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Message from the Chair



Dear Colleagues,

The CINF events in Anaheim were a great success (and the nearly flawless weather was a bonus). The scientific presentations at ACS national meetings have always been a significant value of CINF, and the papers presented at Anaheim certainly confirmed and underscored that value. One particular favorite for me was the session honoring the legendary Professor James B. Hendrickson. I used the Pine, Hendrickson, Cram, and Hammond *Organic Chemistry* textbook as an undergraduate student and had the pleasure of hearing Dr. Hendrickson give a lecture entitled "The Chemistry of Drugs: Legal and Illegal" at my college. What made that particular session so memorable (apart from the topic) was that Dr. Hendrickson brought his own colored chalk and gave a "chalk talk," using different colors to push electrons through the various reaction schemes. It was science! It was art! It was brilliant! The CINF symposium honoring Dr. Hendrickson was a fitting testament to a man who has done great things at the interface between computers and organic chemistry.

The other CINF symposia were no less captivating, including the session on open data, open science, and open knowledge (kindly supported by the Chemical Structure Association Trust), the session on natural products and drug discovery, the session on data archiving, e-science, and primary data, and the lively "Internet and Chemistry: Social Networking" session, co-sponsored with the Younger Chemists Committee. In addition to the symposia, the CINF Scholarship for Scientific Excellence poster session (graciously supported by Accelrys) highlighted research done by the next generation of CINF members.

Of course, another major value of CINF has always been the networking opportunities, and those were present in abundance in Anaheim, including the Sunday reception, Harry's Party, Tuesday luncheon, and Tuesday reception. The CINF luncheon was memorable for the gory PowerPoint presentation on the case of Jack the Ripper by noted criminal profiler Richard Walter. What did this have to do with CINF? Not a thing! But it was a fascinating view of a century-old case through the eyes (and using modern day criminal profiling techniques) of a man dubbed "The Living Sherlock Holmes." That said, I promise that the next keynote speaker at the CINF luncheon in Denver will not show photographs of dead bodies as Richard did.

Speaking of Denver, it was decided to modify the times of future Saturday Committee meetings. Rather than starting with a 7:30 AM breakfast (which, as a non-morning person, I always found borderline criminal), we will start the meeting in Denver at 11:00 AM. This will allow some people to arrive on the day of the Committee meetings rather than the day before. In today's ever cost-conscious world, every little bit helps. The meeting will go a little later (ending at 6 PM rather than 5 PM), with an overall result aimed at more efficient use of time. So, please plan ahead to come to the Fall ACS meeting and get involved in CINF committee activities. It's good for your soul (not to mention your career). I wish you a great summer and look forward to seeing you in Denver!

Gregory Banik, Chair, ACS Chemical Information Division

Letter from the Editor

Greetings! I believe that the *Chemical Information Bulletin* has succeeded since 2010 in its favorable and seamless transition from its print publication into *e-CIB*. David Martinsen did a skillful conversion of the CINF technical program listing from an ACS host to the 2011 spring issue of *e-CIB*. Certainly, the transition was fluent for the summer and winter issues, which are delivered in an electronic format like the former *CINF E-News*. Based on positive comments on the past issues, I continued with extending invitations to symposium organizers, committee chairs and division representatives for their valuable insights of the conference engagements.



I was honored to receive many submissions, so that the readers can now peruse post-meeting reflections on the high-quality programming, collaboration, and recognition of excellence.

The Technical Program section begins with highlights from the Anaheim meeting by a new Program Chair, Rachele Bienstock. Then it dives into a noteworthy symposium organized by Martin Walker honoring fifty years of contributions by Professor Emeritus James Hendrickson (Brandeis University) in using computers for cheminformatics and organic chemistry, and an attention-grabbing two-day symposium *Chemistry and Internet: Social Networking* by Steven Bachrach. Recorded content from two CINF symposiums, *Internet and Chemistry: Social Networking* (13 presentations), and *Natural Products and Drug Discovery: Cheminformatics and Computational Chemistry* (7 presentations), will be freely available to the public at the [ACS Learning Center](http://www.softconference.com/ACSchem/) (<http://www.softconference.com/ACSchem/>) after May 2, 2011. The section concludes with news from the *Multidisciplinary Programming Planning Group* by Guenter Grethe.

The Reports section brings together a breakthrough “InChI story” by Carmen Nitsche, a call for submissions to the *XCITR* (*Explore Chemical Information Teaching Resources*) repository by Guenter Grether, and disturbing updates on the CINF membership continuous decline, not yet reflecting the exceptionally successful ACS membership recruitment efforts in 2010, reporting the official ACS membership number for 2011 at 163,111 – the highest number since 2003 (see the Council report in this section). Then it goes on with a welcome summary of the executive meeting of the Council Committee on Terminology and Symbols by Peter Rusch, and a flash from the CINF social networking events by Graham Douglas.

Three student scholarship winners, Elsa Alvaro (Lucille Wert Scholarship), and Scott Johnson and Matt Kayala (Scholarship for Scientific Excellence), were announced at the 2011 spring meeting.

In conclusion, I would like to thank all who wrote articles for this issue. Many thanks to Mark Luchetti for designing the cover page, to Bonnie Lawlor and Wendy Warr for proofreading this issue, and to Alex Allardyce, Bonnie Lawlor, Carmen Nitsche, and Wendy Warr for taking photographs at the Anaheim meeting. All photos looked exceptionally good to me, so that I referred the readers to the entire [collection](http://www.flickr.com/photos/cinf/) (<http://www.flickr.com/photos/cinf/>).

Judith Currano will be a “guest” editor of the next issue before the 2011 Fall ACS National Meeting in Denver, CO.

Svetlana Korolev, Editor, Chemical Information Bulletin

AWARDS AND SCHOLARSHIPS

2011 Lucille M. Wert Student Scholarship: Winner Announced

The Lucille M. Wert Student Scholarship is awarded annually and 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 CINF Awards Committee reviewed the applications during the Spring ACS Meeting, and is very pleased to announce that the 2011 recipient is **Dr. Elsa Alvaro**.



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.

Travel plans permitting, the Scholarship (\$1500) will be awarded to Elsa during the CINF Luncheon at the Fall ACS Meeting in Denver in August.

Congratulations to Elsa!

Phil McHale, Chair, CINF Awards Committee

2011 CINF Scholarship for Scientific Excellence: Winners Announced

At the Spring ACS Meeting in Anaheim, Accelrys, Inc. generously sponsored two CINF Scholarships for Scientific Excellence. Five applicants presented excellent posters of their work at Sunday's CINF Welcoming Reception, and after some difficult deliberations, the panel of judges selected the two winners. The winners were recognized at the Reception and received their \$1000 scholarships at the CINF Luncheon on Tuesday.



Guenter Grethe and Carmen Nitsche announce the Scholarship winners:
Scott Johnson (left) and Matt Kayala (right)

The two recipients are Scott Johnson of UCLA, whose poster was on *Re-examining the tubulin binding conformation of antitumor epothilones using QSAR and crystallographic refinement*; and Matt Kayala of UC Irvine, who presented on *Learning to Rank Productive Organic Mechanisms*.

