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Message from the Chair



Dear Colleagues,

The CINF symposia and events at the American Chemical Society Meeting in Denver were a great success. With tie-ins to the International Year of Chemistry 2011, the meeting was as enjoyable as it was informative.

One of the most exciting things announced at the meeting was the results of the CINF 2011 elections. Antony Williams from RSC Publishing was elected Chair-Elect for 2012. Tony will take on the role of CINF Chair in 2013 when the current Chair-Elect, Rajarshi Guha, finishes his tenure as CINF Chair in 2012. In addition, Leah Solla from Cornell University was re-elected Secretary, Andrea Twiss-Brooks from the University of Chicago was re-elected Councilor, and Chuck Huber from UC Santa Barbara was re-elected Alternate Councilor. This excellent group deserves hearty congratulations!

Of course, now that the 2011 CINF elections are complete, one of my duties in 2012 as CINF Past-Chair will be to nominate candidates for the 2012 CINF elections. I urge anyone interested in becoming more active in CINF to contact me about being nominated for this election. I have found CINF members to be some of the finest, brightest, and most fun people with whom you could choose to spend time. Also, as the world of chemical information is a small one, it never hurts your career to network with this group of people.

Another important thing that happened recently was the migration of CINF's [Chemical Information Bulletin](#) to the Drupal content management system. The work done by the CINF Communications and Publications Committee and by CINF webmaster, Danielle Dennie from Concordia University, is simply stunning. They deserve our great thanks and praise!

Finally, I would like to thank two people. Carmen Nitsche from Accelrys, CINF Past-Chair, was a godsend to me. Everyone should send her money and buy Accelrys products, she is that wonderful. I also need to thank Svetlana Korolev, who, in addition to doing a magnificent job with the [Chemical Information Bulletin](#), was utterly gracious and polite when I was late with my Letter from the Chair. If you have extra money left over that you haven't sent to Carmen, please send it to Svetlana.

Wishing you all the very best!

Warmest regards,

Gregory Banik, Chair, ACS Chemical Information Division

Was it worth volunteering? Check out the musings of a past CINF Chair, Carmen Nitsche, at https://community.accelrys.com/community/accelrys_blog/blog/2011/09/21/musings-of-a-past-cinf-chair

Letter from the Editor

This is the most comprehensive post-conference issue of the *Chemical Information Bulletin*. Containing the impressive contributions made by CINF symposia organizers and presenters at the 2011 Fall ACS National Meeting in Denver, CO, the issue looks like “proceedings of CINF and related matters.” Since the program is a driving force of the divisional activities, let me focus on it. In this issue you will find the CINF technical program highlights by Rachelle Beinstock. Besides putting together an accomplished program, Rachelle Beinstock is to be recognized on her publishing *Library Design, Search Methods, and Applications of Fragment-Based Drug Design* sponsored by CINF and COMP within the *ACS Symposium Series*.



Out of the seven CINF symposia held at the past meeting, the full reports of four symposia are included in this bulletin. Namely, these are: a symposium on *Chemical Environmental Specific Databases and Searching Information Related to the Air, Water, and our Environment* organized within ACS thematic programming by Andrea Twiss-Books; the two most noteworthy (and well attended by over 80 people each) symposia, *The Herman Skolnik Award Symposium honoring Professor Alexander Lawson* written by Wendy Warr, and *Chemistry in Mobile Spaces* by Martin Brändle and David Martinsen; and furthermore an unconventional session featuring a mix of presentations and videos on *Non-Traditional Careers: What Else Can I Do With a Chemistry Degree?* by Patricia Meindl. Coincidentally, these four symposia have been recorded by ACS, so that you can get access to some original content (15 CINF presentations) at the [ACS Learning Center](http://www.softconference.com/ACSchem/) (<http://www.softconference.com/ACSchem/>) virtually. I included notes about a number of the recorded presentations available for each session at the end of the articles.

Additionally, you will find a report of the 9th *International Conference on Chemical Structures* held on June 5-9, 2011 in Noordwijkerhout, The Netherlands, by Keith Taylor. This triennial conference is organized jointly by seven societies including ACS CINF. The technical section concludes with a synopsis of themes prepared by the *Multidisciplinary Programming Planning Group* for four upcoming ACS National Meetings. Thanks to Guenter Grethe and Richard Love for this information.

Beyond the technical program you will find awards and scholarships announcements, a book review, committee reports and sponsor announcements. Specifically, I would like to bring to your attention a new feature - *Overview of the Council Committee on Patents and Related Matters*. I would like to thank Edlyn Simmons, James Chao and David Smorodin for this article. Looking ahead to the future bulletins, I would like to welcome an overview of the other Council committees having CINF members on them.

In conclusion, I would like to thank all authors for their generous contributions to this issue. My special thanks go to Mark Luchetti for designing the cover page, to Bonnie Lawlor and Wendy Warr for proofreading this issue, and to David Evans, Carmen Nitsche, and Wendy Warr for taking photographs at the Denver meeting, and for making them available (with name tags!) at <http://www.flickr.com/photos/cinf>.

Svetlana Korolev, Editor, *Chemical Information Bulletin*

AWARDS AND SCHOLARSHIPS

2011 Herman Skolnik Award Presented



The Herman Skolnik Award recognizes outstanding contributions to and achievements in the theory and practice of chemical information science and related disciplines. The 2011 Skolnik Award was presented to Professor Doctor Alexander Lawson – better known to us all as “Sandy.” Sandy organized a fascinating full day symposium on “Information Services in Chemical Sciences: Perspectives” with a roster of big name speakers: who else could have persuaded Bob Massie of CAS and Martin Tanke of Elsevier to appear in the same program? A full report on the symposium is elsewhere in this *CIB*. The symposium was followed in the evening by a reception generously funded by Elsevier, which allowed for some light-hearted “roasting” of Sandy by his Elsevier colleagues.

Phil McHale, Chair, CINF Awards Committee

2012 Herman Skolnik Award Winners Announced

Dr. Peter Murray-Rust and Prof. Henry Rzepa are the joint recipients of the 2012 Herman Skolnik Award presented by the ACS Division of Chemical Information (CINF).

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. The winners will also be invited to present an award symposium at the Fall 2012 ACS National Meeting to be held in Philadelphia.



Peter Murray-Rust and Henry Rzepa are recognized for their continued efforts to advance the field of chemical informatics, particularly in electronic and online forms, for opening standards to facilitate first-class science, and promoting new ways to collaborate and exchange chemical data. Through their efforts they have dramatically improved the ways in which molecular data are embedded in published scientific articles, preserving chemical identifiers and facilitating indexing and searching online. Their work has had a huge impact in the fields of chemical document analysis, chemistry on the Internet, and in the orchestration of a viable strategy for making electronic chemistry information as widely accessible and usable as possible in our information age.

Henry Rzepa and Peter Murray-Rust have been closely associated with chemistry on the Internet, and were the only two chemists at an early WWW conference held in CERN in 1994. From this they were involved in the use of XML and development of the Chemical Markup Language (CML).

Other Internet-related projects led by Henry include how a chemical journal might evolve to benefit from the Internet (the CLIC project, jointly with Cambridge University, Leeds University and the RSC), an exploration of online chemical conferencing (the ECTOC series), the ChemWeb discussion forum, the Molecule-of-the-month columns, and co-organizing the first ever Internet-focused session at an ACS national meeting (in 1995) dedicated to the Internet and the Web, along with dedicated workshops in Washington DC, the UK, and at Imperial College. In addition to his Internet-related activities, Peter has also overseen development of software including OSCAR1 for experimental data checking and its extension to OSCAR4 for chemical tagging and other chemical natural-language processing; OPSIN name-to-structure conversion (delivered as Open Source to the community); Chem4Word add-in; and CrystalEye online resource of crystal structure data from the Internet. Peter has also been very active in the principles and practice of Open Data, in chemistry and elsewhere, and he was one of the team that defined the Panton Principles (honored by the SPARC Innovator, 2010).

Peter has B.A. and D.Phil. degrees in chemistry from the University of Oxford, and was a lecturer at the Universities of Ghana and Stirling. After a period in industry as Head of Molecular Graphics at Glaxo Group Research, he turned to academia as Professor of Pharmacy at the University of Nottingham, and is currently Reader in Molecular Informatics and Senior Research Fellow, Churchill College, University of Cambridge.

Henry has a B.Sc. in chemistry from Imperial College, London, and Ph.D. and D.Sc. (London). After a period as a SERC Postdoctoral Fellow at the University of Texas, he returned to Imperial College, London, where he has held the Chair in Computational Chemistry since 2004.

Henry and Peter's pioneering and continued efforts have changed the ways in which chemistry is handled, shared, stored and communicated on the Internet for the better of all, and they are worthy recipients of the 2012 Herman Skolnik Award.

Phil McHale, Chair, CINF Awards Committee

2011 CINF Scholarship for Scientific Excellence: Winners Announced



Three scholarships of \$1,000 were awarded by FIZ CHEMIE Berlin. The recipients presented posters of their work during the CINF Welcome Reception on Sunday evening, and received the awards from Professor René Deplanque during the CINF Luncheon on Tuesday. The three winners were:

Barun Bhatarai (University of Miami):
“SMARTNames: a new framework to organize chemical structural information based on chemically relevant functional groups.”

Felix Rudolph (Max-Planck-Institut für Kohlenforschung (Mülheim an der Ruhr, Germany)): "Development of an Open Source ELN."

Karen Salazar (Louisiana State University): "Introduction of InChI to Researchers in the Department of Chemistry at Louisiana State University."

Phil McHale, Chair, CINF Awards Committee

2011 Lucille M. Wert Student Scholarship Presented



This annual award of a \$1,500 scholarship is 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 2011 Scholarship was presented to Dr. Elsa Alvaro at the CINF Luncheon on Tuesday. Elsa has BS and PhD degrees in chemistry from the Universidad Complutense de Madrid in Spain, and she is currently enrolled in the Master of Library Science degree program at the School of Library and Information Science at Indiana University Bloomington, where she is the Charles A. and

Charles H. Davis fellow in Scientific Information and a Merit Scholar. She is also a graduate assistant at the Chemistry Library and Life Science Library at Indiana University Bloomington, and her avowed calling is to become a chemistry librarian in a research institution.

Phil McHale, Chair, CINF Awards Committee

2012 Lucille M. 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 2012 Lucille M. Wert Scholarship is February 1, 2012.

Details on the application procedures can be found at <http://www.acscinf.org/awards/wert.php>.

Applications (email preferred) can be sent to: margaret.matthews@thomsonreuters.com

Contact address: Marge Matthews, CINF Awards Committee,
633 Dayton Rd. Bryn Mawr, PA 19010-3801, Phone: 215-823-3922.

Chemical Structure Association Trust Jacques-Émile Dubois Grant: Applications Invited for 2012



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, renamed in honor of Professor Jacques-Émile Dubois who made significant contributions to the field of cheminformatics. The Trust is currently inviting the submission of grant applications for 2012.

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. A Grant will be awarded annually up to a maximum of five thousand U.S. dollars (\$5,000). Grants are awarded for specific purposes, and within one year each grantee is required to submit a brief written report detailing how the grant funds were allocated. Grantees are also requested to recognize the support of the Trust in any paper or presentation that is given as a result of that support.

Who is Eligible?

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

Which Activities are Eligible?

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

Application Requirements:

Applications must include the following documentation:

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

4. Two reference letters in support of the application. Additional materials may be supplied at the discretion of the applicant only if relevant to the application and if such materials provide information not already included in items 1 - 4. Three copies of the complete application document must be supplied for distribution to the Grants Committee.

Deadline for Applications:

Applications must be received no later than March 14, 2012. Successful applicants will be notified no later than May 2, 2012.

Address for Submission of Applications:

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

Bonnie Lawlor, Chair, CSA Trust Grant Committee



Submissions for the 2012 Reaxys PhD Prize will open on December 15, 2011. The Reaxys PhD Prize recognizes research and publication excellence in organic, inorganic, and organometallic chemistry. The Prize is open to all students studying for a PhD (or having completed a PhD after January 1, 2011) in chemistry.

Each submission consists of a letter of recommendation from the student's supervisor, a representative peer-reviewed publication, and a CV.

Submissions are reviewed and judged for originality, importance, applicability, rigor or approach and publication quality, by an external board of internationally renowned chemists.

