

Chemical Information Bulletin
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Svetlana Korolev, Editor
University of Wisconsin, Milwaukee
skorolev@uwm.edu

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MESSAGE FROM THE CHAIR

Dear Colleagues -- I hope everyone made it home safely from the drenching Boston meeting. The deluge did not stop us, however, from having a very productive and enjoyable conference. It was terrific to catch up with so many old friends and meet so many new colleagues as well.

In this issue you will find a summary of our activities in Boston. I will just highlight a few items here: As usual we had several excellent networking receptions, thanks to our generous sponsors. For the first time we cosponsored the Sunday reception with the COMP division. This led to a lively and jam-packed event, as we celebrated the 50th anniversary of the *Journal of Chemical Information and Modeling*. The joint event was so successful we are going to try to do this regularly.

We also extended several awards throughout the week. On Sunday we honored Svetla Baykoucheva with the Val Metanomski Meritorious Service Award for her dedication and the constructive energy she has devoted as our bulletin editor. Over the Tuesday luncheon we gave out the Best Presentation Award to Susan Roberts of Vertex for her informative talk “*Integrating chemical and biological data: Insights from 10 years of VERDI*” during the Data-intensive Drug Design session. We also awarded the Lucille M. Wert Student Scholarship to Yuening Zhang of Indiana University. Later that Tuesday I had the honor of presenting the 2010 Herman Skolnik Award to Tony Hopfinger for his contributions to the QSAR field. Tony and Emilio Esposito co-organized the day-long symposium, “*The Marriage, or at Least Dating, of Molecular Simulation and Modeling with QSAR Analysis.*”

The Saturday Division business meetings were very productive. A significant amount of time was allotted to aspects of Division communications, from the website redesign, to managing division business, to engaging more participation in initiatives like the CINFlash sessions. We were fortunate to have Christine Schmidt and Mark O’Brien (ACS) join us for the morning, giving us an in-depth overview of the ACS Network followed by extensive Q&A. We have a tremendous amount of work ahead of us as we put in place a new communications strategy, and the good news is that the ACS network, with its ability to set up private and public areas, will allow us a framework through which we can communicate with the entire membership interactively, and manage committee activities all in one place. So once again I encourage all of our members to join the ACS network and the CINF Group so you can stay connected.

Speaking of CINFlash, I have some terrific late breaking news: we just received a \$7,500 ACS innovation grant to expand the CINFlash concept, encouraging more virtual exchange of information and ideas through live blogging and tweeting, through the ACS Network, and via remote access that will engage participants not just for the session, but for days and weeks after the event itself is over.

Thanks again to all of you for your support during my year as CINF Chair. Greg Banik will be up next as Chair, with Rajarshi Guha moving to his new role as Chair Elect. All the best for the rest of 2010.

Carmen Nitsche, Chair, ACS Chemical Information Division

LETTER FROM THE EDITOR

This is the second issue of *e-CIB* since its transition from the former *CINF E-News* in 2010, as well as the second issue under my editorship. Traditionally, *CINF E-News* has contained reports from ACS national meetings. With this issue I wished for the expanding of the technical program coverage by featuring three CINF notable symposiums from the 2010 Fall ACS National Meeting. I was honored to receive generous contributions from all the authors whom I had contacted. The readers can now be engaged with captivating reports written by Wendy Warr of the *50th Anniversary Symposium of the Journal of Chemical Information and Modeling*, Emilio Exposito of the *2010 Herman Skolnik Award Symposium* honoring Anton Hopfinger, and Leah Solla of *Assessing Collections and Information Resources in Science and Technology*, a joint effort between two societies.



In addition to three symposium highlights, the technical program section has my first interview with Rajarshi Guha, CINF Program Chair 2009-2010. The interviews conducted by Svetla Baykoucheva, CIB Editor 2005-2010, have become such an integral and welcome addition to *Chemical Information Bulletin*, so that I hope to continue a tradition of including interviews in *e-CIB*. With Svetla's consent for this interview I have asked Rajarshi about his experience of the division programming. Readers will find Rajarshi's reflections continue a sequence of behind the stage perspectives of the former CINF Program Chair Leah Solla available at the [CINF website](#).

The technical section concludes with news from the *ACS Multidisciplinary Programming Planning Group* chaired by Guenter Grethe. Our Division is blessed to have such an active member as Guenter. Among his numerous endeavors is overseeing of the *CINF Scholarship for Scientific Excellence* since its establishment in 2005. The Division received a record number of student poster presentations this year. Three scholarship winners from the Boston meeting are featured in this issue. You can find a few audio and slide presentations from three CINF symposiums: *Data Intensive Drug Design* (6 audio: 2 with slides), *The Journal of Chemical Information and Modeling 50th Anniversary Symposium* (7 audio: 6 with slides), *The Emerging Concepts of Activity Landscapes and Activity Cliffs and Their Role in Drug Research* (2 audio: 1 with slides) in the [ACS Fall Meeting recorded content](#). Twenty four slide presentations will be posted at the [CINF website](#).

In conclusion, I would like to thank all who submitted materials for this issue. It contains an announcement of the 2011 recipient of the prestigious Herman Skolnik Award, two new entries on ACS Network and Committee on Chemical Abstracts Service, and many more highlights of the Fall 2010 ACS National Meeting. My thanks especially to Gregory Banik, Bonnie Lawlor and Wendy Warr for taking photos at the meeting (which are posted at [flickr](#) and used throughout the bulletin), to Mark Luchetti for cover design, and to Bonnie Lawlor and Wendy Warr for proofreading this issue. Dave Martinsen will be a "guest" editor of the next *e-CIB* before the 2011 Spring ACS National Meeting in Anaheim, and then I will do a post conference issue. We would be pleased to hear from Division members with any thoughts you may have for future content.

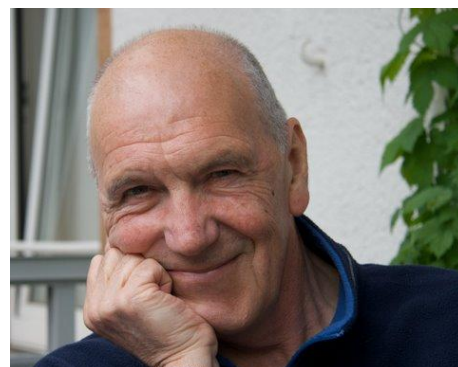
Svetlana Korolev, Editor, Chemical Information Bulletin

AWARDS AND SCHOLARSHIPS

2011 HERMAN SKOLNIK AWARD ANNOUNCED

Professor Dr. **Alexander (Sandy) Lawson** is the recipient of the 2011 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 winner will also be invited to present an award symposium at the Fall 2011 ACS Meeting.