Thanks to Accelrys, Inc., and congratulations to Scott and Matt.

Up to three scholarships will be presented at the Fall ACS Meeting in Denver, kindly sponsored by FIZ CHEMIE Berlin.

Phil McHale, Chair, CINF Awards Committee

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.

Bonnie Lawlor, Chair, CSA Trust Grant Committee

TECHNICAL PROGRAM

CINF Technical Program Highlights



Rachelle's daughter with "Mole"

While it was Anaheim, with Disney close by, I did not spot Mickey in attendance; however there was a large friendly "Mole" willing to hug and greet attendees and pose for pictures.

The 2011 Spring CINF program although brief on quantity was not short on quality. The program featured 67 submissions: 8 poster presentations and 59 oral presentations, which included 6 poster submissions for the CINF Scholarship for Scientific Excellence (financially supported by Accelrys at this meeting). The smaller CINF program is a reflection of the overall downturn in the economy and the fact that many attendees were unable to participate due to travel budgets.

The meeting opened on Sunday with a featured symposium (cosponsored by the Division of Organic Chemistry) honoring James Hendrickson, Professor Emeritus, Brandeis University, on his long career and many contributions to methodologies for computer-aided synthesis and reaction design. Martin Walker paid tribute to his mentor by putting together a superb program. The Symposium honoring James Hendrickson brought many nontraditional attendees to a CINF session from the Division of Organic Chemistry, to the afternoon talks by Paul Wender (Stanford University) and Phil Baran (Scripps Research Institute) particularly.

Sunday afternoon also drew attention to a session "Integration of Combinatorial Chemistry and Cheminformatics as Applied to Materials Science and Drug Discovery" organized by Maciej Haranczyk and Jose Medina-Franco. This symposium featured several seminal talks on effective combinatorial library design. Then, Sunday evening saw a small but high quality group of student posters in our CINF Scholarship for Scientific Excellence session, organized by Guenter Grethe. There were two California award winners, Matthew A. Kayala, of University of California, Irvine, Department of Computer Science, "Reaction Prediction as Ranking Molecular Orbital Interactions" (coauthors: Dr. Chloe A. Azencott, Dr. Jonathan H. Chen, Prof. Pierre Baldi) and Scott A. Johnson, University of California, Los Angeles, Department of Chemistry and Biochemistry, "Re-examining the Tubulin-Binding Conformation of Anti-tumor Epothilones using QSAR and Crystallographic Refinement" (coauthors: Dr. Adam J.T. Smith, Prof. James P. Snyder, Prof. Kendall N. Houk).

On Monday, Simon Wang organized a session on "Natural Products and Cheminformatics," which was selected for videotaping by the ACS. This session, complete slides with talk synchronized, should appear through links on the ACS Anaheim website for later viewing. On the second track the CSA Trust symposium organized by Peter Rusch and Irina Sens on "Open Data" was also held on Monday morning. It featured presentations by Peter Murray-Rust, Matthew Segall, Colin Groom and Irina Sens. Then on Monday afternoon Leah Solla, Robert McFarland and Norah Xiao organized a session on "Data Archiving, e-Science and Primary Data" focusing on how to catalogue and organize increasing amounts of chemistry data effectively.

One of the areas where CINF demonstrated technical innovation was the remote presentation via the Internet of a paper in the "Internet and Chemistry" symposium (cosponsored by the Younger Chemists Committee) organized by Henry Rzepa and Steven Bachrach on Tuesday morning. Although, hearing a disembodied voice deliver the talk was perhaps initially disconcerting, this provided for an effective means of delivering a talk in this day and age of austerity when travel is sometimes difficult. (Perhaps, we should see how many attendees liked this on Facebook?) This two day symposium featured presentations on Open Science projects by Peter Murray-Rust, on Quixote by Jens Thomas, OpenTox by David Gallagher, on new mobile technologies by Steven Muskaf and Alex Clark, on many uses of the web in chemistry by Alex Allardyce, Svetla Baykoucheva, Anthony Williams and Stephen Heller, and on web publishing and scientific literature by David Martinsen, Jan Kuras, Henry Rzepa and Roger Schenck. This well-attended symposium featured all kinds of amusements including one of the older audience members holding up an IBM punch card to show some of the younger members how programming was done "in the good old days..."

The CINF program concluded with the general papers which consisted of several presentations on toxicity, QSAR and computational methods by Adam Lee and Marvin Waldman of Simulations Plus, an oral presentation from one of the student poster award winners, Matthew A. Kayala, UC Irvine, a presentation by Eugene Muratov, representing an international consortium working on a collaborative QSAR modeling project, and a presentation by Richard Nafshum of Oregon State University on the use of computers in teaching chemistry.

Of course, I want to thank Rajarshi Guha for all his assistance with the steps involved in preparing the CINF program for this meeting, and to all the organizers and symposium chairs for all their hard work, as well as the Program Committee for suggestions for programming for this spring meeting and for future meetings. If you have any programming suggestions for future meetings or any programming comments at all, please don't hesitate to get in touch, at rachelleb1@gmail.com

Rachelle Bienstock, Chair, CINF Program Committee

James B. Hendrickson: 50 Years of Computers in Organic Chemistry

A symposium was held in Anaheim, to celebrate fifty years of contributions by Professor Emeritus James B. Hendrickson (Brandeis University) in using computers for cheminformatics and organic chemistry. The morning session began with a thorough review of Hendrickson's work by Guenter Grethe, from his early work on ring conformations, through synthesis design into his modern work on reaction classification. Dr. Josef Eiblmaier (InfoChem) showed some modern approaches to reaction classification, while Dr. Orr Ravitz (SimBioSys) described advances in computer-aided synthesis design.



In the afternoon, the emphasis moved more towards synthetic organic chemistry, with a focus on Hendrickson's concept of an "ideal synthesis." Professor Paul Wender (Stanford University) explained how Hendrickson's systematic approach to synthesis design influenced his own work, then he described some of the new treatments for cancer and HIV that are being developed in his

laboratory. Professor Philip Baran (Scripps Research Institute) also paid tribute to Hendrickson's work, and then explained his own radical biomimetic approach to synthesis based on stereoselective functionalization. The symposium closed with a presentation by Professor Hendrickson himself. He began with a few personal reflections on his work, which also explained his basic approach. He then explained his recently published system of "reaction signatures" which can uniquely and concisely describe any organic reaction.

The symposium attracted around 40-60 people, but most interesting was the mix of the audience, which contained both cheminformatics specialists and mainstream organic chemists. CINF members heard about groundbreaking work in organic synthesis by two of the world's leading synthetic chemists, while the synthetic chemists in the room learned about the relevance of cheminformatics for improving the design and implementation of laboratory synthesis.