Submissions will close on February 15, 2012.

For further details on the 2011 Finalists and Winners, and information on how to submit please visit prize.reaxys.com.

The next CINF Best Presentation Award Symposium, *Beyond the Database: New Models of Scholarship in an eScience World*, will be held at the 2012 Spring ACS National Meeting
<http://www.acscinf.org/awards/presentation.php>

TECHNICAL PROGRAM

CINF Technical Program Highlights



Unfortunately the fall 2011 Denver National ACS meeting began with a hurricane. Hurricane Irene affected travel from the entire East Coast, closing all three New York area airports and putting a severe damper on attendance and resulting in the cancellation of many sessions. However, despite all, CINF sessions still managed to maintain a high level of attendance and interest. The weather was sunny and perfect in the mile high city!

Opening day Sunday morning featured a session complementing the theme for the Denver meeting, *Chemistry of Air, Space and Water*, on “Chemical Environment Specific Databases and Searching Information Related to the Air, Water, and our Environment.” Andrea Twiss-Brooks organized this session with talks that complemented each other without overlap. This session featured talks on the US Geological water survey and USGS National Geochemical Database as well as CHEMLIST. There was a lively question and answer session and audience participation.

Sunday afternoon, Patricia Meindl organized a very apropos session on “Nontraditional Careers What Else Can I do with a Chemistry Degree?” This was a very topical symposium based on the ACS Board’s meeting on unemployment and what the ACS can do. Unemployment among chemists, based on ACS data is currently 3.8%, the highest it has been since 1972!

Monday featured a standing-room only symposium organized by David Martinsen and Martin Braendle on “Chemistry in Mobile Spaces: Chemical Apps for Mobile Devices.” Attendees struggled to capture those QR codes on the presented slides before they disappeared and argued whether iPhone, iPad, or Android smartphones were the platform of the future, while the oldies in the audience struggled with reading the ACS program small text on our phones!

By all means, on Tuesday we were all honored to celebrate with Alexander (Sandy) Lawson on receiving the 2011 Herman Skolnik Award. The Herman Skolnik symposium opened with Robert Massie (CAS) and a fascinating overview of the publishing and information age and how it is evolving, followed by presentations from Martin Tanke (Elsevier), Tony Williams (ChemSpider, Royal Society of Chemistry), and Uwe Rosemann (German National Library of Science and Technology). The afternoon session opened with a presentation by Robert Glen (University of Cambridge) on *apelin* and drug discovery, followed by a presentation from Torsten Hoffmann (Hoffmann-La Roche) on how medicinal chemists in industry keep track of information. Rudy Potenzzone (SciencePoint Solutions), and Wendy Warr (Wendy Warr & Associates) rounded out the afternoon prior to hearing from Sandy himself about his extensive and interesting career. We all want to share our sincerest congratulations to Sandy on receiving this well deserved award!

Wednesday concluded the CINF programming with our CINFlash last minute cutting edge papers and discussion led by Rajarshi Guha. Our general session featured a very full and eclectic group of papers including many presentations on chemical structure representations, consensus modeling and ring representations by David Deng (formerly Roche, now ChemAxon), Jose Medina-Franco

(Torrey Pines Institute for Molecular Studies), and Adrian Kolodzik (University of Hamburg), endocrine disruptor characterization by Tudor Oprea (University of New Mexico), and several presentations on chemical databases by Evan Bolton (National Center for Biotechnology Information), Tony Williams (ChemSpider, Royal Society of Chemistry), Jens Schamberger (Bayer HealthCare AG), and interaction networks by Adam Palmer (Harvard Medical School) and Karina Martinex-Mayorga (Torrey Pines Institute for Molecular Studies). The afternoon session closed with a presentation on the use of InChIs as chemical reaction descriptors by Jonathan Goodman (University of Cambridge) and several presentations on library tools and their usage by Jayne Knoop (CAS), Shu Guo (Central Michigan University), Danielle Jacobs (Rider University) and Donna Wrublewski (University of Florida).

I am grateful to all the symposium organizers who worked so hard putting together an outstanding program for this Denver meeting. Of course, if you have any programming ideas for future meetings, please don't hesitate to contact me – it is too late for the next San Diego meeting (Spring 2012), but it is not too late for Philadelphia (Fall 2012) or future meetings!

Rachelle Bienstock, Chair, CINF Program Committee

Proposed CINF Program for the 2012 Spring ACS National Meeting

<i>Beyond Small Molecules: Pushing the Envelope for Chemical Structure Representation (CSA Trust)</i>	Keith Taylor, keith.taylor@accelrys.com
<i>Systems Chemical Biology: What is Systems Chemical Biology?</i>	Erja Kajosalu, kajosalu@mit.edu Jan Kuras, jan.kuras@chemistrycentral.com Tudor Oprea, toprea@salud.unm.edu
<i>Instruction Tools for Chemical Information Research Assessment</i>	Chuck Huber, huber@library.ucsb.edu
<i>Reaction Searching</i>	Leah Solla, leah.solla@cornell.edu Andrea Twiss-Brooks, atbrooks@uchicago.edu
<i>Mobile Space and eBooks</i>	David Evans, da.evans@elsevier.com Roger Schenck, rschenck@cas.org
<i>InChI Symposium</i>	Rich Apodaca, rapodaca@metamolecular.com
<i>Drug Polypharmacology Design and Prediction</i>	Antony Williams, williamsa@rsc.org Alex Tropsha, alex_tropsha@unc.edu
<i>CINFlash</i>	Shuxing Zhang, shuzhang@mdanderson.org
<i>How Good are Computational Methods for Drug Design?</i>	Rajarshi Guha, rajarshi.guha@gmail.com Orr Ravitz, orr.ravitz@gmail.com
<i>CINF Scholarship for Scientific Excellence</i>	Guenter Grethe, ggrethe@att.net
<i>General Papers</i>	Rachelle Bienstock, rachellebl@gmail.com
<i>Beyond the Database: New Models of Scholarship in an eScience World</i>	Phil Bourne, pbourne@ucsd.edu

Chemical Environmental Specific Databases and Searching Information Related to the Air, Water, and our Environment

The theme of the 242nd National Meeting was the Chemistry of Air, Space & Water. This CINF Sunday morning session in Denver kicked off the theme for the Division of Chemical Information with an introduction to a few of the many available database resources for information on environmental aspects of chemicals in terrestrial, aquatic and atmospheric environments.



Speakers addressed the challenges of creating databases for focused areas of research as well as those encountered in developing unified national repositories of information about manmade chemicals in the environment. Most of the featured resources are available on the web, but future developments may make more information available on smartphones and other mobile technology. Speakers included scientists from government agencies (USGS and USDA), academic librarians, and a representative from CAS. During the course of the morning, speakers provided links to a number of web resources that will be of interest to many readers. A summary of some of these resources, along with the presentation title and author are given here:

Can a compact means of representing the ionic equilibria of multi-acid/base aqueous solute molecules be devised?

R. Don Wauchope, US Department of Agriculture (retired)

Wauchope presented on the development of USDA Pesticide Properties Databases (ARS, NRCS and FOOTPRINT databases) and the SPARC chemical property calculator and its application in predicting ionization of pesticides in the environment.

ARChem's physicochemical calculator, SPARC
<http://archemcalc.com/sparc.php>

USGS National Geochemical Database: Recovering, repackaging, and repurposing 50+ years of historical data

Steven M. Smith, David B. Smith, US Geological Survey

Focusing on elements and compounds primarily of economic interest, but also on those playing a role in environmental health, Smith spoke about the historical and current development of the National Geochemical Database.

National Geochemical Database Project
http://minerals.cr.usgs.gov/projects/geochem_database/

Mineral Resources Data Download Site
<http://mrddata.usgs.gov/>

Quality of water resources from the U.S. Geological Survey: An introduction

Shu Guo, Central Michigan University

Guo presented on an array of resources from the USGS related to groundwater, surface waters, water quality measurements, and marine waters.

USGS Water Resources – links to various water data collected by USGS

<http://www.usgs.gov/water/>

National Water Information System (NWIS) – water quality data

<http://water.usgs.gov/owq/>

WaterQualityWatch – real-time water quality of surface waters

<http://waterwatch.usgs.gov/wqwatch/>

National Water-Quality Assessment (NAWQA) Program

<http://water.usgs.gov/nawqa/>

SPARROW Surface Water-Quality Modeling

<http://water.usgs.gov/nawqa/sparrow>

Public access to toxic release data: Exploring TRI and RTKnet.org

Barbara Losoff, University of Colorado Boulder

Using styrene releases and concerns about exposure as a case study, Losoff compared two interfaces to the Toxic Release Inventory data – the TRI Explorer from EPA and the RTK website.

“What is the Toxics Release Inventory Program?”

<http://www.epa.gov/tri/triprogram/whatis.htm>

EPA TRI Explorer interface

http://iaspub.epa.gov/triexplorer/tri_release.chemical

Right-to-know Network

<http://www.rtknet.org>

CHEMLIST: Chronicling the course of regulated chemistry

Roger J. Schenck, CAS

Schenck presented an overview of international chemical regulatory efforts and of the coverage of the CHEMLIST database.

CHEMLIST

<http://www.cas.org/expertise/cascontent/regulated/index.html>

Finally, I'd like to draw attention to the growing number of information resources for environmentally important chemicals that are available as mobile apps for smartphones and other devices. There are also a couple of interesting news items that highlight use of mobile detection technology coupled with smartphones to help first responders at fire and chemical spill sites.

CAMEO – EPA Emergency management tool

<http://cameochemicals.noaa.gov>

WISER (Wireless Information System for Emergency Responders) – National Library of Medicine

<http://wiser.nlm.nih.gov/about.html>

HazMat Reference and Emergency Response Guide

<http://www.thatsmystapler.com/erg/>

Cell-All: Super Smartphones Sniff Out Suspicious Substances

http://www.dhs.gov/files/programs/gc_1268073038372.shtm

Intel Fireball Lets You know if its Safe to Enter a Burning Building

<http://www.netbooknews.com/35155/intel-fireball-lets-you-know-if-its-safe-to-enter-a-buring-building/>

Andrea Twiss-Brooks, Symposium Organizer

Two recorded presentations (by Don Wauchope and Barbara Losoff) from this symposium are available at the [ACS Learning Center](http://www.softconference.com/ACSchem/) (<http://www.softconference.com/ACSchem/>)

Chemistry in Mobile Spaces

The symposium in Denver on Chemistry in Mobile Spaces highlighted a growing number of mobile chemistry capabilities, and definitely left one with the impression that mobile chemistry research is becoming more of a reality. The symposium did not define mobile devices in advance, and so apps aimed at a variety of devices were included. In reality, there is a difference in what a person is willing to do on a smartphone versus a tablet device, and as one moves from an iPad to a small laptop or notebook, the distinction in devices becomes less clear. There are hybrid laptop/tablets which have a removable display. Plug in the display, and you have a “normal” laptop. Remove the display and you have a tablet. “Normal” is in quotation marks because at the current time, these hybrids are limited to the tablet operating systems, and so do not have the capability or flexibility of a traditional laptop computer. In that sense, we are in a transitional phase. Someday soon, we might be able to have the best of both worlds - a full strength computing environment when we need it for data entry and data processing, coupled with an ultra portable touch interface for reading and entertainment. The focus of the symposium, then, was on the current set of applications and uses for mobile computing devices. These capabilities were definitely focused on search, discovery and consumption of content. Processing and analyzing content were also discussed, but to a lesser degree, and the model emerging there is toward mobile devices interfacing with server- or cloud-based applications. This focus may in fact be a way in which cloud-based services displace local storage, so individuals with multiple devices can have a seamless experience across their devices.

Tony Williams, from RSC/ChemSpider, opened the session with an excellent introductory overview on current apps in chemistry. Included in this brief survey were: Mendeley on iPhone, Wikipedia Chemistry, Theo Gray The Elements, structure drawing for calcs (formula, mass, predictions, DB lookup), ChemJuice, ChemDoodle, ChemMobi (DiscoveryGate), name lookup for ChemSpider, structure lookup for ChemSpider (cs.m.chemspider.com), and structure searchable apps: Yield101, Reaction101 from Alex Clark.

ChemSpider Mobile was just introduced in the last few days, and has had about 250 downloads/day initially. Under development is a substructure search capability as well as reaction searching.