Sandy Lawson is recognized as a pioneer and far-sighted visionary in the fields of chemical structure handling, database searching, chemical nomenclature, reading machines, and linking text and structural information. He has made numerous innovative contributions, often struggling with the limitations of nascent technology, to develop early prototypes to validate concepts, which sometimes only bore fruit when the technology caught up with his ideas. Sandy has spent a large part of his career associated with "Beilstein", initially working with the *Beilstein Handbook*. As early aids to searching in Beilstein, he developed the Lawson Number and the SANDRA program. He was instrumental in the creation and development of the electronic Beilstein Database, including both the organization, data structure, and indexing, and also the development of the powerful CrossFire search engine and interface, capable of handling millions of molecules, reactions, and properties.

Sandy has a deep and abiding interest in chemical nomenclature and has been active on IUPAC Committees for Publications, Databases, and Structural Representation, including Division VIII Chemical Nomenclature of Organic Structures. His expertise led him and his team to develop the first commercial program for generating systematic names from structures, AUTONOM, and then its counterpart, to generate structures from names. More recently Sandy has been involved in the consolidation of Beilstein, Gmelin, and the Patent Chemistry Database into a unified database with a modern and chemist-friendly interface, Reaxys. In his current role within Reed Elsevier, and in earlier organizations, he pioneered building bridges between the structured world of molecules and reactions in databases and the looser but nonetheless related realm of text in journals, and the early DYMOND Linking project presaged later developments such as Project Prospect from the Royal Society of Chemistry.

Sandy Lawson received a B.Sc. from the University of St. Andrews, and a Ph.D. and D.I.C. from the University of London. He did post-graduate work at the Universities of Kent and Mainz, and was an extramural professor at the latter. He has been awarded the Irvine Medal (1966), Forrester Prize (1966), Gold Medal (1985, for Sandra), EuroCase IT Prizewinner (1997, for CrossFire), and the CSA Trust Mike Lynch Award (2008). He has continued to pursue his love of cheminformatics research and development through a series of organizations, including the Beilstein Institute, Beilstein Informationssysteme GmbH, MDL Information Systems GmbH, Elsevier Information Systems GmbH, and latterly Elsevier Properties SA in Neuchâtel.

Sandy Lawson is among the handful of truly excellent cheminformatics scientists at work today, and is widely and thoroughly respected. He is a gentleman's scientist with a tremendous understanding of chemistry and computers. He embodies the best qualities of cheminformatics and is truly worthy of this award.

Phil McHale, Chair, CINF Awards Committee

2010 CINF BEST PRESENTATION AWARD ANNOUNCED



At the 240th ACS National Meeting in Boston, the Division of Chemical Information (CINF) announced the winner of the CINF Best Presentation Award. The Award symposium selected was *Data Intensive Drug Discovery* organized by John van Drie, and held on Sunday, August 22. All the papers were very good, and the judges' choice of winner was **Susan Roberts** of Vertex, who spoke on *Integrating chemical and biological data: Insights from 10 years of VERDI*. This is the central hub for all chemical and biological data in Vertex, and has been providing search, view and analysis tools to Vertex scientists since 2001. It is now being retired and was replaced by a new next generation application, ASAP, in January 2010. Susan was presented with a plaque and a check for \$1,000 at the CINF Luncheon on Tuesday, August 24th.

The CINF Best Presentation Award was instituted in 2009 and is the result of an ACS Innovation Grant awarded to CINF with the intent of encouraging more speakers, higher quality papers, and larger audiences at CINF sessions at ACS Meetings.

Phil McHale, Chair, CINF Awards Committee

2010 LUCILLE M. WERT STUDENT SCHOLARSHIP PRESENTED



The 2010 Lucille M. Wert Scholarship was presented to **Yuening Zhang** of Indiana University at the CINF Luncheon on Tuesday, August 24th. The Scholarship administered by the ACS Division of Chemical Information consists of a check for \$1,500 and a certificate.

An announcement about Yuening Zhang being the recipient of the 2010 Lucille M. Wert Scholarship was made in the Summer 2010 issue of the [Chemical Information Bulletin](#).

Phil McHale, Chair, CINF Awards Committee

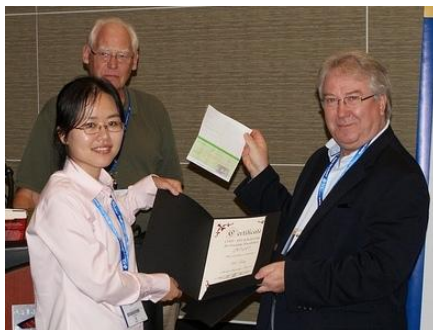
2010 CINF SCHOLARSHIP FOR SCIENTIFIC EXCELLENCE SPONSORED BY FIZ CHEMIE BERLIN ANNOUNCED

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) funded by FIZ CHEMIE Berlin is designed to reward graduate and post-graduate students in chemical information and related sciences for scientific excellence and to foster their involvement in CINF.

Applicants showed their posters at the CINF Welcoming Reception and the Sci-Mix session of the 2010 Fall ACS National Meeting in Boston. Three scholarships valued at \$1,000 each were given out at the divisional luncheon at the same meeting. The winners were presented with cash awards and plaques by Dr. René Deplanque, Executive Director of FIZ CHEMIE Berlin. The names of the recipients and the titles of their posters are:

Rima Hajjo, Division of Medicinal Chemistry and Natural Products, School of Pharmacy, University of North Carolina at Chapel Hill, Chapel Hill, NC,

“A Chemocentric Informatics Approach to Drug Discovery: An Application to the Identification and Experimental Validation of Selective Estrogen Receptor Modulators as Serotonin Receptor Subtype 6 Binders and Potential Anti-Alzheimer’s Agents”. Co-authors: Simon Wang, Bryan Roth and Alexander Tropsha.



Hao Tang, Department of Biochemistry and Biophysics, School of Medicine and Division of Medicinal Chemistry and Natural Products, School of Pharmacy, University of North Carolina at Chapel Hill, Chapel Hill, NC,

“Quantitative Structure Activity Relationship (QSAR) Analysis of US EPA Toxicity Reference Database (ToxRefDB): Toxicity Models help Prioritizing Compounds for Future Toxicity Testing”. Co-authors: Hao Zhu, Liying Zhang, Alexander Sedykh, Ann Richard, Ivan Rusyn, and Alexander Tropsha.