Martin Walker, Organizer, Symposium in Honor of James B. Hendrickson

Internet and Chemistry: Social Networking

To commemorate the very first session at an ACS meeting regarding the Internet, held in Anaheim in 1996, Henry Rzepa and Steven Bachrach co-organized the session: Internet and Chemistry, at the Anaheim meeting in 2011. The session featured talks that were both retrospective and prospective, interspersed with some philosophical meanderings regarding how chemists can further exploit the technological innovations of the web.

Peter Murray-Rust presented a timeline of major developments on the chemical web and discussed the recent "Green Chain Reaction" project, which utilized social networking to look at changes in solvent usage in reported patents over the past decade. Cameron Neylon was unable to physically attend, but provided a movie of his talk, where he discussed reimagining the paper as a discrete set of objects that could be re-used and mashed-up. Cameron also answered questions live through a skype connection. Jens Thomas presented an update of "Quixote," a collaborative project to create an open database of computational chemistry results. The next two talks, by Steven Muskal and Alex Clark, featured new mobile applications on the iPhone and iPad available from Eidogen-Sertanty and Molecular Materials Informatics. In the afternoon, Alex Allardyce discussed the "chemicalize" tool, which adds chemical information and links to existing web pages via recognition of chemical names. Svetla Baykoucheva presented the use of campus guides to present library information to customers. Tony Williams discussed the role of the crowd in creating the ChemSpider site. The first day was concluded with a provocative talk by Steve Heller regarding how the web may be dumbing us down, along with an update on the InChI project.

The second day began with a publications session. David Martinsen discussed new digital publishing technologies, including many innovations implemented by ACS Publications. Jan Kuras reported on the results of the recent SOAP survey of scientists' attitudes towards Open Access journals. David Gallagher discussed the social networking project, OpenTox, which is developing tools for toxicity prediction. Roger Schenck presented an overview of CAS products. Henry Rzepa closed the morning session with a look at how web technologies could dramatically enhance publication by reimagining the classic Watson-Crick DNA paper presented with modern tools. In

the afternoon session, Sam Adams discussed the CLARION project, a way of creating an open data repository. Klaus Gubernator discussed how the Internet enables his company, eMolecules, to sell and deliver chemicals around the world. Steven Bachrach gave a retrospective view of the slow adoption of Internet technologies by the broad chemical community and discussed the social changes needed to make revolutionary progress. The final talk was delivered by Jean-Claude Bradley through Skype. He talked about Open Notebook Science, whereby scientific results are revealed as they occur in a collaborative open framework.

Steven Bachrach, Co-Organizer, Internet and Chemistry Symposium

Recorded content from two CINF symposiums, *Internet and Chemistry: Social Networking*, and *Natural Products and Drug Discovery: Cheminformatics and Computational Chemistry*, is available at the [ACS Learning Center](http://www.softconference.com/ACSchem/) (<http://www.softconference.com/ACSchem/>)

Multidisciplinary Program Planning Group (MPPG)



Since its inception at the 2007 Spring National Meeting in Chicago, thematic programming has become an established and successful fixture at National Meetings. The 2011 Spring National Meeting in Anaheim was no exception. The theme, “The Chemistry of Natural Sources,” was highlighted on banners and posters at the Convention Center and on the cover of the meeting program. The theme organizer, Ann-Christine Albertsson, Professor in Polymer Technology at the Royal Institute of Technology, Stockholm, Sweden, and Editor-in-Chief of *Biomacromolecules*, placed emphasis on topics dealing with understanding, creating and using the chemicals of nature.

Within the broad scope of the theme, she successfully worked with ACS divisions and committees to generate a very interesting program. Seventy-two symposia related to the theme were organized in 185 sessions by nineteen divisions and one committee. CINF participated with a well-attended, full-day symposium on “Natural Products & Drug Discovery: Cheminformatics & Computational Chemistry.” Dr. Albertsson also organized and presided over a very successful Plenary Symposium in which four speakers addressed important issues related to the theme. Nobel Laureate Harry Kroto talked about “Carbon in nano and outer space,” Björn Åkermark lectured about “Artificial photosynthesis, the final solution of humanity’s energy problems,” Steve Kelly elaborated on “How can bioenergy be made sustainable,” and Piet Lemstra concluded the session with his talk on “Petrovs. bio-based polymers.” Finally, 2013 theme organizers and a member of MPPG were involved in the selection of the speaker of the first Kavli Foundation Innovation in Chemistry Lecture in which Virgil Percec talked about “Bioinspired synthesis of complex molecular systems.” Overall, activities related to the theme successfully showed the increasingly important multidisciplinary nature of chemistry and MPPG’s role in providing organization and content.

After Anaheim we are now looking forward to the 242nd ACS National Meeting in Denver (August 28 – September 1, 2011). The theme of the meeting is “Chemistry of Air, Space and Water” and the theme organizer is Ronald C. Cohen from UC Berkeley. Based on early information, the meeting promises to be very successful with interesting topics. About 30 symposia related to the theme have already been identified. The main subtopics listed by the organizer are “Atmospheric aerosols: Chemistry, clouds and climate,” “Chemistry at high pressure: Exploring the interior of planets with laboratory experiments and theory,” “Chemistry as a tool for space exploration and discovery at Mars” and “Nitrogen and human endeavor.” As of this writing, three speakers have already agreed to talk at the Plenary Symposium on Sunday afternoon. The topics and speakers are “Of muck and molecules: Relating bulk aerosol properties to molecular behavior” by Neil Donahue, Carnegie Mellon, “Chemistry of planetary gases, liquids, and ices in extreme environments” by Russell Hemley, Carnegie Institute Washington, and “Nitrogen and the human endeavor” by Alan Townsend, INSTAAR. The Kavli Lecture on Monday afternoon will be delivered by Susan Solomon, NOAA/University of Colorado, Boulder. The title of her talk will be “The enduring challenges of ozone depletion and climate change: How planetary chemistry is changing science and society.”

Going forward, the theme suggested by MPPG and approved by ACS divisions for the 2012 Spring ACS National Meeting in San Diego is “Chemistry of Life” with subtopics such as biomimetics, synthetic biology, systems biology, cell biology, chemical signaling in biological systems, metabolomics, etc. The theme organizer is Dr. Peter Senter, Seattle Genetics. The 2012 Fall Meeting in Philadelphia will be organized under the theme “Materials for Health and Medicine.” Potential subtopics include biological systems and drug discovery, drug delivery vehicles, polymeric materials for medical applications, nanomedicine, nutrition and health, etc. The theme organizer for this meeting has not been selected as of this writing.

In 2013, the National Meetings will take place in New Orleans (Spring) and Indianapolis (Fall). The following themes have been approved: “Energy and Food” and “Chemistry of Motion,” respectively. More details will be forthcoming in due time.

Any questions or comments regarding MPPG and the themes should be directed to Guenter Grethe at ggrethe@att.net.