There are a number of chemical reaction apps, such as Named Reactions, Organic Named Reactions, ReactionFlash, Reaction101, and Yield101.

ChemSpider is looking at the appropriate capabilities within apps. When considering spectroscopy, they questioned whether processing of spectra was needed on a mobile device. The capabilities for viewing, predicting, and analyzing were considered to be useful in a mobile environment. Tony presented SpectralGame (spectralgame.com), a website that was developed by Jean-Claude Bradley, Andrew Lang and him with the purpose to train students in structure determination of organic compounds from spectra. The website does so by taking a spectrum from the ChemSpider repository and suggesting two molecules of which the user has to choose the appropriate one. Besides training, the other purpose of SpectralGame is to use crowdsourcing to curate spectra that were submitted to the ChemSpider platform. Since iOS mobile platforms don't support Java, ChemDoodle can be used instead of the JSpecView Java plugin to view spectra.

Williams announced two apps about to be released: RSC Mobile and Chemistry World. Williams also unveiled the SciMobile Apps Wiki: scimobileapps.com, which is a site where app producers can list their app and highlight its features.

Kurt Zielenbach, from CAS, presented SciFinder Mobile. Rather than an app, this is a mobile-friendly interface to the SciFinder website that was launched in April, 2011. Because it is a web-based technology, it can be platform independent, working on multiple devices and mobile operating systems. This is important for providing broad access to users because although the iPhone and iPad are clear leaders in the device market, the operating system market is more diverse. From June, 2011, Android devices account for 54% market share to 26% for iOS. RIM, Symbian, and Windows Mobile follow with 15%, 3%, and 2% respectively, based on market research from Millennial Media.

Zielenbach noted the history of CAS in mobile devices, pioneering the first representation of a chemical structure on a BlackBerry in 2005 with CAS Mobile. He also presented some interesting statistics on smartphone usage from comscore.com. For example, in Italy and Spain, smartphone uptake is greater than 30%, leading all other countries in North America and Western Europe.

SciFinder offers the highest priority features for mobile access including explore by research topic, substance ID, author name and company name, along with ability to review Keep Me Posted alerts and saved answers. All of these were identified in a global CAS SciFinder customer survey and

implemented. SciFinder features not available on SciFinder Mobile at this time such as structure entry and structure searching were identified as lower priority by users. An important consideration for customers was that SciFinder Mobile should access personalized information from the web-based SciFinder desktop platform, including saved answers and “Keep me posted” alert results. This allows the user a uniform experience across devices.

David Evans, Elsevier Properties SA (EPSA), presented survey results showing what their users are currently using, or would like to use their mobile devices for: reading articles (75%), searching (70%), recording (60%), and analyzing data sets (50%), while only 30% are writing publications. EPSA decided to develop for Apple iOS at this time, partly due to market share, but also because the Android market was too fragmented with several different versions of the OS.

Reed Elsevier had developed a large number of iOS apps, but none specifically in this area. EPSA decided to create an app associated with Reaxys, but to focus on a single purpose and not replicate Reaxys. They presented a series of ideas to their 2010 Reaxys PhD Prize Finalists. Based upon feedback from that group, EPSA decided to create ReactionFlash, a flash card app for learning named reactions.

The development cycle for ReactionFlash addressed some of the limitations of mobile devices. Because structure drawing was not robust on the iPhone, structures were represented as pictures. However, bitmapped pictures were too large, and so the structures were converted to SVG and encrypted, so that the pictures could not be re-distributed. To enable the app to be used offline, the structures for the 200 named reactions are downloaded to the device with the app. This avoids data and roaming charges, an important requirement that the PhD students and postdocs had expressed in the development phase.

Evans also touched on the marketing aspects. Who needs the app? How large is the market? What should the price be set at? How should they promote the app? EPSA settled on two versions of the app, one a free version with 10 reactions, and the other full version with 257 reactions for \$9.99. Evans pointed out that the market for chemistry apps may be too small to generate a reasonable income, and that correct pricing may be essential to achieve relevant uptake. To investigate the response to pricing, EPSA launched a short term \$1.99 “back to school” offer.

Jason Wilde, Nature Publishing Group, discussed NPG’s approach to apps. He had a slightly different set of survey results, showing a significant difference in the number of apps downloaded in the last 6 months by user type. In industry, about 12 apps is the average number downloaded, with current awareness predominant. For students, approximately 8 apps is average, mainly for social networking. For faculty, about 8 apps is also the average, with learning aids becoming prominent. The time distribution of app usage was also discussed and, as expected, the time most users are using their mobile devices is early in the morning, on the way to work.

Wilde chronicled the development of NPG’s mobile products, with Nature Reader for iPhone, launching in February, 2010. A special iPad issue celebrating the 10th anniversary of the publication of the draft human genome sequence in *Nature* was released in July, 2010, and a special issue of *Scientific American* in December, 2010. The Nature Reader was updated and release for iPad in January, 2011, and a clinical medicine e-book, available via the Amazon Kindle store was released

in February, 2011. Wilde noted that the Kindle had problems with scientific content, including mathematics, tables, and images. The comparison of mobile and web usage on nature.com revealed that mobile users register more often, return to the product more often, and spend more time with the product.

In thinking about the future, Wilde commented on a flipbook model, QR Codes (2-dimensional barcodes that can be photographed by a smartphone and converted to a string of text, such as a URL), and the use of HTML5/CSS3 to deliver a dynamic mobile website. Wilde also discussed some potential uses for augmented reality. For example, you position the smartphone camera over an advertisement, and see an enhanced or interactive view of the product. Or you position the camera over a structure in the PDF version of an article, and you see a 3D rendering, or links to CAS or ChemSpider.

Dan O'Brien, ACS Publications, described the ACS strategy in mobile applications. The offerings include the ACS Mobile app, launched on iPhone and iPad in spring, 2010, and on Android in March, 2011. These apps have proven to be very popular, and frequent use of the app for tracking new articles is very common. C&EN Mobile was launched for both iOS and Android in August, as a free app with a capability for in-app purchase of issues of the magazine. O'Brien discussed the pros and cons of app development, and compared these to mobile-friendly websites. The latter are becoming more functional with the advent of HTML5 and CSS3, but there is still a development and maintenance cost for developing for multiple devices. One of the issues O'Brien mentioned is the support for Unicode characters which would allow accurate rendering of the full range of characters used in scientific publications. At this point, support across browsers is not uniform, and the mapping to smartphone operating systems is not completely consistent either.

Also discussed were the technologies that ACS Publications is evaluating for future mobile offerings. The environment is changing rapidly, and a number of new technologies for addressing some of the limitations associated with smartphones are emerging. These include enhanced PDF technology, which allows for reflowing of text depending on the size of the viewing device, Wolfram's Compound Document Format, and applications which can handle the EPUB format. Also included were a discussion of QR Codes, and the presentation was sprinkled with QR Codes to allow attendees to snap a photo of the slide, and quickly link to websites for additional information.

Theodore Gray, Wolfram Research and TouchPress, talked about his app, The Elements, which was developed using Mathematica. The app was referenced by the earlier speakers as an example of a publication which really takes advantage of the native environment of the mobile platform. Gray described his dissatisfaction with the education system and with educational materials in the US, and developed this app to provide an engaging way for students to learn about chemistry. (Note: Gray received the 2011 Grady-Stack Award from ACS for in recognition of outstanding reporting directly to the public, which materially increases the public's knowledge and understanding of chemistry, chemical engineering, and related fields). In addition to the high quality pictures, interactivity, and advanced capabilities (3D rendering of images), the app has direct connections to the WolframAlpha computation engine which provides a host of additional properties about each element.

Steven Muskal, Eidogen-Sertanty, went through highlights of each of the apps offered by his company, many of them in conjunction with Alex Clark of Molecular Materials Informatics.

Eidogen-Sertanty is committed to mobile computing, and has developed mobile apps for a variety of different uses. These apps include a mix of paid and free, and in order to provide the best capability for the mobile device, the apps make liberal use of a cloud infrastructure for data storage and calculations. Muskal noted that the growth of Amazon AWS was much larger than the growth of Amazon.com retail. Some of Eidogen-Sertanty apps include iKinase Pro, which is a paid app, and iKinase, iProtein, Mobile Reagents, Reaction101 for balancing reactions, and Yield101, which are all free. Muskal also mentioned OSRA processing of photographed structures, with name lookup.

Rich Apodaca, Metamolecular Inc., discussed HTML5, JavaScript and CSS3 as sustainable technologies to overcome the cross-platform problems that software producers are facing when developing apps for mobile devices. As a development platform he recommended PhoneGap to create cross-platform apps. This HTML5 platform allows users to author native apps with web technologies, as well as to get access to mobile APIs and app stores of the various mobile OS producers.

Metamolecular Inc. is currently working on ChemTab, software to browse chemical database files (e.g. SD files) on a tablet. ChemTab generates the structures dynamically from molfiles and uses portable JavaScript as the top layer in its software architecture. The connection to lower architecture layers such as the cheminformatics part, the structure editor, UI emulation widget, and native OS APIs is done via a bridge integration software.

Apodaca then presented ChemWriter, a structure drawing software, and ChemVector, a fast browser-based structure renderer. Both were completely written in JavaScript and require no browser plugin.

Muthukumarasamy Karthikeyan, National Chemical Laboratory in Pune, India, described an environment where hand drawn structures could be photographed, using a standalone digital camera, or the digital camera on a smartphone, and sent off to a server for conversion to a chemical structure connection table. A number of chemical OCR packages are available, and Karthikeyan presented benchmarks of the two engines CLiDE and OSRA. There are problems which are inherent in chemical OCR, and these are even more complex with hand drawn structures, where bonds may not be straight, overlapping bonds may be difficult to interpret, the drawing background may not be uniform, or color in contrast to black-white printed structures must be treated. The open source software developed at the National Chemical Laboratory of India applies some of the standard recognition algorithms used in the other chemical OCR engines, but is also able to treat the color and the background problem. In the discussion following, he acknowledged a 25-30% recognition rate for hand drawn structures. The chemical OCR is not really a mobile capability at this time, but the integration of a smartphone camera with a chemical OCR server brings the structure recognition capability to the mobile device.

In summary, there is no shortage of apps and interfaces for both research and education for smartphones and tablets, enough to justify a purchase for any chemist. How well you change your habits to incorporate the device and the apps into your daily workflow is up to you. Chances are, though, that if you aren't already using one of these devices for mobile chemistry, you will be soon.

Martin Brändle and David Martinsen, Symposium Organizers

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are available at the [ACS Learning Center](http://www.softconference.com/ACSchem/) (<http://www.softconference.com/ACSchem/>)

**Herman Skolnik Award Symposium
Honoring Prof. Alexander (Sandy) Lawson
Information Services in Chemical Sciences: Perspectives**

When Sandy Lawson initially planned this symposium he said that he wanted to look to the future rather than the past, and that his theme was “change.” The first two speakers addressed change as it impacts publishers. Bob Massie, President of CAS, talked about long-term implications for learned societies. The STM industry has prospered in the digital age when many other industries have been upended. One sign that it has done so is the ability to maintain prices. Music and book stores have closed; the circulation of most newspapers is in decline. Book publishing cannot control its economics. Asking why STM publishing has prospered, Massie suggested that executive leadership may have been a factor, and some of those leaders have been winners of the Herman Skolnik Award. On the other hand, he noted the observation by Warren Buffett that when an executive with a reputation for brilliance tackles a business with a reputation for bad economics, it is most often the reputation of the business that remains intact. So, while leaders matter, it is more likely we will find elements within the STM business itself to explain its resistance to the ravages of the web.

Why then has STM publishing weathered the storm brought about by the Internet era? First, it was not advertising funded. In addition it did not allow itself to be “dis-intermediated.” Beyond that, the value in STM products lies in the content, not in the users or their interaction with the content. This makes STM products less vulnerable to the viral power of the web. STM publishing also relates uniquely to its professional marketplace: journals link to career paths and other information tools lock-in the specific work functions. So far so good, but where should the industry invest now? Outsell’s “five to watch” for the next two years are APIs, tablets, social messaging, HTML5 and MySQL. Massie predicts that primary publishers will continue to emphasize brand prestige and the career connection, while secondary publishers will continue to emphasize “workflow solutions.” Will other players with the right technologies (Google and Facebook, for example) be a threat in future?