Qian Zhu, School of Informatics and Computing, Indiana University, Bloomington, IN,

“Using aggregative Web Services for drug discovery”.

Co-authors: Michael S. Lajiness and David Wild.



Lajiness accepts the award on behalf of Zhu

Guenter Grethe, Coordinator, CINF Scholarship for Scientific Excellence Coordinator

2012 HERMAN SKOLNIK AWARD: CALL FOR NOMINATIONS

The ACS Division of Chemical Information established this Award to recognize outstanding contributions to and achievements in the theory and practice of chemical information science. The Award is named in honor of the first recipient, Herman Skolnik. By this Award, the Division of Chemical Information is committed to encouraging the continuing preparation, dissemination and advancement of chemical information science and related disciplines through individual and team efforts. Examples of such advancement include, but are not limited to, the following:

- Design of new and unique computerized information systems;
- Preparation and dissemination of chemical information;
- Editorial innovations;
- Design of new indexing, classification, and notation systems;
- Chemical nomenclature;
- Structure-activity relationships;
- Numerical data correlation and evaluation;
- Advancement of knowledge in the field.

The Award consists of a \$3000 honorarium and a plaque. The recipient is expected to give an address at the time of the Award presentation. In recent years, the Award Symposium has been organized by the recipient.

Since its establishment in 1976, the Award has been presented to the following individuals at a national ACS meeting:

Herman Skolnik	1976
Eugene Garfield	1977
Fred A. Tate	1978
William J. Wiswesser	1980
Ben H. Weil	1981
Robert Fugmann	1982
Russell J. Rowlett, Jr.	1983
Montagu Hyams	1984
Dale B. Baker	1986
William Theilheimer	1987
David R. Lide, Jr.	1988
Michael F. Lynch and Stuart A. Marson	1989
Ernst Meyer	1990
W. Todd Wipke	1991
Jacques-Émile Dubois	1992
Peter Willett	1993
Alexandru T. Balaban	1994
Clemens Jochum and Reiner Luckenbach	1995
Milan Randić	1996
Johann Gasteiger	1997
Gary Wiggins	1998
Stuart Kaback	1999
Stephen Heller and Bill Milne	2000
Guenter Grethe	2001
Peter Norton	2002
Frank H. Allen	2003
A. Peter Johnson	2004
Lorrin Garson	2005

Hugo Kubinyi	2006
Robert S. Pearlman	2007
Gerry Maggiora	2008
Yvonne C. Martin	2009
Anton J. Hopfinger	2010

Nominations for the Herman Skolnik Award should describe the nominee's contributions to the field of chemical information and should include supportive materials such as a biographical sketch and a list of publications and presentations. Three seconding letters are also required. Nominations and supporting material should be sent by e-mail to Phil McHale at philmchale@comcast.net. Paper submissions are no longer acceptable.

The deadline for nominations for the 2012 Herman Skolnik Award is June 1, 2011.

Phil McHale, Chair, CINF Awards Committee

2011 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 preferred.

The deadline to apply for the 2011 Lucille M. Wert Scholarship is **February 1, 2011**. Details on the application procedures can be found at: <http://www.acscinf.org> and once there click on "Awards" and then click on "Lucille M. Wert Student Scholarship."

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

Marge Matthews, Coordinator, Lucille M. Wert Scholarship

CINF SCHOLARSHIP FOR CINF SCIENTIFIC EXCELLENCE SPONSORED BY ACCELRY'S : CALL FOR APPLICATIONS

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) funded by Accelrys is designed to reward graduate and postdoctoral students in chemical information and related sciences for scientific excellence and to foster their involvement in CINF.

Up to two scholarships valued at \$1,000 each will be presented at the 241st ACS National Meeting in Anaheim, CA, March 27 – 31, 2011. Applicants must be enrolled at a certified college or university, and they will present a poster during the Welcoming Reception of the Division on Sunday evening at the National Meeting. Additionally, they will have the option to also show their poster at the Sci-Mix session on Monday night. Abstracts for the poster must be submitted electronically through PACS, the abstract submission system of ACS.

To apply, please inform the Chair of the selection committee, Guenter Grethe, at ggrethe@comcast.net, that you are applying for a scholarship. Submit your abstract at <http://abstracts.acs.org> using your ACS ID. If you do not have an ACS ID, follow the registration instructions and submit your abstract for "CINF Scholarship for Scientific Excellence." PACS will be open for abstract submissions on August 3, 2010, and will close on October 18, 2010. Additionally, please send a 2,000-word abstract describing the work to be presented in electronic form to the Chair of the selection committee by January 31, 2011. Any questions related to applying for one of the scholarships should be directed to the same e-mail address.

Winners will be chosen based on the content, presentation, and relevance of the poster and they will be announced during the reception. The content will reflect upon the student's work and describe research in the field of cheminformatics and related sciences. Winning posters will be marked "Winner of Accelrys-CINF Scholarship for Scientific Excellence" at the poster session.

Guenter Grethe, Coordinator, CINF Scholarship for Scientific Excellence

APPLICATIONS INVITED FOR CSA TRUST JACQUES-ÉMILE DUBOIS GRANT FOR 2011

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 2011.

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 four thousand U.S. dollars (\$4,000). 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, 2011. Successful applicants will be notified no later than May 2, 2011.

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 REFLECTIONS: AN INTERVIEW WITH RAJARSHI GUHA

Dr. Rajarshi Guha is currently a research scientist at the NIH Chemical Genomics Center in Rockville, MD and is an Adjunct Professor of Informatics at Indiana University. He works on cheminformatics and bioinformatics topics related to high throughput screening for small molecules and RNAi. He also has active interests in novel data exchange and data analysis paradigms ranging from the use of Google services to large-scale parallel processing for chemical data.

Dr. Guha has been a member of the ACS and CINF since 2003 with an outstanding service as the CINF Division Program Chair during 2009-2010.



Svetlana Korolev: Rajarshi, the Fall 2010 ACS National Meeting was the last meeting for you as the CINF Program Chair, could you share highlights of the CINF technical program in Boston?