Guenter Grethe, Past-Chair, Multidisciplinary Program Planning Group

Schedule of Future ACS National Meetings

242 nd	Fall 2011	August 28 - September 1	Denver, Colorado
243 rd	Spring 2012	March 25 - 29	San Diego, California
244 th	Fall 2012	August 19 - 23	Philadelphia, Pennsylvania
245 th	Spring 2013	April 7 - 11	New Orleans, Louisiana
246 th	Fall 2013	September 8 - 12	Indianapolis, Indiana

REPORTS FROM THE 2011 SPRING ACS NATIONAL MEETING

InChI gains CINF support

Despite all of the efforts that have gone into chemical representation, chemists still face challenges when exchanging basic information about specific molecules. Molecule names, of course, are notoriously difficult, with compounds often having dozens, if not hundreds of synonyms. Various registration systems also exist, from CAS numbers, to MDL numbers, to ChemSpider IDs – but these numbers are “dumb” in that they don’t convey any aspects of the underlying chemistry in-and-of themselves. Actual chemical structure representations, such as MolFiles or SMILES, are an effective way to exchange exacting chemical specifics of a molecule. But even here we face issues due to varying conventions, multiple non-canonical representations, and good old fashioned human error. And to top it all off, we face the fact that in many of these cases the representations are proprietary in nature and may require payment.

It is in this environment that some ten years ago IUPAC undertook a project to establish an open, non-proprietary international standard, assigning unique machine-readable representations to chemical structures – now known as the InChI standard. The original work on the standard, development of the appropriate algorithm, and creation of software to generate InChIs was carried out under the auspices of IUPAC at the National Institute of Standards and Technology (NIST).

In 2009 the InChI Trust was established to create a mechanism by which the standard could be maintained and developed further. This work is overseen by the InChI Trust board of directors, which includes a member of IUPAC. Any corrections, improvements, or extensions of the InChI must be approved by IUPAC before release.



The CINF Division is keenly interested in all efforts to foster the exchange of chemical information, since many of our members within the academic, government and commercial spheres are involved in its creation, dissemination, and interlinking. So our division has avidly watched the advancement of InChI and became an InChI supporter in late 2010. This will allow us to attend the InChI Trust’s annual general meetings and contribute our members’ perspectives on InChI related projects. If you would like to be the CINF representative at the next meeting in the Fall, please let me know at Carmen.Nitsche@accelrys.com.

Several IUPAC working groups continue to explore ways to expand the InChI standard. Current projects include representation of Markush structures, polymers and mixtures, organometallics, and electronic states, as well as an InChI for Reactions. As these efforts advance, we expect that InChI will encompass an ever broader range of chemical representation – facilitating a free exchange of more and more types of chemistries.

Carmen Nitsche, Immediate Past Chair, CINF Division



Your Submissions Wanted!

*XCITR (<http://www.xcitr.org>) is a repository for exploring and sharing chemical information teaching resources. **Register today to contribute materials that you have produced for sharing with others or access XCITR materials for teaching or personal use.***

XCITR (Explore Chemical Information Teaching Resources) was developed to meet the need for an international repository of chemical information educational material. XCITR is intended not only for librarians and instructors in chemical information, but also for chemistry professors, instructors in other disciplines related to chemistry, information specialists, students, high school teachers, and even technical writers. XCITR is a hub in which librarians, instructors, and information providers can deposit and access important and useful teaching materials. Educational materials about library services and collections are also welcome.

Teaching materials in XCITR can be used for free and, if the author permits, modified according to individual needs. To help insure that items deposited fall within the scope of the collection, an editorial board will briefly review all depositions before they are made publicly available in XCITR. Allowed document files are Office files (Word, PowerPoint, Excel) and PDF. Additionally, embedded videos from YouTube and slideshows using SlideShare are permitted. The inclusion of embedded websites is under development.

XCITR was opened to the public last year and contains a small, but growing, collection of *ca.* 50 documents. Items in the collection range from book resources for K-12 to a set of videos about searching PubChem. Check the XCITR website for a complete list of topics. In addition to material dealing with cheminformatics topics, we solicit teaching material from the areas of bioinformatics and computational chemistry. Software developers and database providers are encouraged to submit training materials and help manuals if publicly available.

XCITR is a collaborative project between the Computer-Information-Chemistry (CIC) Division of the German Chemical Society (GDCh) and the Division of Chemical Information (CINF) of the American Chemical Society (ACS). XCITR is hosted by FIZ CHEMIE Berlin, Germany. The website was developed by a group at FIZ CHEMIE Berlin and contains all the features of modern Web 2.0 technology, including user-dependent display and functionality, tag cloud and keyword linked documents, and many more. Users are encouraged to access the site and see for themselves. For questions and comments, please contact Guenter Grethe at ggrethe@att.net or Gregor Fels at fels@uni-paderborn.de.

Guenter Grethe, XCITR Project Coordinator

Information Competencies for Chemistry Undergraduates: the elements of information literacy.
Special Libraries Association, Chemistry Division and American Chemical Society, Chemical
Information Division. 2nd ed. May 2011. [<http://units.sla.org/division/dche/il/cheminfolit.pdf>]

Report of the CINF Membership Committee



I am the only member of the CINF Membership Committee now, so if anyone would like to serve on the committee it would be greatly appreciated!

The CINF Division membership stands at **1,037** at the end of February 2011.

Though the total number is still decreasing, the descent has slowed. We actually have gained in three categories, retired, emeritus and undergraduate student members, on both ends of a career maturity spectrum.

I analyzed the numbers of new and departing members from March 2010 to February 2011 and made the following observations:

More than 50% of our new members chose CINF as their free division. Hopefully, these members will continue considering CINF as their primary division after their first year of membership. (Editor's note: In joining the Society individuals may choose one free division for one year and additional divisions to be billed with their membership dues). Less than 10% of our new members choosing CINF as their free division have been leaving it. Most of them continue their memberships in other ACS divisions.

From the demographics report we seem to be losing members from industry the most. The job title report shows memberships in all of the following categories going down:

- Chemical Technician,
- Production/Operations Manager,
- Purchasing Manager/Buyer,
- Sales Marketing/Business Development, and
- Supervisor/Project Leader/Foreman.

The other job title categories seem to be remaining stable percentage - wise.

I would like to encourage people to fill out their membership forms more completely as a number of categories have over 50% "N/A" marks, which keep us from being able to make many deductions as to where our membership is heading.

Jan Carver, Chair, CINF Membership Committee



www.acs.org/memberGetmember

Summary of Executive Meeting of the Council Committee on Nomenclature, Terminology and Symbols (NTS)



It was reported that the International Committee on Weights and Measures has postponed action on new definitions of some SI Base Units until 2015, leaving time for input from other interested organizations. In a straw poll, the Committee on Nomenclature, Terminology and Symbols (NTS) voted in favor of drafting and submitting a policy statement about redefinition of the kilogram and the mole. A review of the 2011 International Year of Chemistry activities called attention to a symposium organized by Carmen Giunta, a member of NTS, on “*What’s In a Name? Histories of Units and Constants*” in the Division of the History of Chemistry on Tuesday, March 29, 2011.