There are two ways an industry can adapt: retain the essential character, but adapt new technologies and approaches, or change into something different. The issue for the future is whether STM publishing will be able to adapt without changing its fundamental nature. Finally, Massie pointed out that this is the “Asian century.” Will the Herman Skolnik awardee in 2025 be a Chinese or Indian technologist?

In the second talk, Martin Tanke, Elsevier’s Managing Director of S&T Journal Publishing, honed in on the learned journal or, more precisely, “beyond the journal.” Will journals continue to exist? Yes, says Tanke, as long as they truly support the scientist’s workflow. Finding information is crucial to the processes involved in applying the scientific method. Faced with information overload, scientists end up repeating the work of others as they move through the disconnected data containers. Journals have a role in integrating the containers. Journal content must be smarter. Publishers must tag and enrich articles, open up publishing platforms, embrace applications, and redefine how journals work on the web.

Smarter content arises from semantic search and navigation. RSC, Nature and other publishers are all innovating in semantic technologies. One Elsevier example is entity extraction and marking up of

reactants, conditions and solvents in a Reaxys synthetic procedure. Enabling the research community to collaborate drives innovation. Tanke showed community-built applications that have appeared since publishers opened up APIs. PANGAEA is a mashup with geographical data. The Genome Viewer on SciVerse Science Direct is part of Elsevier's "Article of the Future" project (<http://www.articleofthefuture.com/>). It connects articles with the NCBI database. Article of the Future improves readability and discoverability and is extensible. New content is created as a scientist reads an article. The display has three panes: on the left is navigation, in the middle is a "traditional" reading pane, and on the right is a task-based pane that adds value and context.

Interoperability of journal content with raw research data sets is also important. Reflect, winner of the Elsevier Grand Challenge, tags and highlights proteins, genes, chemicals, and Wikipedia, and pulls information from EMBL and other databases. Author-created supplementary data files can be visualized and given added-value functionality with InChIKeys, Google and Reaxys links, all inside an article. The Reflect-Network application within SciVerse Applications and SciVerse ScienceDirect addresses the workflow challenges of life sciences researchers.

A lot has been achieved, said Tanke, but there is still work to be done. Publishers must set up an environment that works across all sciences not just chemistry; continue development of taxonomies and ontologies; devise authoring tools; work with suppliers; and achieve a balance between manual and automated approaches, since fully automated semantics might not scale.

Tony Williams of RSC spoke next, mainly about collaboration in the cloud, and open data. ChemSpider has been called the "Google and Wikipedia of Chemistry." Its vision is linking all chemistry on the Internet. Its roles are hosting and exposing data for the community and curating and validating chemistry-related data. ChemSpider is just one of many Internet resources that can be searched by chemical name, structure skeleton, molecular formula, etc. Unfortunately, errors proliferate because of data sharing between the databases. Some public databases are "trusted" as primary sources and that trust is granted without investigation. Williams says you should never trust a public domain database. Indeed, he believes that you should never trust *any* database: always ask questions.

ChemSpider is curated in a never-ending, crowdsourced effort. Data curation is tough and, sadly, the "crowd" is small: only 131 people have ever become involved, but that does include a few "master curators." Reciprocal curation is thus a good idea. Identifier dictionaries of InChIKeys and synonyms allow curators of other databases to check if their data match ChemSpider's. DrugBank is already using this facility. Batch validation also works (for example, checking if there is a count for chlorine in the molecular formula of a compound that has "chloride" in the name). To validate spectra, ChemSpider has constructed a game called SpectralGame (<http://spectralgame.com>) and a learning tool (<http://spectraschool.rsc.org>).

The community can also contribute reactions to ChemSpider SyntheticPages, but submissions have been few to date. Williams suspects that one problem is that chemists fear that a SyntheticPages entry will be considered "prior publication," preventing formal publication in a high impact journal. ChemSpider would grow if it had access to supporting information from journal articles. Williams ended his talk with a plea for data to be open. Examples include OpenPHACTS

(<http://www.openphacts.org/>) and RSC LearnChemistry. Williams is convinced that more collaboration can benefit us all.

Jan Brase of TIB (Technische Informationsbibliothek Hannover, the German National Library of Science and Technology), speaking on behalf of Uwe Rosemann, addressed change in libraries. The Digital Agenda for Europe outlines policies and actions to maximize the benefit of the digital revolution for all. Supporting research and innovation is a key priority for the Agenda and is essential if Europe wants to establish a flourishing digital economy by 2020. Brase said that the answer to the deluge of data is not to turn off the tap but to build boats.

TIB's GetInfo portal is being opened up to data, maps, movies, PowerPoint files, graphs etc. The data can be held elsewhere as long as there is a persistent link. TIB has been issuing such links in the form of DOIs for data sets since 2005, and in 2009 it was a co-founder of DataCite (<http://datacite.org/>) which helps researchers to find, access, and reuse data. It aims to establish easier access to scientific research data on the Internet, increase acceptance of research data as legitimate, citable contributions to the scientific record, and support data archiving that will permit results to be verified and re-purposed for future study. Now TIB is addressing new media types, visual search, and visualization. Challenges are to ensure quality and preservation, and migration to even newer media.

PROBADO is a visual search in architecture. Brase gave an illustration of indexing based on room connectivity graphs, after which visual searches such as "buildings with 15 rooms over three floors" can be carried out. Graphical queries, such as drawing a chair, are possible. In chemistry, CLiDE (<http://www.simbiosys.ca/clide/>) and chemOCR (<http://infochem.de/mining/chemocr.shtml>) extract chemical structures that are held as images, and produce live structures. TIB is collaborating with Thieme on publication of research data by assigning DOIs to data such as spectral peaks that occur in articles published by Thieme.

What if you could just draw a curve and search for curves "just like this one"? TIB is working with the Fraunhofer Institute IGD (Institut für graphische Datenverarbeitung) and the Technical University of Darmstadt on query by example and query by sketch in visual search. Note that the curve for cell phone use in India might be the same as that for the weather in Hawaii. Brase concluded by saying that the ultimate goal of dissemination of scientific and technical information is interlinking and search across all digital assets. The methods may have changed but the mission remains the same.

The next two papers illustrated changes in chemistry, the central science, and in particular how chemistry reaches out into biology. Robert Glen of the University of Cambridge gave an academic viewpoint and Torsten Hoffmann of Roche an industrial viewpoint. Glen's team has faced the challenge of probing a new found target without any prior knowledge of suitable pharmaceutically active molecules. In particular they tackled Apelin, a difficult target, for which there were no small molecule leads. Apelin is a G-protein coupled receptor (GPCR) which is a potent vasoconstrictor.

The approach of Glen's team was to model the receptor and associated endogenous ligands to understand the criteria for binding (and mechanism of action) combined with compound selection to optimize chemical structures for efficacy and affinity. Using this approach and rational design they

have discovered novel agonists, partial agonists, antagonists, and some micromolar small molecule leads.

Using previously published alanine scanning data (Fan, X. *et al.* Structural and Functional Study of the Apelin-13 Peptide, an Endogenous Ligand of the HIV-1 Coreceptor, *APJ. Biochemistry*, **2003**, 42(34), 10163–10168), they investigated the changes in the biological activity and linked this to structural and dynamic features of both ligand binding and receptor dynamics. They also constructed cyclic peptides and used NMR and constrained MD to study the shape of the peptides. Analysis was done with replica exchange molecular dynamics. A beta-turn at the RPRL motif was important for binding affinity (Macaluso, N. J. M.; Glen, R. C. Exploring the RPRL' Motif of Apelin-13 through Molecular Simulation and Biological Evaluation of Cyclic Peptide Analogues. *ChemMedChem* **2010**, 5(8), 1247-1253). Analogues were synthesized, pharmacophores were generated, and molecular dynamics was used to study them.

Glen and co-workers analyzed the binding modes, interactions, and dynamics and related these to potency, agonism and antagonism. They then attempted to make an antagonist by stabilizing the antagonist conformation and they designed peptides with two “anchor” groups and a variable linker. The first competitive antagonist was discovered. Biased agonism is a new emerging concept in GPCR pharmacology. Glen used molecular dynamics to show the differences between apelin (a full agonist) and a biased agonist; he showed the audience the motion of the 7-helix and associated -C terminal loop which seems to be associated with biased agonism.

His team has combined this methodology with access to ethically sourced human tissue, an approach which eliminates many of the problems associated with animal testing and which also allows investigation of not only healthy, but diseased tissue. Drugs can then be targeted at the diseased state, which is more relevant in a clinical setting. As an aside, I was interested to note the multidisciplinary, international nature of Glen's research team.

Torsten Hoffmann of Roche subtitled his talk “if we only knew what we already know.” This was a good way of expressing the challenge of knowledge capture and retrieval in medicinal chemistry. He started by explaining the workflows involved in carrying out medicinal chemistry research. He did this with reference to RG1678, a potent and selective GlyT1 inhibitor for the treatment of schizophrenia. A benzoylpiperazine hit was identified through high throughput screening, but it contained a nitro group (with potential for mutagenicity) and it had some undesirable properties that needed to be improved in lead optimization. A methylsulfone replacement was found for the nitro group, and, after SAR explorations, a series of compounds was found which had good overall physicochemical properties, high metabolic stability, oral activity, and no undesirable cytochrome P450 and off-target activity. The scaffold was also patentable. RG1678, in this series, has an excellent overall profile. It was safe and well tolerated in Phase I trials and had an excellent pharmacokinetic profile; in Phase II it improved the negative symptoms of patients with schizophrenia; and phase III studies are ongoing.

Hoffmann identifies three types of knowledge in discovery chemistry. Explicit knowledge can be shared in the form of hard data, scientific formulas, codified procedures or universal principles. External knowledge is communicated in journals, books, and at conferences. Tacit knowledge is

personal and hard to formalize; Roche Chemistry Knowledge (ROCK) is a unique knowledge capturing tool for capturing tacit knowledge.

An editorial board controls the ROCK submission and review process. The knowledge can be browsed, or substructure-searched in combination with keywords. Scientists can retrieve both the knowledge and the experts involved within a few mouse-clicks. ROCK creates a knowledge-sharing culture, fosters a life-long learning attitude, and offers a reward and recognition scheme. It is regularly used by medicinal chemists at all Roche sites.

Hoffmann next showed a truly fascinating movie of the perceptive pixel technology in use at Roche (http://www.youtube.com/watch?v=MIz_25ehzs0). Molecules on cards can be moved around in a touch screen interface, like moving CD covers in iTunes. Chemists can scribble on a card, can erase a section of a molecule, can create piles of cards, and name and save them, and can drag an avatar onto a card pile. It is not only chemistry that can be handled: it is also possible to drag and drop clinical data in the interface.

In the future, users expect next neighbor analyses by user-defined similarity searching, visualization enhancements and navigation options of search results in 2D and 3D, pattern recognition tools for broadest possible knowledge access, and intuitive human-computer interfaces for portable devices with wireless access.

The next paper covered some other futuristic aspects of capturing and reusing data. Talking about enriched research documents at the cutting edge, Rudy Potenzone of SciencePoint Solutions wonders why we are not focusing on authoring tools now that the “e-paper” has arrived and we are on the verge of a major revolution. Authoring technology enables scientists to create elaborate versions of the results of research, capturing the full context of research in progress: the formal scientific report, and the very methods used, with a full data repository, and complete workflows. The resulting documentation offers the information for completely reproducible results.

The scientific e-paper will help to improve the quality of science, facilitate the intellectual transfer of the core discoveries, fully document the provenance of the research, and preserve the knowledge with complete context. Services such as visualization and analysis will be easily accessible on top of the data. This heralds an era of accessible, reproducible research.

When Microsoft introduced OpenXML in Office 2007 it paved the way for workflow options and add-ins such as Chem4Word (<http://research.microsoft.com/chem4word>), GenePattern (<http://GenepatternWordAddin.codeplex.com>), the Research Information Centre Project (a virtual research environment for SharePoint, <http://ric.codeplex.com/>), and the chemical Semantic Web in oreChem (<http://research.microsoft.com/en-us/projects/orechem/>).