Rajarshi Guha: The Fall 2010 meeting had a pretty extensive program covering topics ranging from big data to the applications of RDF and the semantic web in chemistry. At this meeting we also co-hosted the JCIM 50th anniversary symposium with COMP. Sunday started off with the first session of the RDF symposium, highlighting tools and methods to handle this type of data along with a session on the assessment of collections and information resources. In the afternoon, we had the Best Presentation Award symposium – this time it was the Data Intensive Drug Discovery symposium run by Dr. John Van Drie. This was a great symposium, with a variety of very stimulating talks, all addressing how the data deluge is affecting the drug discovery workflow. Monday saw the JCIM symposium, with talks from luminaries of cheminformatics describing their research over the years. In parallel, we had the RDF symposium continue with various applications of RDF in chemistry. The afternoon session saw a symposium on consumer health information and the impact of social networking services. Monday also saw the first version of CINFlash – the lightning talks session. As an experiment it ran pretty well and we got a lot of excellent feedback on improving it in the future. On Tuesday, we had the Herman Skolnik Award symposium, organized by Tony Hopfinger & Emilio Esposito, who put together a great set of talks. Wednesday saw two excellent symposia – one on structure activity landscapes and one on chemical structure representations. My only complaint was that I couldn't attend both simultaneously. Thursday ended with a good selection of General Papers, covering modeling, prediction, and characterization and integration of chemical information.

We also had a number of novel technological features at this meeting. It turned out that a speaker with three talks in the program was unable to make it to the USA – rather than having a program with three holes, we decided to connect to the speaker via Skype. I switched through his slides and we were able to get crystal clear audio and video of the remote speaker (thanks to great wireless at the convention center). These remote talks went very well, and while I wouldn't want future speakers to get ideas, Skype is a very nice backup for emergencies.

This was also the first meeting I got involved with Twitter. We had three or four people at the CINF symposia tweeting from the sessions that they were attending. While I've only recently joined the Twitter bandwagon, I was pleasantly surprised to see that it was quite useful to keep track of parallel sessions. As part of the fun, I also put together a real-time aggregator to get a summary of all the messages emanating from the ACS meeting (<http://rguha.net/atv/atv.html>) - as you can see CINF was pretty prolific.

SK: Would you assess the last meeting as the most successful program during your tenure?

RG: The last meeting was quite successful – we had a good set of symposia including a new experimental symposium and I'm happy that I was able to end on a high note. But I think I'd consider the Spring 2010 meeting as my most successful one. While the Program Chair can't really control how many papers get submitted, I was very pleased to see 140 papers submitted for that meeting (the highest since 2004, I think). Obviously, the venue being San Francisco helped! But beyond that we had an excellent selection of symposia including a great one on materials informatics – that one was a gratifying example of recognizing a subfield via submissions to General Papers and translating that to a fully fledged symposium, which from the varied feedback I've had, will be run in various incarnations in the future. The visualization symposium was one that I was very pleased to see run – the topic being close to my heart. I think one of the most memorable features was that these two symposia were run by newcomers to the Division and they did a fantastic job. From what I understand, they will continue to contribute to CINF programming in various ways in the future. The Spring 2010 meeting was also pretty hectic since we had 21 sessions running – resulting in triple tracking. Another nice aspect was the large size of General Papers – 24 papers. Over the last two years I've seen a general upward trend in the size of General Papers, which is encouraging as it indicates an increasing interest in the Division and also serves as a source of future programming topics.

SK: Do you think that you have gained maturity in handling of the Division technical program over the past two years?

RG: I think one of the main things that occurred over these two years is that I have developed a higher level view of CINF programming in terms of topics that are relevant to the Division. This has been helpful, especially with the thematic programming initiatives from the ACS, as it lets us match our programming to proposed themes (as far as possible). In addition, while topics such as "Chemical Structure Representation" may be regarded as old hat, having an overview of CINF programming over the years allows us to rerun these topics, but addressing the latest issues. Getting feedback from members about whether certain topics have been addressed or whether a symposium didn't work too well has been useful in terms of future programming. Obviously, this type of feedback takes some time to work itself into the program, so it's manifested itself towards the end of my tenure. Finally, having a high level view of programming is very useful in exploring new topics and areas that may not have been traditionally considered in the Division, but are become more and more relevant in our field. Of course, having two years of experience certainly helps when organizers need to make last minute changes or PACS is not being co-operative – no panic attacks!

SK: Have your expectations of the Program Committee Chair position proved to be true to the experience? Where there any aspects unforeseen? Would you agree that the Program Committee

Chair is the most prestigious and challenging position in the CINF Division? What have you learned from this experience?

RG: I'm very thankful that Leah Solla provided a brain-dump when I started! She was very thorough in bringing me up to speed. And given that she was always very responsive to my questions, I must say that I didn't hit too many unexpected things. Probably the most unexpected thing is the degree of socializing that I have done to solicit program topics and organizers. Not being a very social person, this was initially a little tricky – but over time it became easier. I think the effort paid off as I was able to bring in a number of people into contributing to CINF programming.

Probably someone other than the ex-Program Chair should comment on the prestige of the position – I'm biased! The role is certainly one of the central roles in the Division. At the same time, without the help of the Fundraising Chair and the Program Committee, I would not have been able to put together high quality programs. But I will admit that it is one of the more challenging and certainly one of the most visible positions. In the end, members attend national meetings, in large part, for the technical programming. While networking is a vital part of any meeting, I think having relevant and interesting symposia provides “hubs” around which people congregate. Given the diversity of the membership, it is certainly challenging to develop a balanced program that addresses a broad variety of interests. Also, being responsible for scheduling of sessions does present challenges in keeping people happy – nobody likes to be scheduled on Thursday!

I've learned a number of things from this experience – time management probably being a major one. As developing the program is done on nights and weekends, I've had to be quite efficient to make sure everything stays on track. I've also gained a much broader view of the field of chemical information. Prior to taking on this role, I was primarily focused on cheminformatics and computational aspects of the field. Over the last two years I've gained a deeper appreciation for the information science side of things – coupled with my involvement in Open Source, Data & Access, I think I have gotten a much better idea of the interrelated issues that are currently of interest in the field.

SK: Please talk about initiatives that you have implemented during your tenure, e.g., a call for new speakers, CINFlash. What were the driving forces for these innovations? How have they worked out?

RG: When taking over as Program Chair, one of my concerns was how to expand a range of programming topics and get more people involved with CINF. While we have a pretty large collection of topics that we can run from time to time, as well as a Program Committee with a diverse range of expertise, I thought that crowd-sourcing topics would be useful. With this in mind, I put out a “Call for Symposia” on various mailing lists, to solicit symposium topics (and organizers). That first call went out in April, 2009 and we got a decent response – 4 proposals. Due to the fact that we prepare programs in advance, we could not fit in all the proposals we got. However, we did manage to incorporate two proposed symposia into the subsequent programs. More importantly, a number of people were encouraged to contribute to CINF programming and though they could not organize a symposium in 2009, they have shown interest in working on later meetings, and I believe that they will be organizing in 2011 and 2012.