The Committee is still seeking ways to contribute to the chemical education thrusts and concerns of various units of the Society.

With the help of a National Research Council staff member, the Committee reviewed the relationships among American Chemical Society (ACS), International Union of Pure and Applied Chemistry (IUPAC), and National Academy of Sciences (NAS), bringing attention to some duplication of the Committee structure and some conflict of purpose or point of view. NAS, rather than ACS, is the U.S. organization that interacts directly with IUPAC. In most other countries, the adhering body is the residing chemical society representing chemists. This difference in IUPAC representation may cause U.S. chemists to be less aware of the scope of the IUPAC activities. ACS development of international outreach programs has resulted in strengthening of ties between IUPAC and ACS.

As a follow-up of an exploration of the future of the Committee begun at the previous meeting, NTS engaged in a lengthy discussion and analysis of committee members’ responses to questions about the Committee’s duties and opportunities.

Peter Rusch, Chair, Council Committee on Nomenclature, Terminology and Symbols

Report from the ACS Council Meeting

The Council of the American Chemical Society met in Anaheim, CA on Wednesday, March 30, 2011 from 8:00am until approximately 10:45am in the Grand Ballroom of the Hyatt Regency Orange County Hotel. The meeting opened with a moment of silence in respect for the Councilors who have passed away since the last Council meeting. The minutes of the Council meeting held in Boston, MA in August 2010 were approved and Dr. Carolyn Ribes was confirmed as the Vice-Chair of the Council. Additional key items from the meeting are as follows:

Nominations and Elections

President-Elect: The Committee on Nominations & Elections (N&E) had identified four nominees for the office of 2012 ACS President-Elect. They are as follows: Judith L. Benham (a former Chair

of the ACS Board of Directors); Dennis Chamot (a current member of the ACS Board of Directors); Diane Grob Schmidt (a current member of the ACS Board of Directors); and Marinda Li Wu (a current member of the ACS Board of Directors). The four nominees answered questions at the Town Hall meeting that was held on Sunday and each gave a three minute presentation at the Council meeting. Council voted to select Dennis Chamot and Marinda Li Wu as the final two candidates who will appear along with any petition candidates on the ballot in the fall.

N&E also developed interim guidelines for the use of audience response devices (clickers) at Council meetings to capture votes.

Other Elections

The Committee on Nominations and Elections announced the results of the election to select candidates from the list of nominees to represent District III and District VI on the Board of Directors for the term 2012-2014. Nominees for District III included Susan B. Butts, Pat N. Confalone, David J. Lohse, and Judith A. Summers-Gates. Nominees for District VI included G. Bryan Balazs, Bonnie A. Charpentier, Carlos G. Gutierrez, and Victor J. Hruby. By mail ballot, the Councilors from these districts selected Pat N. Confalone and David J. Lohse as District III candidates; and Bonnie A. Charpentier and Carlos G. Gutierrez as District VI candidates. Ballots will be mailed on or before October 10 to all members in District III and District VI for election of a Director from each District.

The Committee on Nominations and Elections also announced the selection of the following candidates for Directors-at-Large for a 2012-2014 term: Ken B. Anderson, William F. Carroll, Jr., Charles E. Kolb, and Barbara A. Sawrey. The election of two Directors-at-Large will be conducted in the fall. Ballots will be mailed to the Council on or before October 10, 2011.

Change in Committee Charter Charge

The Committee on Committees put forth a recommendation to change the wording of the Charge of the Committee on Technical Affairs as a result of the 2009 disbandment of the ACS Division of Chemical Technicians. The ACS Committee on Technical Affairs (CTA) met in Boston last fall and voted to accept new language for the ACS Constitution & Bylaws regarding CTA's mission. Council voted and approved the request that the term "chemical technicians" be replaced by "Applied Chemical Technology Professional," a term that is considered more accurate and is widely used.

ACS Dues for 2012

Council voted and accepted the recommendation from the Committee on Budget and Finance with regard to the 2012 membership dues (an increase of \$2.00 - from \$146 to \$148). The increases to ACS dues are based upon an escalator defined in the ACS Bylaws (Bylaw XII, Section 3,a). The dues are calculated by multiplying the base (current) rate "by a factor which is the ratio of the revised Consumer Price Index for Urban Wage Earners and Clerical Workers (Service Category) for the second year previous to the dues year to the value of the index for the third year previous to the dues year, as published by the United States Department of Labor, with the fractional dollar amounts rounded to the nearest whole dollar."

Base rate 2011: \$146.00

Change in the Consumer Price Index, Urban Wage Earners, Services Category:

December 2010 CPI-W Services:	257.382
December 2009 CPI-W Services:	254.519
Change in CPI-W Index:	1.125%

2012 Dues, fully escalated: $\$146.00 \times 1.01125 = \147.64

2012 Dues, Rounded: \$148.00

Change in Name of Local Section

Council voted to accept the petition of the Northeast Oklahoma Section to change its name to Northern Oklahoma Section. This is a result of a recent merger of the North Central Oklahoma Section and its territories into the Northeast Oklahoma section. The proposed change more closely reflects the combined territories of the two sections.

Change in Calculation of Division Allocations

The Divisional Activities Committee (DAC) recommended that there be no change to the procedure that is currently used to distribute the Divisional Allotment (which is 9% of dues) among the Divisions. The current procedure was approved by Council in 2008. Council voted and accepted the recommendation.

Themes for Future National Meetings

The Multidisciplinary Program Planning Group (a subcommittee of the Divisional Activities Committee) has recommended the themes for upcoming national meetings in 2014. For the spring national meeting in Dallas it will be “Chemistry of Power and Advanced Materials” and for the Fall meeting in San Francisco it will be “Chemistry on a Crowded Planet.”

Support for Non-Councilor Committee Members

The Council Policy Committee (CPC) has approved a program to reimburse non-councilors for committee participation at 50% of the Councilor reimbursement level. Committees that currently reimburse are not affected and will continue according to their own reimbursement guidelines. Committee chairs and other interested parties will be consulted and further informed later this year. The program will be presented to the Committee on Budget and Finance to be considered for future implementation.

2010 Financial Results

The Committee on Budget and Finance gave a summary of the ACS 2010 Financial results. Revenues totaled \$463.7 Million dollars (\$2.4 Million over budget). Net from Operations was \$23.8 million, or \$11.9 million favorable to budget. As of December 31, 2010 the Society has unrestricted net assets of \$130.5 Million. This does not meet the financial goal of \$180 million in unrestricted net assets, but it does represent a significant growth from the \$60 million that existed at the end of 2008. The favorable 2010 finances resulted largely from cost containment initiatives and lower-than-

budgeted salaries and fringe benefits as well as from strong performances in investments and in the information services (CAS and Publications).