There are also several commercial data sharing and analysis services. Harvard’s Dataverse Network project (<http://thedata.org>) enables data archiving and preservation through re-formatting, standards and exchange protocols. It provides control and recognition for researchers through data management, branding and formal data citation. Workflow and pipelining tools include Taverna, KNIME and Pipeline Pilot. Taverna is integrated with the myGrid open suite of tools (<http://www.mygrid.org.uk/>) designed to “help e-scientists get on with science and get on with scientists.” The Project Trident Scientific Workflow Workbench

(<http://tridentworkflow.codeplex.com/>) is built on Windows Workflow Foundation.

Potenzzone concluded that the e-paper will provide a significantly more capable platform for science and for the scientific community, but it will further erode the *status quo* system of rewards and tenure. As far as the business of science is concerned, e-papers mean that publishers must evolve into “cool providers” of tools and “hot” distribution centers; A&I companies will need to redefine their role; and software vendors have a real opportunity, if they can adapt. The developments Potenzzone discussed offer opportunities for improving reproducibility of scientific results; for data sharing and collaboration; for reliable maintenance of provenance; for faster availability and efficient query tools; for controlled access to data; for finding related data and research partners; for assuring that data will be preserved; and for improved knowledge transfer.

The final invited talk was my own. Since my brief was to summarize the preceding papers it seems pointless to repeat myself in a written report that summarizes all the talks. Readers who want to hear the live and more humorous version can access the official ACS recording. What must be recorded here in print are the many tributes paid to Sandy Lawson himself. The official accolade lists his main achievements, but during the symposium much was said about him as a person. He was praised as a gentleman, and a mentor, and someone who has survived with a reputation for impeccable ethical behavior despite the industry controversies that arose during his long career.

In my talk I picked out a few topics such as new interfaces (noting that no one mentioned multilingual search) and data reuse and open data. The underlying theme of the day was not “databases” but access to, and reuse of “data.” I am sure that our awardee will not mind my mentioning that Reaxys gives immediate access to actionable data, although Reaxys was not the central theme of his talk.

In his award address, Sandy Lawson discussed some challenges and opportunities in preserving the scientific record. As more and more information gets published, the time-pressed reader feels more and more of a need for a focus on relevance. Chemistry databases are not passive media, they are interactive and have considerable underused opportunity to improve on pinpointing relevance *via* a specific description of a series of observations in words to which the users can respond.

Lawson cited three statements from Lawson, A. J. The Beilstein Database. In *Handbook of Chemoinformatics: From Data to Knowledge*; Gasteiger, J., Ed.; John Wiley & Sons: Chichester, UK, 2003; Vol. 5, pp 608–628:

“...the quality of a database...lies in the quality of its indexing power, to be able to reduce the suggested list of articles to a manageable number, without discarding relevance...”

“... expect secondary indexing systems...to retreat somewhat from an insular, stand-alone, center-stage posture... [with] query formulators taking a less prominent role...”

“...much will be driven directly from the source article itself, coupled with a natural language interpreter...to encourage the user to follow up suggestions...”

These three statements in three (almost) consecutive sentences are essentially tying the concept of focus on relevance to a verbal exchange.

Databases of one sort or another are necessary if users are to find documents. A document “does not exist” for the user either when (a) it is not found at all, or (b) when it is lost amongst a host of other irrelevant documents. In either case it is a question of relevance. Lawson dealt with the first point in his talk about natural language interfaces at the Herman Skolnik Award symposium for Guenter Grethe (Lawson, A. Question, query and relevant response: pick any two. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, United States, August 26-30, 2001, CINF-062). In the current talk he concentrated on the second point: a very common problem facing all users of primary and secondary information systems.

The focus on relevance is more about inspecting answer sets, and less about formulating queries. Relevance is a judgment that lives in the eye of the user. Trying to express relevance exactly in query formulation requires chemists to “know” the nature of the answers (and how they are expressed) before even looking. Lawson believes therefore that an *answer set* should “know” about chemistry and be able to correlate the inspection of the set for relevance to the user, and be able to respond “what it thinks” in conversational terms. Lawson’s approach is based on remote dynamic interpretation of database metadata, by a Visual Basic Web Service, an app, that is communication between two electronic devices over a network. Document content (words and graphics) can be converted into a document summary (in words and graphics). Lawson says this should be done even though there are titles and abstracts because titles and abstracts are *fixed* (on the historical unique focus of the author), but the user’s focus on relevance is *not fixed*: it is based on the user’s current thought and current query.

Lawson presented a proof of the concept. His prototype is bidirectional, i.e., it can “listen” and “talk” directly to a database system (here Reaxys). The requirements are to analyze a document and present its results for inspection in two ways: either as a synthetic backbone, or as a list of methodologies. The prototype worked well on two papers, one of which had an abstract and one of which did not, but the more interesting test was application to a “crowd” of documents.

In this example the app was applied to not one document, but to 101 documents all at once. Lawson formulated a query which even after refinement resulted in 840 reactions from 101 publications. This is far too many publications to be read or scanned. Each publication has its own single focus. If “relevance” is equivalent to [(user’s focus) AND (publication focus)], which publications should Lawson now read? The focus on relevance is about inspecting answer sets. The analysis is automatic and a black box for the purposes of the present talk.

Lawson’s engine listed the top seven methods in the whole hit set, and has the ability to call exactly these methods up from Reaxys. The app does not “know” everything: five out of the seven methods were named (e.g., “amidation with nitriles”), but two were not. In practice the app is currently about 60% successful. Lawson viewed each of the seven methods, one by one, and judged them in the light of his own relevance view. This reduced the hit set to two methods from seven publications. The final fine-tuning uses manual inspection by focusing on the method as a percentage of the total article content. Two documents stood out with a high focus on relevance. This is 2% of the original 101 publications.

Using the engine, one preparative method was chosen, and there were just two documents to read. Had the searcher hoped to find these documents by use of keywords, title, or abstracts in the

(Reaxys) query, he or she would have had to guess correctly and settle for some combination of generic chemical name and transformation terms. With Lawson's engine, the user merely has to recognize the term when he or she sees it, supported by the structures presented. This talk was not really about a new method or feature of any particular database; rather it was about general principles of communicating relevance in graphics and also words, reducing the load on users, by removing some aspects of "you need to know" at query formulation, and harnessing the power of databases from outside of the formal database user interface. Lawson concludes that both principles can contribute significantly to preserving the scientific record as a live entity moving forward.

Wendy Warr, Symposium Co-Organizer and Presenter



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Library Design, Search Methods, and Applications of Fragment-Based Drug Design

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Non-Traditional Careers: What Else Can I Do With a Chemistry Degree?

The symposium attempted to showcase a variety of career paths that are available to chemists either straight out of school or as a career change later in life.

The first speaker was Antony Williams, the creator of ChemSpider (www.chemspider.com). His first message was “follow your head and heart when making career decisions!” and his second observation was that “great careers don’t just happen – they are created by you.”

Slides of his presentation are available at:

<http://www.slideshare.net/AntonyWilliams/aligning-scientific-expertise-with-passion-for-a-career>

The next speaker was Bill Milne, a retired chemist and former editor of the *Journal of Chemical Information and Modeling* (1989-2004), who has found a second career teaching scientists how to present their ideas effectively, i.e. how to write better papers!!

Sarah Hasford, a patent lawyer with Connolly Bove Lodge & Hutz, LLP, began as a patent examiner before returning to law school. She outlined the joys and frustrations of the examiners that need to review each patent – sometimes they can be very specialized down to only doing certain types of drug patents and sometimes they can be more varied.

Norman Schmuff, Associate Director for Product Quality in the Drug branch of the Food and Drug Administration, told the audience about his path from lab to product quality.

Patricia Meindl, a University of Toronto chemistry librarian, described a career spent in both government and academic science libraries.

The symposium also premiered two videos in a series of interviews that had been created via the ACS Innovative projects fund grant. The first was an interview with David Martinsen from ACS Publications and the second was with Thomas Krimmer, who until recently was the marketing manager for the chemistry publications of Thieme Publishers – he has recently moved within the company to now head the marketing of the medical publications.

Patricia Meindl, Symposium Organizer, Chair, CINF Career Committee

A recorded presentation by Antony Williams from this symposium is available at the [ACS Learning Center](http://www.softconference.com/ACSchem/) (<http://www.softconference.com/ACSchem/>)



Ninth International Conference on Chemical Structures

The Ninth International Conference on Chemical Structures (ICCS9) was held in Noordwijkerhout in the Netherlands over the period June 5-11, 2011. ICCS is regarded as the premier venue for discussing all aspects of the management and understanding of chemical structures in electronic systems. The success of the conference depends on the quality of its technical presentations and the active participation of its attendees. The nature of the Noordwijkerhout center contributes significantly to the nature of conference. It is easy to get to, but once you are there, there is little to do but participate in the presentations and network with your peers. The 195 attendees rose to the challenge and contributed to the 34 oral and 158 poster presentations. Vendors' participation was also high.

Concerns that in these tough economic times registration might be restrained proved unfounded; a testament to the value of the conference. Financially the conference trust is well funded, enabling some 15 student bursaries to be awarded, and virtually guaranteeing a 10th conference in 2014.

The essence of ICCS is the high quality of technical presentations. The call for papers was oversubscribed and it proved challenging to select the final 34 oral presentations and 158 poster presentations. All sessions were well attended and less formal discussions continued in the social areas.

The conference was again chosen as the preferred venue to award the fourth CSA Trust Mike Lynch Award to Dr. Engelbert Zass of the Eidgenössische Technische Hochschule (ETH), Zürich. Dr Zass opened the conference by receiving the award and delivering the keynote address titled, *The Intermediary Reloaded - On the Need for a "Go-Between" to Information Users and Producers*, on Sunday evening.

ICCS9 was the latest in a series that began in 1973 as a workshop on Computer Representation and Manipulation of Chemical Information sponsored by the NATO Advanced Study Institute and thereafter was held under its new name every third year starting in 1987. The conference has a reputation for supporting outstanding networking opportunities and unscientific observation of the 195 attendees supported this reputation.

Block out the first week in June 2014 and plan to participate in the 10th conference. This conference will celebrate its 30 plus years of excellence and once again continue the tradition of outstanding presentations and networking opportunities.

Keith Taylor, ICCS Chair

Slides of the lectures and posters are available at the ICCS website
<http://www.int-conf-chem-structures.org>

Thematic Programming at Future ACS National Meetings

Chemistry of Life
243rd American Chemical Society National Meeting
March 25 – 29, 2012
San Diego, CA

Chemistry is involved in all aspects of our lives, starting from what controls the structures and functions of biologically important molecules, to the mechanics of how complex organisms interact with each other. In the past decade, detailed insights into what governs these interactions on a molecular basis has allowed us to rationally design new therapies for diseases with large unmet medical needs such as neurological, infectious and autoimmune disorders, and to develop targeted treatments for cancer.

Understanding the *chemistry of life* at the cellular level has allowed scientists to control critical checkpoints for cell division and differentiation. At the macro level, advancements in this area have allowed us to address perplexing issues in health and in the environment. Enhancing our understanding of the *chemistry of life* will impact our ability to solve many of the most pressing issues within our society.

The San Diego meeting will focus attention on advancements made in basic and applied research toward understanding the *chemistry of life* at the molecular and macroscopic levels. Many of the divisions and committees programming at the San Diego meeting may participate in the theme by developing interdisciplinary symposia on drug development, cell biology, neurochemistry, synthetic biology, and systems biology. These will convey advances in these areas with a focus on critical unsolved problems.

Dr. Peter Senter, San Diego Thematic Program Chair,
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Materials for Health and Medicine
244th American Chemical Society National Meeting
August 19-23, 2012
Philadelphia, PA

Materials that are used to replace or restore function to a tissue/organ and are continuously or intermittently in contact with body fluids are defined as biomaterials. Material-based medical devices, such as prosthetics, contact lenses and hip replacement implants, are widely employed to provide mechanical support or physical corrections to patients with compromised organs. More advanced products, such as drug-eluting vascular stents and growth-factor releasing bone grafts, present biologically relevant molecules in a controlled manner so as to elicit the desired biological

responses to the implants. The most sophisticated implant materials are living tissues created using tissue engineering methodologies through the combination of a scaffold matrix, progenitor cells and/or bioactive agents. Innovations in materials science and engineering have dramatically improved human health and revolutionized modern medicine.