My other effort was CINFlash, a lightning talk symposium that we ran for the first time in Fall, 2010. The idea of short (6 to 8 minutes) talks had been floated in the past by Dave Martinsen, and though I had heard that it might be difficult to run it during an ACS meeting, we decided to try. I had seen videos of Ignite talks – 5 minutes, 20 slides on auto - and they seemed like a lot of fun. Another motivation for this was that submissions for ACS meetings must be decided 6 months before the meeting; so either the material is a year old or else the author expects (hopes!) to get the results described in the abstract by the time the meeting comes around. One of the key features of CINFlash was that we would not go via PACS. Instead we accepted short (less than 100 words) abstracts from mid - June until two weeks before the meeting, on pretty much any topic in chemical information and cheminformatics. Given that we were considering 6 to 8 minute talks, we weren't looking for scientifically heavy talks. Rather, we wanted people to have some fun. Rob McFarland, Roger Schenck and I reviewed abstracts received via Gmail. In the end we had 5 people willing to go along with our experiment, which I think worked out relatively well. I must admit that some of the speakers were impressively creative in their use of 8 minutes! The audience was pretty unanimous that we run the session in the future. The session had a lively audience discussion at the end where we exchanged ideas on how this type of symposium could be improved and I think we got a lot of excellent suggestions. One of the main issues with the symposium was that it wasn't publicized very well. So expect to see revamped version of CINFlash next fall in Denver.

SK: Rajarshi, as Program Chair have you been getting any data about CINF programming from ACS? Could you share with us what sorts of data those are and if they provide any curious facts?

RG: Laura Mehlon was kind enough to provide me with a dump of the abstract data from the 220th National meeting (Fall, 2000) till the 238th National meeting (Fall, 2009). The data includes presentation dates, abstract titles, author titles and affiliations and so on. This is a great resource to examine how the CINF program has changed from meeting to meeting. I won't go into too much detail, but will highlight a few interesting aspects of the data.

To begin with, Figure 1 shows how the number of symposia and the median number of papers per symposium has varied over the years. In general there is a negative correlation between the number of symposia scheduled in a meeting and the median number of papers in any given symposium ($R = -0.69$, $p = 0.0009$). This is an expected result, but suggests that the number of contributions is static overall.

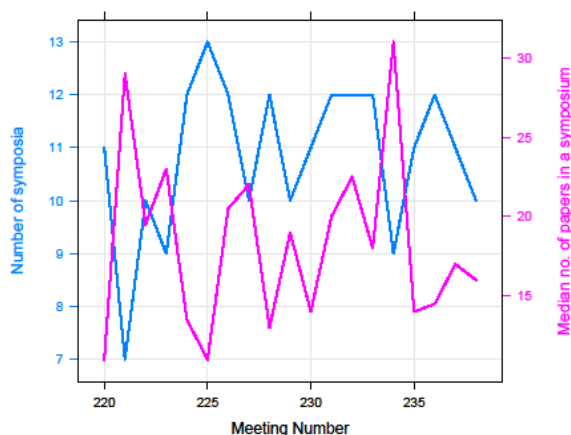


Figure 1. Summary of the number of CINF symposia per meeting and the median number of papers per symposium

If we consider the number of papers per meeting (Figure 2), we see the spikes in the graph corresponding to West Coast locations such as San Diego (229th meeting, Spring 2005) and San Francisco (232nd meeting, Fall 2006). The low value for the 238th national meeting (Fall 2009) is due to incomplete data. I know that the submissions have been increasing since that meeting (but at this time I do not have the data to plot). As I mentioned before we saw the highest number of CINF submissions (140 papers) since 2004 for the Spring 2010 San Francisco meeting.

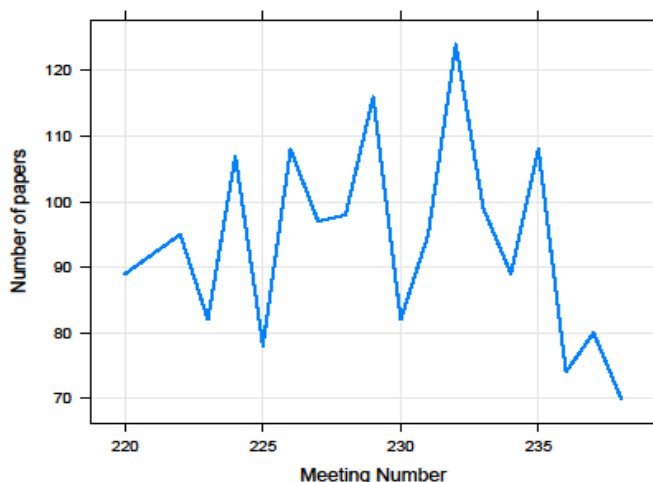


Figure 2. Total number of CINF papers per meeting.

Next we consider some aspects of the authors contributing papers to the CINF program. For instance, if we consider the fraction of authors from industry, government and academia (based on email domains) in a given meeting (Figure 3), we see a cyclical trend for industry and government, but a slight upward trend for academics. Interestingly, the contributors from industry overshadowed academia and government prior to the 225th meeting (Spring 2003). Note that this does not consider the fact that many papers may involve industry, government and academia, but does provide some information on who's contributing to CINF programming.