Member Statistics

Membership recruitment efforts were exceptionally successful in 2010. It is particularly impressive that due to efficiencies in recruiting efforts, the net cost to recruit the more than 25,000 new members decreased from \$122 per member in 2008 to \$67 in 2010 despite increases in costs for postage and printing. The official membership number for 2011 stands at 163,111 – the highest number since 2003. Membership totals since that time are as follows:

2003: 159,332
2004: 158,127
2005: 158,422
2006: 160,491
2007: 160,052
2008: 154,024
2009: 161,783
2010: 163,111

2011 Spring National Meeting Attendance

The attendance at the 2011 spring national ACS meeting in Anaheim, CA totaled 14,047, broken down as follows: Regular Attendees, 7,336; Students, 4,682; Guests, 333; Exhibitors, 1,097; Exhibit Attendees only, 599. The total attendance at this meeting was about 4,000 less than the spring 2010 meeting in San Francisco, CA, but was about 3,300 higher than the 2009 spring meeting that was held in Salt Lake City, UT (total attendance 10,668). Spring meeting attendance since 2004 is as follows:

2004: Anaheim, CA:	14,141
2005: San Diego, CA:	15,385
2006: Atlanta, GA:	12,546
2007: Chicago, IL:	14,520
2008: New Orleans, LA:	13,454
2009: Salt Lake City, UT:	10,668
2010: San Francisco, CA:	18,076
2011: Anaheim, CA:	14,047

The spring national meeting in 2012 will be held in San Antonio, TX.

Job Market for Chemists

The poor job market for chemists was a major theme throughout all of the reports given at Council. As of 2009 the unemployment rate for chemists was 3.9% and is assumed to be higher this year. A major issue is the length of time of unemployment. 50% of those identified as being unemployed have been without a job for an extended period of time – some for two years or more.

The job fair at the spring national meeting had 795 job seekers and 39 employers looking to fill 182 positions. Because employers have fewer jobs to offer they are not coming to national meetings. As a result, ACS is holding virtual job fairs. The first one was held in November 2010 with 2,513 job seekers, 26 employers and 196 open positions. Another virtual job fair will be held in 2011.

ACS is working to promote and support entrepreneurship, with the goal of creating more jobs here in the United States. They are forming a single unit that will offer affordable help to entrepreneurs; they will increase advocacy at the state and federal level to improve the business environment; they will partner with academia to promote career pathways; and they will increase public awareness of the value of early-stage entrepreneurship.

Petition to Charter Two New International Chemical Sciences Chapters

Council voted to accept the request from the International Activities Committee (IAC) to approve the charter of two new international chemical sciences chapters: The Shanghai International Chemical Sciences Chapter and the Thailand International Chemical Sciences Chapter. Both petitions were signed by ACS members in good standing and residing in the territory. The applications met all of the requirements of the ACS Constitution and Bylaws (Bylaw IX). Proposed operation budgets were submitted and they do not include allotments of Society funds. The ACS Board of Directors has authorized these actions and now having received Council approval, the Chapters will begin operation.

Bylaw Changes for Consideration Only

There was one Bylaw change on the agenda and it is for Council consideration only. It will be voted on at the fall Council meeting in Denver, CO.

Petition on Position Statements

The ACS Constitution makes it clear that any position statement that expresses the position of the Society as a whole requires the approval of the Board of Directors. ACS Bylaws (Bylaw IX) regulate the issuance of position statements by any "Society Body" other than the Board. These bodies include Local Sections, Divisions and presumably, ACS Committees. As currently written, Bylaw IX could potentially conflict with the Board Regulations governing position statement development. This petition is intended to allow for a clear and consistent position statement development process for the Society.

This petition seeks to amend Bylaw IX so as to assure that the Board of Directors has primacy in issuing position statements that establish policy for the full Society, and that Society bodies other than the Board may issue statements on issues that fall solely in their jurisdiction so long as they do not impair other Society bodies' ability to do the same.

The financial implications of the petition are being assessed. The Committee on Constitution and Bylaws finds the petition to be legal and consistent with other provisions of the Society's documents. However they believe that there are a number of ambiguities that impact the ability of the proposed language of the petition to achieve its intended purpose and recommend that they be addressed prior to Council vote.

Actions of the Board of Directors

The Board's Committees, Advisory Boards and Working Groups

The Board of Directors received reports from the Committees on Professional & Member Relations (P&MR), Grants and Awards (G&A), and Planning, along with its Executive Committee.

The Committee on Grants and Awards presented the Board with a screened list of nominees for the 2012 Priestley Medal and the 2012 Award for Volunteer Service to the ACS. The Board **VOTED** to approve the screened lists, and will now vote on, and announce, the winners of these two awards after its June meeting. On the recommendation of G&A, the Board **VOTED** that Regulation III, Section 13, paragraph 2 (and related language) be removed from the Charter, Constitution, Bylaws and Regulations (Bulletin 5) of the American Chemical Society, because effective January 1, 2011, the ACS Petroleum Research Fund no longer provides a 1% allocation to the ACS Green Chemistry Institute.

The Chair briefed the Board on items arising from the Executive Committee meeting, including agreement of the Board's role at the Leadership Institute and attendance at various other conferences and events.

On the recommendation of the Board Logistics and Training group, the Board agreed to change the group's name to the Board Operations and Technology Team. Several topics were presented with regard to improving the effectiveness of Board operations.

The Board received a thorough report from the Presidential Task Force on Innovation in the Chemical Enterprise: New Technologies for the Society, New Jobs for Chemists. The Board heard the task force report recommendations on how ACS could help entrepreneurs create U.S. jobs for chemists. The Board reached consensus in support of the next steps outlined by the task force. The recommendations from this report will be sent to all Councilors.

Strategic Issue: ACS Worldwide Strategy

At this meeting, the Board continued its discussion of a Society Worldwide strategy as a follow-up to the strategic issues retreat in January, and is also involving the Planning Committee in a more thorough review to engage other members and stakeholders in these discussions. The Board plans to wrap up its ACS Worldwide strategy discussions by year-end.

Plan for a Financial Planning Conference

Every three to five years, the Board, with the Committee on Budget and Finance, holds a conference to discuss in greater detail the Society's finances and its financial objectives. In Anaheim, the Board was briefed on the preliminary plans and desired outcomes for the 2011 Financial Planning Conference, to be held in June. The theme for this conference is "Ensuring the Society's Financial Sustainability and Growth in a Period of Extraordinary Change."

The Executive Director/CEO Report

The Executive Director/CEO and several of her direct reports updated the Board on the activities of CAS (Chemical Abstracts Service), the ACS Publications Division, and the Society's General Counsel. The General Counsel report included an update on the ACS vs. Leadscope litigation. ACS' appeal, which is supported by several prominent Ohio organizations and the Ohio Attorney General, has been accepted by the Ohio Supreme Court, and is under review by that body. As a follow-up to the Publications report, the Board **VOTED** to approve three editor reappointments to ACS journals.

Compensation of Society Executive Staff

The Board received a report from its Committee on Executive Compensation and **VOTED** to approve several actions relative to compensation for the Society's Executive staff. The compensation of the Society's Executive staff receives regular review from the Board.