Recent advances in molecular biology and genomics/proteomics have significantly influenced the design and application of biomaterials. Meanwhile, various materials fabrication tools and strategies have been adapted to the construction of biomaterials with increasingly complex functions. Recent work in this field ranges from fundamental studies aimed at manipulating biomaterial properties to control biological responses to the design of biomaterials for use in disease diagnosis and therapeutic treatment. The continued advances in materials science and engineering, translation of these advances to address biological challenges, and their integration with cell biology offer many promising approaches for the application of these materials in the repair and regeneration of functional tissues.

The Philadelphia ACS meeting will showcase the advancement of materials in health and medicine. Many ACS divisions can participate in the *Materials in Health and Medicine* theme by developing interdisciplinary symposia. Topics that are of interest to the ACS community include (1) understanding of the complexity of biological systems at molecular and cellular levels; (2) molecular design of novel biomaterials; (3) probing the interactions between materials and cells/tissues; (4) designing strategies to modulate the *in vivo* and *in vitro* responses of synthetic materials; (5) designing novel devices for diagnostic purposes and (6) adaptation of microfabrication tools for biological and medical studies.

Professor Xinqiao Jia, Philadelphia Thematic Program Chair
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Chemistry of Energy and Food
245th American Chemical Society National Meeting
April 7-11, 2013
New Orleans, LA

The theme for the New Orleans meeting will be the *chemistry of energy and food*. This topic will involve many of the ACS divisions, since it can accommodate interests ranging from biotechnology, agricultural and food chemistry, to environmental aspects including food vs. fuel issues, emerging chemistry of nanotechnology, new analytical methods to ensure food and environmental safety, and the chemistry of biofuels and bio-based products from a variety of “green” feedstocks. Energy production and the food supply came under scrutiny during the 2010 Deepwater Horizon oil supply crisis, when a small army of scientists assessed the damage to the ecosystem, including the safety of seafood from the affected areas. The oil leaking into the Gulf of Mexico contained polycyclic

aromatic hydrocarbons including some that are carcinogenic. Fortunately, the levels found in shrimp, finfish, and crabs fell below the levels of concern set by FDA, but widespread effects of the released oil, chemical dispersants, and other technologies used to mitigate the spill on the ecosystem and longer-term productivity are still undergoing intense study and follow-up. The Japan earthquake and its after effects on coastal nuclear power plants in Japan represent another, still unfolding, connection between energy production, food safety, and the ecosystem.

New sources of energy and bioenergy are under intense development in the Gulf region and elsewhere. New feedstocks and conversion technologies are being explored, and the first integrated biorefineries are far along in planning and/or implementation. What we are learning in terms of the potential of “green” energy to lessen global climate change, impacts on the food vs. fuel debate, effects of bioenergy production on water availability and quality, and other societal and environmental effects – particularly the areas where chemistry can contribute – will be explored in a plenary session and divisional programming.

Food quality and health, including food safety, healthful chemical constituents of food and beverages, and the sustainability of the food supply are capturing the attention of multidisciplinary teams involving chemists as well as food technologists, microbiologists, sensory scientists, agricultural engineers and other scientists and engineers. The benefits of such cooperative efforts will be explored as part of the *chemistry of energy and food* theme, including potential pay-offs in terms of affordable, healthy, delicious, and sustainable foods far surpassing what the average consumer puts on the dinner plate.

Professor James N. Seiber, New Orleans Thematic Program Chair
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Chemistry in Motion
246th American Chemical Society National Meeting
September 8-12, 2013
Indianapolis, IN

Chemistry impacts myriad facets of the transportation industry, from the fuels that are needed to power vehicles to the materials from which the vehicles are designed. Energy, the environment, and economics are intimately joined with regard to the creation of a successful transportation network, and chemistry impacts each and all components of that equation. Chemistry is a dominant factor for optimizing the use of precious resources, the development of new technologies to power and build our transportation infrastructure and to minimize the environmental consequences of a society built upon energy and mobility.

Cars, rail and planes are the dominant examples of *chemistry in motion*. Those modes of transportation have historically relied upon energy from fossil fuels and high density materials of

construction. Petroleum, however, is becoming a more precious and valued resource and the economy of transportation depends on the mass of the vehicle, the efficiency of the power plant and the drag and friction associated with motion of the vehicle. As a result, society demands more economical production of petroleum-based fuels, development of alternative fuels and lightweight building components and more efficient and aerodynamic designs of our transportation vehicles. That, in turn, requires advances in catalysis, the development of bio-based and renewable production of fuels and lightweight, structural materials, the development of new economically-viable sources of power such as hydrogen fuel cells and photovoltaics, as well as health and environmental effects of those technologies. On the one hand, chemistry will facilitate the refinery of the future, and on the other hand it will provide the means to replace those refineries with sustainable technologies and bio- or agro-based renewable methods to use chemistry for motion.

The Indianapolis meeting will showcase contemporary research and future technologies that will transform the transportation industry in the 21st century. Divisions can participate in the *chemistry in motion* theme by programming and developing joint symposia on catalysis, biofuels, alternative energy, lightweight materials, health and the environment and tribology.

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Submitted by Richard Love, ACS

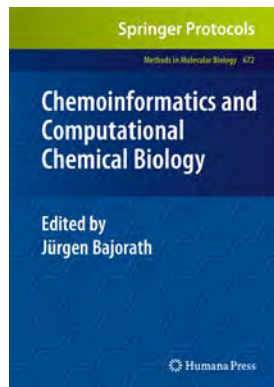
Schedule of Future ACS National Meetings

243rd	March 25-29, 2012	San Diego, California	<i>Chemistry of Life</i>
244th	August 19-23, 2012	Philadelphia, Pennsylvania	<i>Materials for Health & Medicine</i>
245th	April 7-11, 2013	New Orleans, Louisiana	<i>Chemistry of Energy & Food</i>
246th	September 8-12, 2013	Indianapolis, Indiana	<i>Chemistry in Motion</i>
247th	March 16-20, 2014	Dallas, Texas	TBD

Book Review

Chemoinformatics and Computational Chemical Biology, (Methods in Molecular Biology no. 672)
J. Bajorath, Ed., Springer, New York, 2011, \$159.00 (Hardcover). 588 pages.

ISBN: 978-1-60761-838-6



When I first received this book I sent out a bid for volunteers to write review. No one stepped forward so I'll give it a try. Since the relevant journals do not or no longer publish book reviews, *CIB* is apparently the only medium for reviews on chemical information, cheminformatics, and related subjects.

Forty-one authors wrote 22 chapters for this compendium, including CINF notables Wendy Warr, Peter Willett, and Rajarshi Guha. The book is an update and an extension of a previous volume in the series.¹ Several topics in chemical biology are discussed as well as in cheminformatics *per se*.

The book begins with an excellent introductory chapter by Wendy Warr (37 pages, 273 refs.). A general history of cheminformatics up until 2000 is provided, followed by summaries of recent trends which are further elaborated upon in the remaining chapters. This review will be largely confined to the introduction.

Cheminformatics is still in search of a uniform title. The former seems to be the most preferred, but chem(o)informatics, chemoinformatics (per the book title), and chemical information are also used. In fact, the journal for publishing papers in the area, *J. Chem. Inform. Modeling*, continues to use "chemical information" although we veterans of the development of chemical information might disagree with this "subset", although relevant, used as a subject title for the entire field.

A definite link with "classical" chemical information is representation of chemical structures. The Morgan Algorithm (CAS; proprietary), InChI (ChemSpider *inter alia*, open), and SMILES (varied, proprietary) are discussed and referenced. In addition, developments in computing environments, open systems, the predominant influence of industry, docking, *de novo* design, molecular similarity, prediction of metabolism, pharmacophores, data reduction and visualization, and text mining are summarized. These latter subjects along with others (Bayesian methods, combinatorial libraries, statistical techniques) are discussed in detail in the remaining chapters.

Readers less familiar with the topics will find the introduction worth studying. Those with more detailed backgrounds (and those wishing to gain proficiency) in the various topics will find this book and excellent resource.

1. Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery (Methods in Molecular Biology no. 275), Bajorath, J., Ed., Springer, New York, 2004.

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REPORTS FROM THE 2011 FALL ACS NATIONAL MEETING

What's up, InChI?



The CINF Division became an InChI Trust supporter last year. So this year we were invited to attend the annual general meeting, held on Sunday August 28 during the ACS National meeting in Denver. Leah Solla and I were able to attend. The proceedings were led by Jason Wilde (Publishing Director at Nature Publishing Group and Chairman of the InChI Trust) and Alan McNaught (Secretary, IUPAC Division VIII InChI Subcommittee and Company Secretary, InChI Trust). Trust members attending included Accelrys, ACD/Labs, Elsevier, FIZ CHEMIE Berlin, RSC, Springer, and Wiley. After taking care of several administrative votes, the committee provided updates on the various InChI activities underway:

InChI (v 1.04) is being released shortly under more liberal licensing terms, to alleviate concerns brought to the Trust by corporate participants. The InChI [Source Code Documentation](#) (v1.03) is also available today.

Member and Supporter Logos are now available for posting on member and supporter websites.

The InChI Validation program has been launched allowing users to certify their implementation of InChI. The programs test your installation against a broad set of structures (which are provided with the suite). Once the programs are run and the results sent back to the Trust, an "InChI certified" logo will be sent to the organization.

InChI Extensions: Under the guidance of IUPAC, several sub-teams are now working on expanding InChI to new areas of chemical representation:

Reaction InChI (RInChI): the reaction working group has completed their recommendations, and work is ready to begin.

Polymers/Mixtures: The polymers/mixtures working group also has submitted its recommendations, and work to incorporate the new representations should begin once version 1.4 is released.

Markush: This project is the most complex undertaken to date. The initial recommendations have been submitted, but financing of the work still needs to be sorted out.

Upcoming reports: IUPAC has two more working groups underway, focusing on organometallics and electronic states, whose reports are due over the next year.

Of particular relevance to CINF was our discussion on how to reach out to the chemistry community more effectively. We all agreed that this was an area in which to engage the members and supporters more extensively. For example, InChI training materials should be included in the [XCITR](#) repository, and InChI might also be a good candidate for a short course, perhaps co-sponsored by CINF, COMP and CHED. One initiative already underway: the Trust is contracting with Bill Armstrong at LSU to prepare some InChI training materials. And for San Diego Antony Williams and Alex Tropsha are organizing an InChI symposium.

By Carmen Nitsche, Immediate Past-Chair, CINF Division

Report from the CINF Communications and Publications Committee

The CINF Communications and Publications committee met in Denver on August 27th. The following items were discussed:

1) Conversion of the *Chemical Information Bulletin (CIB)* website to Drupal

Congratulations were offered to Danielle Dennie on the conversion of the *Chemical Information Bulletin (CIB)* website to Drupal. All present at the meeting agreed that the last *CIB* issue looked really good. The next step is to convert the remainder of the CINF website to Drupal using the same contractor (supervised by Danielle) as before. There is \$2,500 remaining from the ACS grant to do the conversion and there are additional funds left over from another CINF grant that may be tapped into if needed and the CINF Executive Committee approves. There is still material on Rick Williams' old website (mostly slides from CINF technical programs at previous ACS meetings) that needs to be moved to the new site. Danielle will take care of this. It was noted that the new website is being hosted by the same organization that hosted the site for Rick.

Judith Currano said that using the new Drupal website for *CIB* was easy. She did have some difficulty creating a PDF, but Danielle did provide instructions and once received, these were easy to follow.

2) *CIB* content

Judith Currano reported on the content of the last issue of the *CIB*. As usual, it contains committee reports, but she also added the agendas of the committee meetings to be held at Denver. She solicited input via the ACS Network and the CHEMINF-L list. She used her judgement on what was to be included, excluding some blatant self-advertising as more suitable to the press release section available to CINF sponsors. All present agreed that the content was useful. In the future she will continue to include "feature" articles and will be adding new columns, such as a "CINF Reviews" that will contain highlights from the chemical information literature, and perhaps she will include database reviews similar to the book review section. Bonnie Lawlor suggested that a call for input be included in a visible section of the *CIB*. Song Yu agreed to look after the CINF Reviews section.

3) ACS Network

Judith asked if the ACS network has a Wiki capability as she thought perhaps that a "Cool Articles that I have Read" wiki could supply material for the CINF reviews editor. David Martinsen said that he does not believe that a wiki capability exists, just the blog feature.