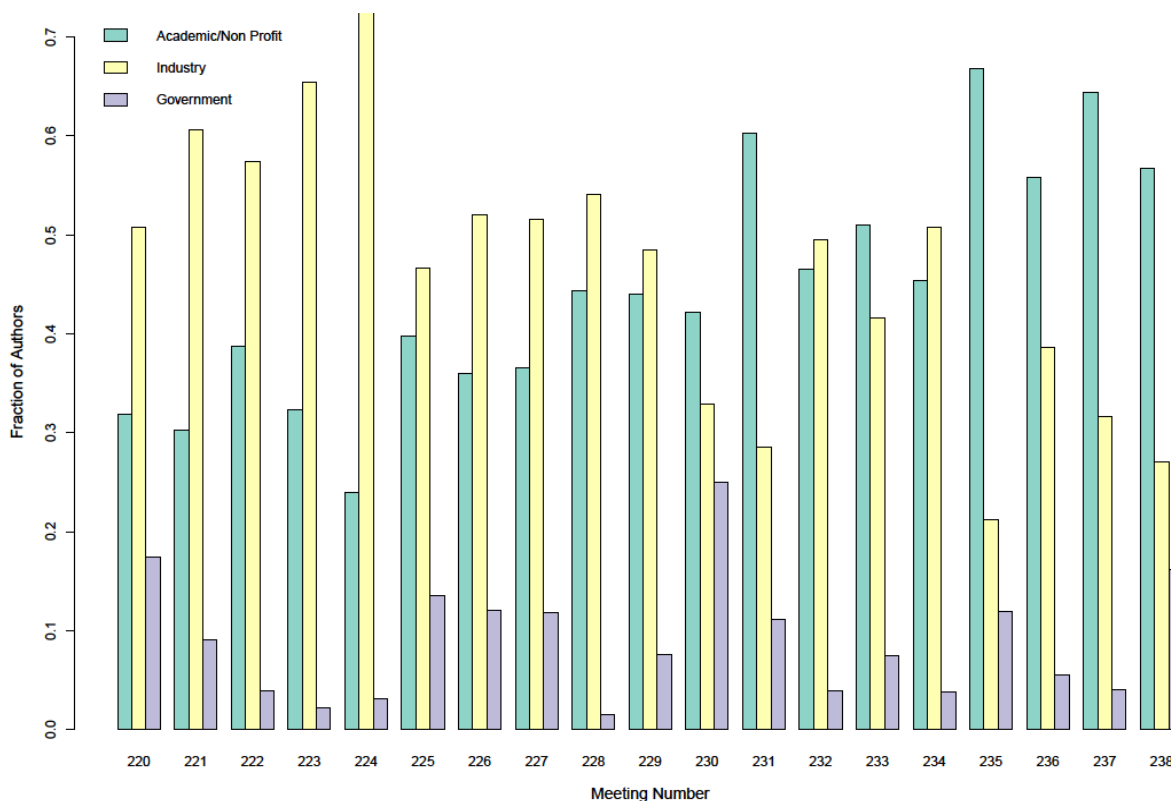


Figure 3. Fraction of authors from industry, academia and government per meeting

Thursday programming (which is usually General Papers) has always been a thorny issue for CINF due to the smaller size of the Division and correspondingly smaller pool of papers, we tend to not have too many papers on Thursdays. This, coupled with the generally low attendance on that day, doesn't make for very interesting sessions. Over the last 3 meetings however, we've seen a steady increase in the number of submissions to General Papers and a lot of interesting content. Unfortunately, for this analysis I don't have access to 2010 data. Thus till the end of 2009, we see a general decline in the number of papers that get allotted to the last day.

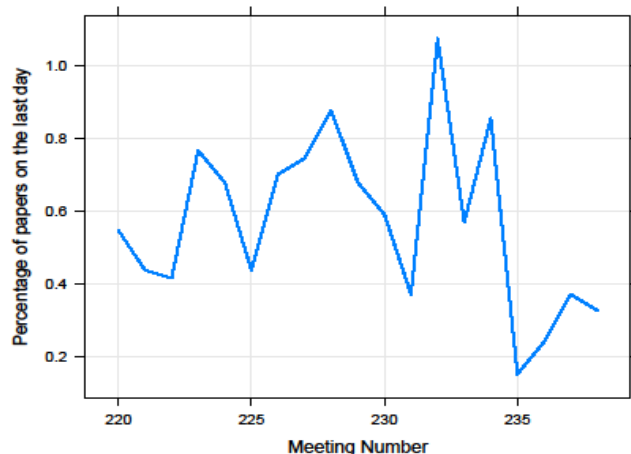


Figure 4. Percentage of papers per meeting that are presented on the last day corresponding to CINF General Papers mostly

It's also interesting to look at who have been the most prolific contributors to the CINF program.

Author	Number of Papers
Michael Woods	39
Marvin Coyner	18
Peter Murray Rust	17
Pierre Baldi	17
Chihae Yang	16
David Wild	15
Ferenc Csizmadia	15
Marc Nicklaus	15
Henry Rzepa	14
Valerie Gillet	14

This is not a completely rigorous analysis (readers of this article are surely familiar with the problem of name disambiguation!). The table alongside lists the top 10 authors based on how many times their name appeared in the CINF program abstracts 2000 - 2009.



Spring 2011 National Meeting & Exposition
March 27-31, 2011
Anaheim, California, USA

friendly. Examples include “Chemistry for Life” and “Chemistry for Health and Disease.” Given the many links between CINF topics and members with the pharmaceutical industry, these two themes are quite easy to satisfy. But it’s important to note that CINF programming is not explicitly constructed to match a theme. Our first priority is to create a program that is of interest to our membership and the community. The theme of a meeting certainly informs that process, and if we can connect multiple symposia to the theme all the better. Given the multidisciplinary nature of CINF, this is probably an easier job than for other divisions as we can connect to themes from various directions (information sources, legal issues, informatics approaches, modeling and so on).

SK: Would you like to comment on the new ACS abstract submission system (PACS)?

RG: Prior to 2009, the OASYS system was used to submit and organize abstracts. While a bit clunky, it was a known system and preparing the program was relatively straight forward. For various reasons ACS shifted to the new abstract submission system called PACS. Given that it’s a new system, there is a learning curve for people who are used to OASYS. But I will admit that it has been a painful experience – it was (at least until the Boston meeting) an unpolished system, that was released to users (program chairs, symposium organizers, etc.) in an untested form. However, to their credit, ACS held open meetings to listen to complaints and issues regarding the system. Major bugs have been fixed in time for the Anaheim and subsequent meetings, so I guess we’ll have to see how it turns out. I will note that there is a PACS Advisory Board, of which I am a member and have been providing input with respect to usability issues, training of users, and so on. I do think that as ACS and the vendor fix the bugs, it could be a very powerful system for management, reporting and in general keeping track of programming - related data. The ability to directly access programming data from the ACS database would be especially powerful for determining long term impact of programming decisions and policies.

SK: Who is going to be your successor as the CINF Program Chair? Could you give us a sneak preview of the CINF technical program planned for the 2011 National meetings?

RG: Dr. Rachelle Bienstock from the National Institute of Environmental Health Sciences will be the next CINF Program Chair. She has been an active member of the Program Committee for the past three meetings and has also organized symposia in CINF. In other words, she knows about the magic that we do to put together a program! She’s provided great input on various aspects of our program and has a number of interesting program topics lined up for future meetings.



As for upcoming programming, I won’t go into too much detail, as Rachelle will be providing highlights of upcoming programming separately. Anaheim (Spring 2011) will see symposia on open data, combinatorial chemistry, and reaction modeling, as well as symposia relating to natural resources. Denver (Fall 2011) will include symposia ranging from the state of openness in science to high content screen analysis. As you can see, we’re maintaining the CINF tradition of topical diversity.

