division’s technical programs and to promote communication between members at social functions.

This year we had a large number of sponsors for the Fall 2014 ACS National Meeting in San Francisco, California, and CINF members and friends got to enjoy networking occasions at four splendid gatherings. (A photo from the CINF Welcoming Reception at left).

On Sunday the CINF Welcoming Reception was sponsored by Bio-Rad Laboratories, InfoChem, Kilmorie Clarke, PerkinElmer, Springer, Journal of Chemical Information and Modeling, and AAAS/Science.

On Monday the Harry’s Party (recognized for its 50th anniversary noble tradition) was sponsored exclusively by ACS Publications.

On Tuesday the CINF Luncheon was sponsored exclusively by RSC Publishing, and the 2014 Herman Skolnik Award Reception honoring Dr. Engelbert Zass was funded by Elsevier/Reaxys, Thieme Chemistry, ACS Publications and Chemical Abstracts Service.

Our sponsors also help to support other divisional activities at the meetings including Scholarships for Scientific Excellence for graduate students and postdocs in chemical information. At the 2014 Fall Meeting the four scholarships were sponsored exclusively by Royal Society of Chemistry.

The Division gratefully acknowledges contribution from all our sponsors!

Looking forward to spring 2015, several opportunities are available to support the Division’s social events, speakers, and other conference related material. Our sponsors are acknowledged on the CINF web site, in the Chemical Information Bulletin, on printed meeting materials, and at all events for which we use their contributions. Additional venues and benefits are reviewed in our Sponsorship Opportunities brochure at: http://www.acscinf.org/PDF/CINF_Sponsorship_Brochure.pdf.

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

Phil Heller, Chair, Fundraising Committee
Email: Fundraising@acscinf.org
Tel: 917-450-4591

Philip Heller, Chair, CINF Fundraising Committee

CINF photos from the Fall 2014 ACS National Meeting are at:
https://www.flickr.com/photos/cinf/sets/
Photos by Wendy Warr
Sponsor Announcements

Did you know the ACS publishes **more than 1,400 peer-reviewed e-books**, many of which are authored or reviewed by CINF Members?

ACS eBooks Fast Facts:

- More than 1,400 titles
- Over 27,000 chapters
- Peer-reviewed down to the chapter level
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*Michael Woodruff, ACS Publications*

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*Science Advances*: **This is the start of something big.** AAAS is pleased to introduce *Science Advances*, an online-only gold open access journal which will publish its first papers in February 2015. The journal will offer high-quality original research in life, physical, and social sciences, as well as computer science, engineering, and mathematics.

*Ebola Virus Special Collection*: Given the current widespread and lethal outbreak of the Ebola virus, *Science* and *Science Translational Medicine* offer a freely available collection of research and news articles on the viral disease to researchers and the general public.

*Minah Kim, AAAS/Science*
Springer Launches *ChemTexts*

The first textbook journal worldwide will publish material for academic education in chemistry and biochemistry

Beginning in 2015, Springer will publish a new online-only journal called *ChemTexts – The Textbook Journal of Chemistry* (ISSN: 2199-3793). With four issues a year and 250 pages per issue, *ChemTexts* will impart contemporary knowledge in all subdivisions of chemistry to students at an exceptionally high didactic level.

*ChemTexts* can be used by students for learning, by lecturers for teaching, or by researchers and professionals as a recap of essential knowledge. On the pedagogical level, the journal primarily supports bachelor and master programs, but material at higher level is also considered. Typically, each text consists of a self-consistent treatment of a topic which could be part of a textbook. Beyond informative illustrations, the texts may also include supplementary material such as animated presentations or videos.

“The idea first came to me when I observed students interacting with a textbook that I had recently published,” said editor-in-chief Fritz Scholz from the University of Greifswald in Germany. “It was clear that they preferred to download individual chapters of the textbook via the internet, rather than carry the whole book around with them.”

*ChemTexts* introduces a completely new concept in scientific publishing: the provision of texts for educational purposes that mirror the current state of knowledge. Unlike many textbooks, the chapters are carefully peer-reviewed to guarantee scientific correctness. Only those texts are published which represent genuine improvements over existing textbook material. If authors provide a translation of their English text in their native language, then Springer will also make that translation available as supplementary material. “Knowing that most of the SpringerLink users are actually students who would benefit from this new journal, I was excited when Fritz Scholz approached me with the idea,” said Springer publishing editor Steffen Pauly. “Springer’s innovative spirit became evident through all the support that the *ChemTexts* proposal got from colleagues in other departments.”

For further information: [http://www.springer.com/40828](http://www.springer.com/40828)

Kazumi Nishihara, Springer

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Deborah Kernan, BioRad

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*Chemical Information Bulletin, 2014, 66 (4)*
Exciting New Content and New Features in Upcoming Science of Synthesis Release 4.0.1

Science of Synthesis (SOS) provides a critical review of the synthetic methodology developed to-date in the fields of organic and organometallic chemistry. The content is compiled and updated by a community of over 1,750 renowned chemists worldwide.

The upcoming release of SOS 4.0.1 (Q4, 2014) will include 13 new content volumes which comprise approx. 8,000 printed pages in total. Eight of the volumes are Science of Synthesis Knowledge Update volumes dating from 2012 to 2014. Highlights include a comprehensive review of asymmetric transformations catalyzed by gold salts published between 2005 and 2011 by M. J. Campbell and F. D. Toste; a new chapter outlining many of the methods used to synthesis α-aryl ketones and α-hetaryl ketones by J. C. Collings; and an entirely new chapter on thioaldehyde and thioketone S-sulfides (thiosulfines) overviewing methods for their in situ generation as well as their application by G. Mlostoń and H. Heimgartner.

The other five volumes comprise part of the much-acclaimed Science of Synthesis Reference Library series. Cross Coupling and Heck-Type Reactions consists of three volumes written by 96 experts and edited by G. A. Molander, J. P. Wolfe and M. Larhed. It includes the best methods currently available for the formation of new carbon-heteroatom and carbon-carbon bonds using metal-catalyzed cross-coupling reactions. The two volumes Multicomponent Reactions written by 63 leading chemists in the multicomponent reactions field and edited by T. J. J. Müller critically review the state of the art of domino, sequential, and consecutive multicomponent reactions.

In addition to new content, this release will include a new HTML5 structure editor which will allow users to draw chemical structures from within the web browser's page and which will not require any plugins (e.g., Java). Also, functionality will be included that enables users to find specific Science of Synthesis articles quickly using additional operators in the text search box.

To get access to the product or a free trial please visit the website at: www.thieme-chemistry.com

M. Fiona Shortt de Hernandez, Georg Thieme Verlag KG

SciFinder and ChemDraw Software Connection

Chemical Abstracts Service (CAS) and PerkinElmer are excited to provide their shared research solution, pairing SciFinder, the world’s most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences, with ChemDraw software, the drawing tool of choice for chemists to create publication-ready, scientifically intelligent drawings for use in ELNs, databases and publications. This collaboration between two industry innovators allows users to draw a structure using the ChemBioDraw Ultra 14 offering and then initiate a SciFinder session to search the structure. ChemBioDraw Ultra software automatically detects whether the structure is a single substance, or the reactant or product of a reaction. Researchers can now save considerable time when using both products.

To learn more, visit us at http://perkinelmer.cas.org/.

Jamie Weiner, CAS
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