The group looked at the CINF information that is currently available on the ACS Network. The Chemical Information Group set up by Sue Cardinal has a mix of annual reports, *CIB*'s, financial reports, etc and it was determined that this "group" is totally open and accessible by anyone in the world. After some discussion, it was agreed that this high-level group would be used for outreach to members and to promote CINF to non-members. Documents, such as annual reports, would be posted in that section, but also posted to the CINF website.

Carmen Nitsche has already created a group for the CINF Executive Committee on the ACS Network and will create one for CINF Functionaries. Both groups will be private. It was agreed that we would not create a secret group. It was also agreed that we would recommend that each CINF Committee establish its own group on the ACS Network and that the ACS Network will ultimately be the focal point for all CINF communication.

5) Duplication of content on the CINF website

It was agreed that the *CIB* will be the entry point for all the material that it usually contains (meeting information, abstracts, etc.) and this material will not be duplicated elsewhere on the website. When someone wants to access that information directly from the CINF website tabs, the information will be accessed via links to the *CIB*.

6) CIB editors for 2012 and beyond

Judith Currano agreed to serve as Editor for the pre-meeting *CIB* issues in 2012 and Svetlana Korolev agreed to serve as Editor for the post-meeting *CIB* issues.

7) Communications and Publications Committee membership

All current Communications and Publications Committee members agreed to remain on the committee with the exception of Rick Williams whose term has expired. Any other members scheduled to stand down in 2011 will have their terms automatically extended to 2014. Song Yu and Carmen Nitsche will be officially added to the committee, both with terms from 2011 - 2014. Bonnie Lawlor will serve as the Committee's liaison to the CINF Membership Committee.

8) Communications and Publications Committee Chair for 2012

Bill Town will remain as Chair for 2012. If he is unable to travel to any ACS meeting in 2012, an "Acting Chair" will be appointed to run the meeting and report to the Executive Committee.

9) Increasing usage of the CINF website

The Committee will look into the possibility of using Twitter and Facebook as tools to "push" information to CINF members and to engage younger participants.

Bill Town, Chair, CINF Communications and Publications Committee



<https://communities.acs.org/thread/3904>

Report from the CINF Membership Committee

At the CINF Executive Committee meeting in Denver Greg Banik volunteered to chair the committee starting in 2012. Other members who volunteered to join the committee membership are Bonnie Lawlor and Leah Solla. We would appreciate any ideas that anyone has on retaining or attracting new members, and any ideas pertaining member benefits. For example, is there any way that we can make a directory available to the division members? This would certainly aid new members getting to know the current members and would be a benefit to our membership.

The Division membership continues to decline, but seems to have slowed down. As of August 2011, CINF members' count is 1028 (6 new members and 9 terminated in August). Student members, though small in number, have increased percentage wise.

When I write to the members who have resigned I usually do not receive many replies. However, those who do respond have a number of reasons, ranging from an economic hardship prohibiting them to be involved in any national organizations to a personal case demanding them to aid an ailing family member. These are all sensible reasons. No one has yet to write that they disliked CINF or anything to that effect. It is just many other factors impacting their lives preventing them to continue membership in the ACS CINF Division.

I would really like for us to think about being more active at regional meetings to see if we could increase our division membership that way.

Jan Carver, Chair, CINF Membership Committee

Report from the ACS Council Meeting

Items of particular interest to members of the Division of Chemical Information

For those who provide information services and products related to National Chemistry Week and Chemists Celebrate Earth Day themes, the chair of the Committee on Community Activities (CCA) reported that the October 16-22, 2011 National Chemistry Week theme continues the International Year of Chemistry (IYC) focus of health with "Chemistry—Our Health, Our Future!" National Chemistry Week 2012 will mark the 25th anniversary of this celebration and will focus on a theme of nanotechnology. Chemists Celebrate Earth Day 2012 theme will be "Rethinking Recycling: It's Easy to Be Green." For resources and more information visit the ACS Education web page at <http://www.chemistry.org/education> and look under "Community Outreach" ACS also received an NSF grant to support outreach and education activities for IYC and beyond.

The chair of the Committee on Professional Training announced plans to introduce a library survey as part of revising guidelines. The supplement on developing student skills in chemical information retrieval is also being revised, and the committee is also discussing its list of recommended journals that may be used to meet the minimum requirement for ACS approval.

Good news for those who serve on ACS Committees, but who are not either local section or division councilors: the ACS Committee on Budget and Finance (B&F) considered a proposal from the Council Policy Committee (CPC) regarding the Committee Travel Expense Reimbursement Policy approved by CPC in March 2011. The policy would allow reimbursement of travel costs to committee meetings held during the ACS national meetings for non-councilor committee members. After some discussion, the Board **VOTED**, as recommended by B&F, to adopt the non-councilor reimbursement policy as presented by CPC (at the rate of 50% of the Councilor travel reimbursement) effective 2012. More details on how to request this reimbursement are forthcoming. On the recommendation of the Committee on Publications, the Board **VOTED** to approve the reappointment of two journal editors and the appointment of a new editor. The Board also **VOTED** to approve an appointment to its Governing Board for Publishing. No further details were provided in the written agenda book.

ACS finances are generally in good condition. With \$18.3 million net from operations, the Society is projected to end the year approximately \$5 million favorable, and is in compliance with four of five Board guidelines for financial health.

On the recommendation of the Committee on Budget and Finance (B&F), the Board **VOTED** to approve an advance member registration fee of \$360 for national meetings held in 2012. The Board also considered several program funding requests, and on the recommendation of B&F **VOTED** to reauthorized funding for inclusion in the 2012 proposed budget for the following programs:

- ACS Fellows
- ACS Leadership
- ACS Scholars
- ACS Global Research Experiences, Exchanges, and Training Program (GREET)

The Board also **VOTED**, as recommended by B&F, to include funding in the 2012 and 2013 budget for a new program – the ACS Entrepreneurship Initiative.

The Chair of the Board gave an update on the Leadscope case. She reported previously that ACS had appealed to the Ohio State Supreme Court and that the Court has agreed to hear the case. In written briefs filed in support of the Society's position (that the lower court rulings were both unfair and unconstitutional), ACS has been joined by several organizations, including other scholarly societies. In April, the Leadscope defendants filed two motions seeking to dismiss the Society's appeal. In June, the Ohio Supreme Court denied their motions and has scheduled oral arguments for September 7 in Columbus, Ohio.

Selected other business before Council

Election Results for Council –elected committees

- The Committee on Nominations and Elections presented to the Council the following slate of candidates for membership on the Committee on Committees beginning in 2012: Matthew K. Chan, Richard S. Danchik, Rigoberto Hernandez, Roland F. Hirsch, James M. Landis, Jr., Helen (Bonnie) A. Lawlor, Zaida C. Morales-Martinez, Howard M. Peters, Sara J. Risch and Jason E. Ritchie. By electronic ballot, the Council elected Rigoberto Hernandez, **Bonnie Lawlor**, Zaida C. Morales-Martinez, Howard M. Peters and Sara J. Risch for the 2012-2014 term.

- The Committee on Nominations and Elections presented to the Council the following slate of candidates for membership on the Council Policy Committee beginning in 2012: Spiro D. Alexandratos, Lawrence Barton, Michael J. Brownfield, John W. Finley, Mark D. Frishberg, Peter C. Jurs, Mamie W. Moy, and Eleanor D. Siebert. By electronic ballot, the Council elected Lawrence Barton, Peter C. Jurs, Mamie W. Moy, and Eleanor D. Siebert for the 2012-2014 term.
- The Council Policy Committee presented to the Council the following slate of candidates for membership on the Committee on Nominations and Elections beginning in 2012: R. Gerald Bass, Cherlynlavaughn Bradley, William H. (Jack) Breazeale, Jr., Catherine C. Fenselau, Lydia E. M. Hines, Robert L. Lichter, Anne T. O'Brien, Robert A. Pribush, Andrea B. Twiss-Brooks, and Steven W. Yates. By electronic ballot, the Council elected William H. (Jack) Breazeale, Jr., Catherine C. Fenselau, Lydia E. M. Hines, Anne T. O'Brien, and **Andrea B. Twiss-Brooks** for the 2012-2014 term.

Candidates for President-Elect and Board of Directors

The candidates for the fall 2011 ACS national election were announced as follows:

Candidates for President-Elect, 2012

Dr. Dennis Chamot, Associate Executive Director, Division of Engineering and Physical Sciences, National Research Council of the National Academy of Sciences, Washington, DC

Dr. Marinda Li Wu, Founder and President, Science is Fun!, Orinda, CA

Candidates for Directors-at-Large, 2012-2014

- Dr. Ken B. Anderson, Professor of Geochemistry, Southern Illinois University at Carbondale, IL and CEO, Thermaquatica Inc., Carbondale, IL
- Dr. William F. Carroll, Jr., Vice President, Industry Issues, Occidental Chemical Corporation, Dallas, TX
- Dr. Charles E. Kolb, President/CEO Aerodyne Research, Inc. Billerica, MA
- Dr. Barbara A. Sawrey, Associate Vice Chancellor, Undergraduate Education, University of California, San Diego, CA

Candidates for District III Director, 2012-2014

- Dr. Pat N. Confalone, DuPont, Vice President, Global R&D, Crop Protection, Wilmington, DE
- Dr. David J. Lohse, Retired, Distinguished Research Associate, ExxonMobil Research & Engineering Co., Annandale, NJ

Candidates for District VI Director, 2012-2014

- Dr. Bonnie A. Charpentier, Vice President, Regulatory and Quality Metabolex, Inc., Oakland, CA
- Dr. Carlos G. Gutierrez, Professor of Chemistry, California State University, Los Angeles, CA Council

The Council received one amendment (petition) to the ACS Constitution and Bylaws for action: The Petition on Position Statements. The Council **VOTED** to approve the Petition on Position Statements, which allows for clear and consistent position development for the Society.

As part of a regular performance review, the Council **VOTED** to continue the joint Board-Council Committees on Community Activities and on Publications. Continuation of these two committees also requires Board of Directors concurrence.

As of September 1, 2011, the ACS fall national meeting had attracted 10,076 registrants. Totals in select categories are as follows: Regular attendees 6,088; Students 2,376; Guests 218; Exhibit Only 394; and Exhibitors 1,000. The history of attendance at ACS fall national meetings since 2004 is as follows:

2004: Philadelphia, PA	14,025
2005: Washington, DC:	13,148
2006: San Francisco, CA	15,714
2007: Boston, MA:	15,554
2008: Philadelphia, PA:	13,805
2009: Washington, DC:	14,129
2010: Boston, MA:	14,151
2011: Denver, CO:	10,076 (decline assumed to be due to the timing – week before Labor Day, not the location)

The Society Committee on Education (SOCED) reported on a joint SOCED-CPT Task Force to examine the implications of the Association of American Medical Colleges-Howard Hughes Medical Institute report *Scientific Foundations for Future Physicians*. Task Force members are gathering information on innovative programs that may be relevant to the recommendations in the report. It was also announced that U.S. participants in the international Chemistry Olympiad held in Ankara, Turkey, had earned 2 gold and 2 silver medals.

A special discussion item was put on the Council agenda for this meeting. ACS President Nancy Jackson presented and moderated a discussion on how ACS can best cultivate a culture of safety in U.S. universities and colleges. At the 2011 ACS national meeting in Anaheim, the Committee on Chemical Safety launched an effort to identify ways to assist academia in strengthening and building strong safety cultures. Devastating incidents in academic laboratories and observations by many that graduates do not have strong safety skills have elevated concerns about the safety culture in academia. (There was a report of another incident that appeared directly after the ACS meeting in Denver). Following Dr. Jackson's presentation, Councilors engaged in robust discussion on this very timely topic, with numerous suggestions by 42 different Councilors.

After a lively discussion, the Council **VOTED** 53% - 47% to dissolve the Division of Petroleum Chemistry and to combine its assets and members with those of the Division of Fuel Chemistry under the new name of the Division of Energy and Fuels, effective December 31, 2011. The discussion centered largely on the name, rather than the merger.

The first ever fully integrated onsite and virtual career fair in Denver offered job seekers and virtual participants via webcam the opportunity to interact with each other and to connect with prospective employers and programs to sharpen their career skills. The Virtual Career Fair attracted 3925 job seekers and 14 employers, and featured 362 jobs. The in-person event in Denver had 765 job seekers, 51 employers and 261 jobs.