Other Society Issues

The Board received a report from the President-Elect on plans and priorities during his presidential year. The Board also reviewed and discussed the presidential succession budget - particularly in light of increasing international and domestic travel demands.

The Board **VOTED** to ratify several consent actions taken since its December meeting, including editor appointments, an appointment to the Board Committee on Executive Compensation, and a reappointment to the Governing Board for Publishing.

The Society's International Activities

The American Chemical Society and the Federation of Asian Chemical Societies (a federation of 28 chemical societies of countries and territories in the Asia Pacific region) agreed to a three-year collaboration alliance characterized by mutual benefits, impact, and commitment to cooperation in service to chemical scientists, engineers and professionals represented by the respective organizations. The signing of this memorandum of understanding took place during a special ceremony at the Board's regular session.

The Board also received reports from several international guests representing the following scientific societies: the Chemical Society for Canada, the Latin American Federation of Chemical Associations, the German Chemical Society, the International Union of Pure and Applied Chemistry (IUPAC), the Mexican Chemical Society, the Royal Society of Chemistry (RSC), and the Federation of Asian Chemical Societies.

Bonnie Lawlor and Andrea Twiss-Brooks, CINF Councilors

CINF Social Networking Events

The ACS Division of Chemical Information (CINF) hosts key social networking events at each ACS national meeting and secures support for CINF symposia speakers to assure successful symposia and social gatherings. The division depends on the generous contribution by our sponsors to support these events where chemical information professionals can meet, mingle, share and connect. We have a lot of fun, too!

The **CINF Sunday Welcome Reception** united about 100 members and guests representing all corners of the chemical information space for a really fun network gathering. Colleagues caught-up, old friends reminisced and new acquaintances connected thanks to our five co-sponsors:

[ACS Publications](#), [Bio-Rad Laboratories](#), [CambridgeSoft](#), [InfoChem](#) and [Thieme Chemistry](#).

The **CINF Scholarships for Scientific Excellence** poster session was also held at this reception and two scholarship winners were each presented with \$1,000 award by our generous scholarship sponsor, [Accelrys](#).

Harry's Party was hosted by [FIZ CHEMIE Berlin](#) on Monday evening in a breezy suite at the Sheraton Park Hotel. About 80 friends of CINF, both old guard and new faces, enjoyed superior fare, fine imbibables and the company of friends and colleagues. If you missed us at this meeting please join us at the next.

The **CINF Tuesday Luncheon** provided fare and dark entertainment to 70 attendees, who were thrilled by our special speaker, Richard Walter. Mr. Walter, who is cofounder of the [Vidocq Society](#) and was featured in Michael Capuzzo's book *The Murder Room*, presented *Jack the Ripper Unveiled*. CINF thanks [RSC Publishing](#) for supporting this special luncheon and [Bio-Rad Laboratories](#) for providing travel and honorarium for Mr. Walter.

The **CINF Tuesday Reception** was attended by about 80 mainstay CINF members and affiliates in the Anaheim Convention Center. It was fantastic to see all the old guard and new faces enjoying great fare and rewarding time to renew friendships and make new acquaintances. 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 Spring ACS National Meeting are available at
<http://www.flickr.com/photos/cinf>*



Chemical Information Sources Discussion List

May 1, 2011, marks the 20th anniversary of the traditional date that was fixed for the beginning of the Chemical Information Sources Discussion List (CHMINF-L). I say traditional date because I didn't realize on April 26, 1991 when I originally established the list that I needed to do something else to actually activate it. That happened on May 1. (May Day seems like a much more appropriate anniversary date for CHMINF-L anyhow!)

Some of the older subscribers will remember the incredible mail loops that occurred in the early years of CHMINF-L, seemingly every time I went on vacation! It was a couple of weeks before I became aware that we could set up a searchable archive for the postings. If you take a look at the [archives](http://listserv.indiana.edu/archives/chminf-l.html) (<http://listserv.indiana.edu/archives/chminf-l.html>), you'll find the earliest posting is May 16, 1991. By May 23, there were 116 subscribers, and now there are around 1350, many of whom have been with us since the beginning.

It is very gratifying to see that this "old-technology" list still has some life left in it. CHMINF-L has truly been a social network for librarians, chemists, publishers, and database producers for two decades now. My thanks to Roger Beckman for helping make CHMINF-L a success and to Brian Winterman for taking on the job of listowner when I gave it up several years ago.

Gary Wiggins, CHMINF-L Founder

*Happy Birthday to you,
Happy Birthday to you.
Happy Birthday dear CHMINF-LLLLLL,
Happy Birthday to you!
(and many more!)
Just think, another year and you can
drink legally!*

Bob Buntrock

*Congratulations and thanks to you Gary
and all the others who make this social
network such a useful source.*

Best wishes.

Gene Garfield

*I join Bob and Gene in wishing the list a happy birthday and in thanking Gary for
getting it started and all the others who have helped support it.*

George Thomson

*"Old Technology" or not, this list has
been one of the best things going as far
as I'm concerned. Almost nothing has
helped me more in my daily chem
library activities!!!
Three cheers and more for Gary.*

Kitty Porter

*Happy Birthday List!
What a wonderful resource it has been.*

Wendy Warr

Comments on the "CHMINF-L's 20th Anniversary" are at the [CHMINF-L archives](http://listserv.indiana.edu/archives/chminf-l.html)
(<http://listserv.indiana.edu/archives/chminf-l.html>)

SPONSOR ANNOUNCEMENTS



Accelrys, Inc. announced March 29, 2011 the Accelrys Modeling and Simulation Suite, a pillar of the new Accelrys Enterprise R&D Architecture. As a key element of the company's strategy for optimizing the R&D value chain, the suite offers a unique platform approach to scientific modeling and simulation that reduces costs, enhances productivity and improves outcomes, quality and sustainability in R&D through the automation and expert use of predictive science.

The Accelrys Modeling and Simulation Suite includes [Discovery Studio](#) software, [Materials Studio](#) software, the [Pipeline Pilot](#) Life Science and Materials Modeling and Simulation Collections, as well as the new [QSAR Workbench](#), a packaged solution from Accelrys Professional Services. This suite offers scientific organizations engaged in pharmaceutical, chemical and materials R&D access to the broadest, deepest predictive science capabilities ranging across small molecules, biomolecules, chemicals and materials.

For more information, please follow this [link](#)



New packaged service offering automates and speeds the development, validation and deployment of predictive QSAR models

Accelrys, Inc. announced March 29, 2011 the release of [Accelrys QSAR Workbench](#). Developed in a collaboration between the Accelrys Professional Services team and pharmaceutical company GlaxoSmithKline, the Accelrys QSAR Workbench is a commercially available, web-based solution that automates and accelerates the development, validation and deployment of predictive Quantitative Structure-Activity Relationship (QSAR) models.