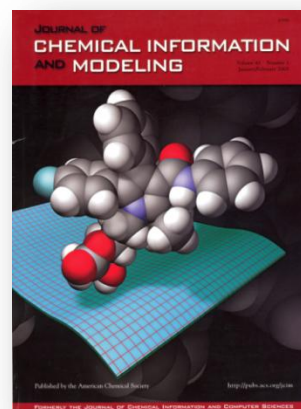
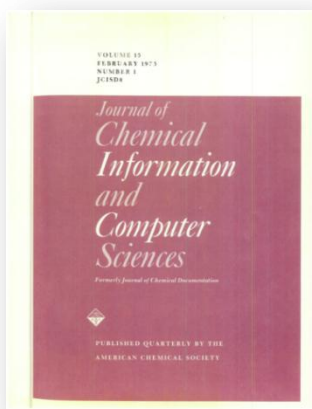
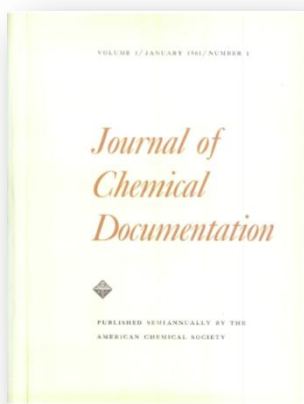
SK: Thank you, Rajarshi, for sharing with us your experience and insights of the CINF Program Committee Chair. Please accept my sincere congratulations on your moving up to the Division Chair-Elect position in 2011!

50th Anniversary JOURNAL OF
**CHEMICAL INFORMATION
AND MODELING**

SYMPOSIUM, ACS National Meeting, Boston, August 23, 2010

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The first issue of the *Journal of Chemical Documentation* appeared in 1960. The name of the journal changed to the *Journal of Chemical Information and Computer Sciences* (“*JCICS*”) in 1975 and to the *Journal of Chemical Information and Modeling* (“*JCIM*”) in 2005.



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This year, 2010, is thus the 50th anniversary of the journal. The anniversary was marked by a symposium shared between CINF and COMP Divisions at the fall 2010 ACS National Meeting and was celebrated by an excellent reception sponsored by ACS Publications, where we all enjoyed useful networking and renewal of old acquaintances (<http://pubs.acs.org/page/jcisid8/anniversary/50/index.html>).

Over the fifty years of the journal there have been only four main editors (<http://pubs.acs.org/page/jcisid8/anniversary/50/editors.html>). Herman Skolnik (whose name is honored by the CINF Award) was the editor from 1960 to 1982. Tom Isenhour served as editor from 1982-1989, and he was succeeded by Bill Milne (1989-2004). Associate Editors were appointed in 1989: Pierre Buffet (1989-1997), Reiner Luckenbach (1989-1999), Kenny Lipkowitz (1993-2005), Tony Hopfinger (since 1993), Dušanka Janežič (since 2001) and myself (since 1989). Bill Jorgensen has been editor-in-chief of *JCIM* since 2005. He also edits *JCIM*'s very successful, new sister journal, the *Journal of Chemical Theory and Computation* (“*JCTC*”).

The first speaker at the 50th anniversary symposium was Johnny Gasteiger, whose first paper appeared in *JCICS* in 1977. Volume 46, issue 6 of *JCIM* in 2006 was his sixty-fifth birthday present: an issue in his honor. Johnny related how his early publication on the separation of π and σ systems

(Gasteiger, G. A Representation of π Systems for Efficient Computer Manipulation. *J. Chem. Inf. Comput. Sci.* **1979**, *19*, 111–115) had devolved into a system, RAMSES, overcoming the limits of the connection table (Bauerschmidt, S.; Gasteiger, J. Overcoming the Limitations of a Connection Table Description: a Universal Representation of Chemical Species. *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 705–714). The Molecular Structure Encoding system (MOSES) is a C++ toolkit based on RAMSES. Johnny also outlined his work on reactions, the most current system being THERESA; the calculation of structure descriptors (now available in ADRIANA.Code); 3D structure generation (CORINA); artificial neural networks; and biochemical pathways (BioPath). The research efforts of Johnny's team over the years have led to range of products now marketed (under the aforementioned names) by Molecular Networks (<http://www.molecular-networks.com/>).

Bill Milne's talk also had a historical perspective. He started by outlining the history of the journal (some of which I have given above), but his main theme was those cheminformatics problems that have been solved and those that are proving intractable. Structure drawing, substructure search, and structure codes fall into the first category. Conversion of names into structures (and *vice versa*) and ligand-protein binding are largely solved. Properties estimation is "somewhat solved." Much of the research in these fields has been published in the journal. Protein-protein binding requires much more exploration, and Markush searching is an open problem, according to Bill, but he did not have time to go into detail about the many papers in *JCICS* on the subject.

A unique aspect of cheminformatics is that it has been heavily influenced and shaped by the needs of the pharmaceutical industry. Dimitris Agrafiotis reflected on experiences of the past and explored the possibilities he saw for the industry in the future: possibilities lying in the convergence of chemistry, biology, and information technology. First he talked about the world before and after "ABCD" (Agrafiotis, D. K. *et al.* Advanced Biological and Chemical Discovery (ABCD): Centralizing Discovery Knowledge in an Inherently Decentralized World. *J. Chem. Inf. Model.* **2007**, *47*, 1999–2014). Nowadays there are sophisticated tools for SAR analysis (Agrafiotis, D. K.; Wiener, J. J. M. Scaffold, Explorer: an Interactive Tool for Organizing and Mining Structure-Activity Data Spanning Multiple Chemotypes. *J. Med. Chem.* **2010**, *53*, 5002–5011), but ABCD goes beyond decision support, and also embraces electronic laboratory notebooks and sequence searching, for example.

The system must also go beyond discovery. Mining of electronic medical records involves handling massive amounts of data usually in SAS datasets. An ABCD plugin will address that problem, too. Pharma is an industry in stress. The good times are over; the future will be defined by in-licensing, pre-competitive collaborations, Asian expansion, a surge in biologics, the increasing roles of government and academia, translational research, public data, the open source movement, commoditization of medicinal chemistry and other functions, outsourcing, consolidation of software vendors, tougher problems, and return on investment.