Links of interest

www.acs.org/acspresidents - Information on ACS past presidents

www.acs.org/creatingjobs - Location for the ACS Presidential Task Force on Innovation report, "Innovation, Chemistry and Jobs"

www.acs.org/iyc2011 - Location for International Year of Chemistry activities

<https://communities.acs.org/message/8125#8125> - A link on the ACS Network for ACS Strategic Plan Discussion – public

www.acs.org/goalsurvey - Location for the ACS online goal survey for helping to develop the 2012 strategic plan

www.acs.org/councilreports - Location for all Council reports of the current meeting (fall reports to appear after September 12)

www.acs.org/bechemists - Information on a campaign to remind recent graduates of the benefits of ACS membership

www.acswebinars.org/vcf2011 - Information on the ACS webinars and virtual career fairs

Andrea Twiss-Brooks and Bonnie Lawlor, CINF Councilors

Report from the Council Committee on Nomenclature, Terminology and Symbols

The Committee on Nomenclature, Terminology and Symbols held its open meeting on Monday, August 29, 2011. They received a report on the discovery of two new elements: number 114 and 116. Presently, neither names nor symbols have been proposed for either element by the discovery teams. When such proposals are made, the Committee will review them and may make comments during the open comment period.

The ACS Office of Public Affairs arranged interviews of members of the Committee with editors of the popular press seeking information on the naming of these new elements. According to the ACS Office of Public Affairs, more than 200 news outlets covered this story including ABC News Online and National Public Radio.

In previous reports from the Committee, Council was informed regarding the redefinition of the kilogram and the mole. The Committee began its work with two goals. To understand:

- What is being done; and
- What it means to the practice of chemistry.

The Consultative Committee on Units (CCU) of the International Bureau of Weights and Measures (BIPM) met in October 2010 and completed its proposed redefinitions. The revised, proposed definition for both the kilogram and the mole were presented in Dr. Rusch's ACS Comment that appeared in the May 30, 2011 issue of *Chemical & Engineering News*. These new definitions have generated a large amount of comment. Much of it from outside the metrology community has been unfavorable. Even though the final numerical values of the Planck constant, used to define the kilogram, and the Avogadro constant, used to define the mole, have not been fixed, it is anticipated

that the new definitions will be presented to the General Conference on Weights and Measures in October 2011 for approval. Once the numerical values of these constants are fixed, these definitions will replace the current definitions.

At its open meeting the Committee elicited comments from ACS Members on these definitions. In particular, it sought comments on how these definitions might affect the practice of chemistry and how ACS might react to the chemical-education implications of the definitions. Members of the chemical educational community were present to contribute.

The Committee did receive comments from the American Society for Mass Spectrometry (ASMS) stating that there will be no impact on current mass spectrometry practice due to the mass of carbon-12 no longer being defined as 12 exactly. The Committee is considering preparation of a position statement on the impact of these new definitions on the practice of chemistry.

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Overview of the Council Committee on Patents and Related Matters

The ACS Committee on Patents and Related Matters (CPRM) is a Joint Board-Council Committee currently chaired by Dr. James Chao. The Committee draws its membership from Councilors and non-Councilors who have an interest in intellectual property matters, particularly patent matters, affecting the chemical enterprise. Both the Board and the Council call upon the Committee to study and make recommendations on matters of importance to the ACS. The Committee focuses on three main areas: educating ACS members about intellectual property issues important to the chemical enterprise; nominating chemists for national awards to recognize the innovations and contributions to society of chemists; and monitoring legislative and regulatory developments influencing intellectual property. CPRM serves as an important part of the ACS Strategic Plan. The goals and activities of the Committee align with the ACS Strategic Plan in several important ways.

Goal 1 of the ACS Strategic Plan provides that ACS will be the indispensable professional and information resource for our members and other chemistry-related practitioners. CPRM, particularly through its Education and Outreach Subcommittee, strives to provide information on intellectual property issues that are useful and necessary to chemists, other chemistry-related practitioners and the general public. CPRM provides a variety of resources on patents and related matters via the Committee's web site:

http://portal.acs.org/portal/acs/corg/content?_nfpb=true&_pageLabel=PP_TRANSITIONMAIN&node_id=320&use_sec=false&sec_url_var=region1&_uuid=d5ae26a7-28d3-4ff9-ab5d-921421ddb41. The Committee's leading publication, "What Every Chemist Should Know About Patents," is now in its third edition. Recently, the Committee published a Supplement to ensure that this resource is as up-to-date as possible. CPRM has begun publishing a series of informative pamphlets on career options in the fields of intellectual property for chemists and other scientists. CPRM members serve as resources to other ACS committees and to regional meetings.

Goal 4 of the ACS Strategic Plan provides that ACS will be a leader in communicating to the general public the nature and value of chemistry and related sciences. One of CPRM's missions

is to seek to highlight and acknowledge the intellectual property contributions of chemists. CPRM's Awards Subcommittee solicits and develops nominations for the National Inventors' Hall of Fame and the National Medal of Technology. This subcommittee guides the nominations through the appropriate ACS approval process to gain endorsement from the Society. For example, as the direct result of CPRM's efforts, the Wyeth Pharmaceutical team of Ronald Eby, Velupillai Puvanesarajah, Dace Viceps Madore and Maya Koster received the National Medal of Technology for their discovery, development and commercialization of Prevnar, the first vaccine to prevent deadly and disabling consequences of pneumonia in children. As President Bush noted in awarding this honor, the impact of Prevnar on the public health is unparalleled, and has allowed the United States to reach its Healthy Children 2010 goal for pneumococcal disease reduction nine years ahead of schedule. Next month, the National Women's Hall of Fame will honor its 2011 inductees. Included in a very prestigious class of honorees will be Dr. Helen Free, whose nomination the Committee recommended to the ACS Board of Directors.

Goal 5 of the ACS Strategic Plan provides that ACS will be a premier advocacy organization for members and the profession, creating and communicating policy statements in accordance with our Congressional charter. The Committee is the only ACS governance entity which actively monitors intellectual property issues of importance to chemists and other practitioners of the chemical enterprise. Intellectual property rights are an integral component to innovation. In turn, innovation has been a major component to the health and growth of the U.S. chemical enterprise. The Committee uses the information garnered from its monitoring to further its mission of proposing policy statements in accordance with the ACS Congressional charter. The Committee works closely with the ACS Office of Legislative and Government Affairs to ensure that the interests of ACS members are included in the debate and discussion about legislation and/or regulations affecting intellectual property. To this end, the Committee drafts proposed position statements on behalf of ACS and its members and recommends positions to the ACS Board of Directors.

This process has become essential. The ACS counts among its members, chemists and chemical engineers who rely on an efficient and effective intellectual property protection regime to bring their discoveries and inventions to the marketplace. The Committee closely studied intellectual property issues of importance to chemists and other practitioners of the chemical enterprise and concluded that failing to reform our patent system could hinder science and our nation's ability to compete in the global arena. Further, the Committee concluded that appropriate patent reform will have a direct, positive effect on the ability of our domestic business, scientific, technological and educational communities to meet the growing demands of an international economy. Consequently, the Committee recommended, and the ACS Board of Directors approved, a Statement on Patent Reform. Several of the major points for which ACS advocated were included in the new Patent Reform bill signed by President Obama on September 16 of this year.

The Committee welcomes liaisons from several committees and divisions. If you have any interest in the Committee's work, please do not hesitate to contact Jim Chao, Chao_j@bellsouth.net, or the Committee's staff liaison, David Smorodin, d_smorodin@acs.org.

James Chao and David Smorodin, Council Committee on Patents and Related Matters

CINF Social Networking Events

The Division of Chemical Information (CINF) was pleased to host our traditional social networking events at the ACS national meeting in Denver, Colorado. The division depends on generous contributions by our sponsors to nurture successful symposia and social gatherings where the chemical information community congregates, socializes, shares and bonds. Our sponsored symposia and receptions were great fun as well.

The **CINF Sunday Welcome Reception** was supported by a record six sponsors uniting an especially diverse mix of 80 to 90 chemical information enthusiasts covering the complete spectrum of CINF affairs. The attendees enjoyed an exceptional menu and energizing conversation to kick off the Denver meeting. Many thanks to our host of supporters: **Digital Science**, **InfoChem**, **OpenEye**, **PerkinElmer**, *Journal of Chemical Information and Modeling*, *Greenhouse Gases: Science and Technology*.

The 13th **CINF Scholarships for Scientific Excellence** poster session at the Sunday Reception provided three scholarship winners with \$1,000 awards by our generous scholarships sponsor, **FIZ CHEMIE Berlin**. Please let your students and interns know about these prizes at <http://www.acscinf.org/awards/sciexcel.php>.

Harry's Party, also hosted by **FIZ CHEMIE Berlin** on Monday evening, reunited the CINF cadre in a view suite at the Westin Tabor Center Hotel. About 90 friends of CINF enjoyed the mountain views, excellent food and drink, and engaging conversation with old friends and new colleagues. If you missed Harry's Party in Denver, please join us in San Diego next spring.

The **CINF Tuesday Luncheon** provided delicious fare and sweet entertainment to about 85 diners who were entertained by our special presenters, Howard & Sally Peters, speaking on "Chocolate, Food of the Gods." The presentation was as interesting and entertaining as the chocolate samples were sweet and delicious. CINF thanks **Bio-Rad Laboratories** and **RSC Publishing** for teaming up again to support this event.

The **Herman Skolnik Award Symposium & Reception honoring Dr. Alexander "Sandy" Lawson** was attended by at least 100 CINF members and affiliates in the Colorado Convention Center. Sandy fielded a roster of symposium speakers that included many stars of the chemical information sphere who provided thoughtful insights into and entertaining anecdotes about Sandy's extensive career. It was fantastic to see the old guard and new faces enjoying great fare and an entertaining award presentation at Sandy's expense. Many thanks for the support of the exclusive sponsor, **Reaxys**.

The second **CINFlash Symposium** was held Wednesday afternoon and, though lightly attended, offered some interesting and thoughtful speed-presentations. CINFlash will no doubt be even better in San Diego. CINF thanks **Accelrys** for supporting this symposium with snacks and refreshments.

The CINF division would not be able to host these social networking events without the generous support from all our sponsors to whom we extend our sincere thanks.

Graham Douglas, Chair, Fundraising Committee

Photos from the 2011 Fall ACS National Meeting are available at
<http://www.flickr.com/photos/cinf>

SPONSOR ANNOUNCEMENTS



Accelrys has launched a comprehensive Academic Program specifically focused on meeting the needs of academic communities - from students, teachers and researchers to IT support staff and university administrators - around the world. Demonstrating Accelrys strong commitment to science and higher education, the new Academic Program makes it easier for researchers to access and share state-of-the-art scientific software solutions that support collaboration, enhance innovation and accelerate discovery in university labs.

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For more information read [Press Release](#) or visit www.accelrys.com/academic



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For more information visit <http://accelrys.com/events/webinars/>

Chemistry & Industry: New Publisher!



From October 2011, the Society of Chemical Industry (SCI) magazine, *Chemistry & Industry* will be published by John Wiley & Sons, one of the largest publishers of chemistry information in the world.

Under Neil Eisberg's continued editorship, the magazine will publish news-breaking, topical and international chemistry-based articles, focusing on scientific and industrial innovation that will result in commercially significant developments in the next ten years.

<http://www.soci.org/Chemistry-and-Industry/>

IC_{SYNTH} Version 1.4

InfoChem is proud to announce the release of IC_{SYNTH} version 1.4 in September.



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

“The major improvement of version 1.4 is not immediately visible” says Dr. Heinz Saller, chief developer for IC_{SYNTH}. “We have invested a great deal of work in optimizing the algorithm responsible for the precursor search and therefore for the synthesis suggestions.”

Also new in IC_{SYNTH} 1.4 is the possibility of grouping the precursors according to the core structure or to the set of created bonds. In addition the ratings for the different synthesis paths can now be exported.

For more information about IC_{SYNTH}, please visit our homepage (<http://infochem.de/products/software/icsynth.shtml>) or contact us (info@infochem.de).



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For more information see <http://www.cambridgesoft.com/pki/>.

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