As a packaged service offering for Modeling and Simulation within the Accelrys Enterprise R&D Architecture, the QSAR Workbench supports better, faster outcomes and reduced costs through the automation and expert use of predictive science. Built on the [Pipeline Pilot](#) platform, the QSAR Workbench utilizes native QSAR methods and easily integrates with other statistical tools — helping experts and non-experts alike save time, reduce costs, collaborate more effectively and speed research by leveraging robust, predictive models.

For more information, please follow this [link](#)



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

ACS Mobile is Now Available for Android

ACS has unveiled a new Android version of the award-winning ACS Mobile application, which was already available for the iPad, iPhone, and iPod Touch.

ACS Mobile provides scientists with an up-to-the-minute live stream of peer-reviewed research content published across the ACS's portfolio of 39 scholarly research journals, and is augmented by "Latest News" from *Chemical and Engineering News (C&EN)*.

The application enables readers to customize their mobile experience, alerts them to new research results across several scientific disciplines, and enables them to quickly search or browse a comprehensive database of current as well as archival scientific information.

The availability of this new ACS application comes at a time when the use of the Internet on mobile devices, including the adoption of a new wave of electronic tablet devices, is soaring. In preparation for launch of *ACS Mobile*, ACS Publications undertook comprehensive reader surveys and detailed analyses of mobile device usage on the Society's web delivery platform.

ACS Mobile was recognized as both the "Best New eProduct in Physical Sciences and Mathematics," and "Best New eProduct/Innovation in ePublishing." This year's recognition marks the second time that the ACS has received the distinction of a Best New eProduct PROSE award.

In 2008, the Society's dynamic journal and book web delivery system, the ACS Web Editions Platform, garnered top honors for "Best New eProduct/Best Website or Platform." The Professional and Scholarly Publishing Division of the Association of American Publishers annually confers the highly prized PROSE (Professional and Scholarly Excellence) awards for publishing achievements across the sciences, medicine and humanities.

To learn more about the ACS Mobile application or download it, go to <http://www.acsmobile.org>



reaxys®

ReactionFlash iPhone Application

Elsevier announced April 27, 2011 the launch of ReactionFlash, a new iPhone app to help in learning and understanding named reactions.

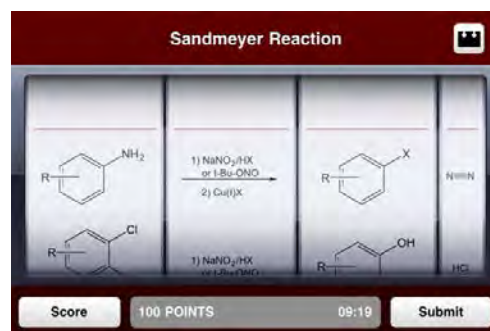
Named reactions – usually named after their discoverers – are a fundamental part of every chemist's toolkit. Not only does the app give you the reaction, it also shows you the known mechanism, recent literature examples from Reaxys, and even allows you to test your skills with the ReactionFlash quiz. No more chemistry flash cards to learn from, ReactionFlash is the app that every chemist should have!

With ReactionFlash you can:

- Learn Named Reactions
- Explore their mechanisms
- Review concrete examples from Reaxys
- Test your knowledge

To download the app please click [here](#)

For further details please see <http://www.reaxys.com/info/reactionflash>



RSC Publishing Celebrations in Anaheim

Journal celebrations, product demos and workshops, plus lots of prizes were given away at the Royal Society of Chemistry (RSC) Publishing booth at the ACS Spring 2011 National Meeting in Anaheim.

Monday saw the announcement of the latest new journal [RSC Advances](#) and Managing Editor Sarah Ruthven and other staff on RSC Publishing were on hand to talk to the many interested researchers.

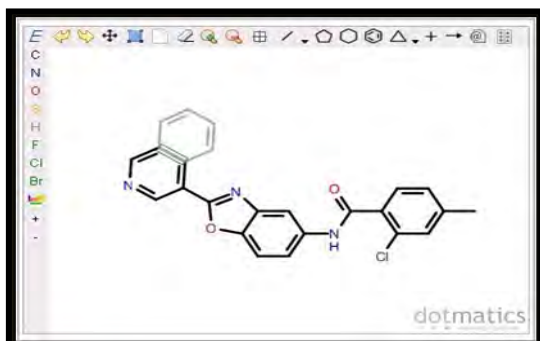
The [reception](#) on Tuesday saw guests toasting the successful launch of [Catalysis Science & Technology](#).

[ChemSpider](#) demonstrations and workshops proved popular, and the [bookshop](#) attracted great interest.

Dotmatics Limited Collaborates with RSC ChemSpider

Dotmatics Limited announced April 14, 2011 that it will provide its web-based structure drawing tool, Elemental, to [ChemSpider](#). Elemental provides a zero install drawing tool that lets users draw simple chemical structures or complex structure queries directly within a webpage.

Antony Williams, Vice President of Strategic Development for *ChemSpider*, comments -

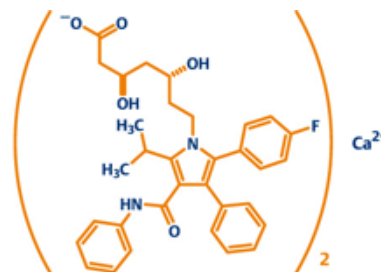


“Elemental offers ease of deployment and flexibility in structure drawing to our community of users and we are happy to embrace this web-based structure drawing platform as an entry point to the rich resources of ChemSpider.”

For more information, please follow this [link](#)

 **Thieme Chemistry** Free trials to Pharmaceutical Substances

Thieme is pleased to offer institutional trials for Pharmaceutical Substances – a one-stop source of information relating to the **industrial synthesis and commercial applications of every licensed drug** of significance. The structure-searchable resource is an ideal tool for researchers, process chemists and for teaching in the field of medicinal and pharmaceutical chemistry.



Pharmaceutical Substances -

Essential for lecturers in the field of medicinal and pharmaceutical chemistry:

- Capability to search for **marketed drugs** relating to a structure or reaction
- A rapid overview of a **therapeutic area** or **chemically related substances**
- Industrial **synthetic routes** discerned from complex patent descriptions
- Insights into **industrial processes** and toxicity issues
- **Commercial information** such as trade names and vendors/manufacturers for six world markets
- **Concise records** ideal for hand-outs and quick reference

Essential for research and process chemists:

- **Full synthetic route for the industrial manufacture of each drug** elucidated from the patent literature
- Unique source of **reactions that perform on an industrial scale**
- **Overview of the pharmaceutical industry** from a synthetic chemist's perspective
- Insights into a **therapeutic area and chemically related substances**

Essential for product managers:

- **Patent information** including approval date and expiration
- First determination of the **market size & competition** for an API - essential for development of new and generic pharmaceuticals
- Source of **markets for synthesis intermediates**
- Comprehensive coverage of **older APIs** and substances approved **worldwide**
- **Merger and acquisition tracking** ensuring that vendor information is up-to-date in a rapidly changing industry

To set up a trial and for further information please contact:

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