In contrast, Val Gillet described some very recent research not yet submitted to *JCIM* (although early results will appear in *Molecular Informatics*). Her team has been working on applications of wavelets in virtual screening, in particular using GRID fields that model the interactions that a small molecule can make with a receptor. These fields are cumbersome to store and compare, but they can be compressed using wavelet transformation. This is a technique for representing signals by decomposing them into components: smoothed, or approximated components, and details or

differences that can be ignored. Gillet's team has experimented with Harr compression (as used in JPEG) and Haar thumbnails. They have applied wavelet thumbnails (low-resolution approximations of finely sampled GRID fields) without loss of information. Val also demonstrated other applications, including the development of an alignment method to enable the comparison of the wavelet representations of GRID fields in arbitrary orientation.

Jürgen Bajorath's presentation was remarkable in that it was given remotely using Skype, because Jürgen was prevented from traveling at the last minute. This is not the first time that CINF has used this technique (the first was a presentation by Tony Williams in Salt Lake City in 2009), but it still caused some excitement. Rajarshi Guha changed the slides in Boston while Jürgen presented, with video, from Bonn, Germany.

Jürgen described some research on privileged substructures. Many privileged substructures have been proposed, but the existence of truly privileged structural motifs has remained controversial. Many scaffolds thought to be specific to a target class occur in compounds active against other types of targets. Jürgen's team investigated whether molecular scaffolds do exist that exclusively occur in ligands of individual target families. They used Bemis-Murcko scaffolds, carried out systematic data mining of publicly available compound data (BindingDB and PubChem) and defined target communities on the basis of ligand-target networks. The nodes were targets, the edges target pair sets, and the edge width the number of shared compounds. In 18 target communities, 206 diverse hierarchical scaffolds were identified, each represented by at least five compounds, that exclusively bound to targets within one of the target communities. In contrast, most scaffolds that exclusively bind to a single target within a community are only represented by one or two compounds in public domain databases. A subset of community-selective scaffolds displays a notable tendency to produce compounds with different target selectivity. The analysis was extended to ChEMBLdb and it was found that BindingDB and ChEMBLdb contain complementary target and scaffold information.

Peter Johnson spoke next, describing work on automated retrosynthetic analysis carried out by workers in Leeds together with SimBioSys and Pfizer. Many systems for computer aided organic synthesis design were developed in the last century (LHASA, SYNCHEM, IGOR, EROS, WODCA, SynGen, etc.) but none has achieved significant user acceptance, partly because such systems required manual creation of reaction knowledge bases, a time - consuming task that requires considerable synthetic chemistry expertise. ARChem (a program developed by Peter and his co-workers) circumvents this problem by automated abstraction of transformation rules from very large databases of specific examples of reactions (Law, J. *et al.* Route Designer: a Retrosynthetic Analysis Tool Utilizing Automated Retrosynthetic Rule Generation. *J. Chem. Inf. Model.* **2009**, *49*, 593–602).

Mapping reactions and finding the initial reaction core are solved problems; the hard part is extending the core to non-reacting atoms. Identifying the precise structural characteristics of each reaction often requires knowledge of the reaction mechanism. Another challenge is minimizing the combinatorial explosion inherent in automated multistep retrosynthesis. One process involved in that is removing interfering functionality. This can be done using statistics on functional groups derived from reaction databases. Peter's team has been working on optimum constraint of the extended core and reducing, rather than increasing the number of rules derived by ARChem; chemists can be used to generate meta rules for reaction mechanisms. Peter concluded by illustrating some other

improvements to ARChem, such as ordering of search results, which matter to the user, but do not represent great technical advances.

Like many of the speakers, Michael Gilson has been on the editorial advisory board of *JCIM*, but Michael's talk in the anniversary symposium was more related to *JCTC* than to *JCIM*, and indeed the work presented has been published in *JCTC* (Gilson, M. K. Stress Analysis at the Molecular Level: a Forced Cucurbituril-Guest Dissociation Pathway. *J. Chem. Theory Comput.* **2010**, *6*, 637–646). Michael presented molecular dynamics simulations consistent with long-ranged entropy effects throughout a protein upon binding a peptide, and explained why the concept of mechanical stress may be useful in thinking about such effects. His results suggest that computational stress analysis can provide mechanistic insight into supramolecular systems.

Elizabeth Amin also presented the results of some recently published research, this time published in *JCIM* (Chiu, T.-L. *et al.* Identification of Novel Non-Hydroxamate Anthrax Toxin Lethal Factor Inhibitors by Topomeric Searching, Docking and Scoring, and in Vitro Screening. *J. Chem. Inf. Model.*, **2009**, *49*, 2726–2734). The lethal factor (LF) enzyme is secreted by *Bacillus anthracis* as part of the anthrax lethal toxin. To date, no LF inhibitor is available as a therapeutic or preventive agent. Amin's team has identified five promising novel LF inhibitor scaffolds with low micromolar inhibition, using topomeric shape-based searching techniques.

Tudor Oprea addressed the issue of “druglikeness.” He and Oleg Ursu have used extended connectivity descriptors computed by the Morgan algorithm and extracted them as SMARTS queries. In a method rooted in the information gain concept, already applied to derive selection rules in decision trees, they aimed at a better separation between drugs and non-drugs (Ursu, O; Oprea, T. I. Model-Free Drug-Likeness from Fragments. *J. Chem. Inf. Model.* **2010**, *50*, 1387–1394). The most discriminating atom environments (having the highest information gain) were selected as model-free druglike filters.

Tudor concluded, however, that there is a danger in relying indiscriminately on machine learning techniques that artificially separate drugs from non-drugs, especially in regard to the *Available Chemicals Directory* (ACD). This is likely to influence the usefulness of such classifiers negatively, as 40% of the “non-drugs” are similar to drugs. Oprea uses the term “model-free” to emphasize the fact that his method does not use kernel functions and does not force ACD into a negative label, but he admits that any learning process actually relies on models. Ultimately, “druglikeness” is defined by regulatory agencies and cannot be predicted. Oprea defined three difficulties: the drug dataset is small (some people claim that there are 8,000 drugs, but Tudor can find only 3,800); the drug character of molecules changes over time as withdrawn from the market; and drugs have high heterogeneity (from lithium to cyclosporine).

Alex Tropsha talked about “chemocentric informatics,” or enabling bioactive compound discovery through structural hypothesis fusion. The information resources available to us have broadened dramatically, including large chemical genomics databases (e.g., ChEMBL, PubChem, PDSP, ToxCast), digital libraries (e.g., PubMed), gene expression profiles (e.g., cmap), and others. To address some of the limitations of QSAR models, Alex suggests adding cheminformatics to “omics.” He described the use of digital libraries (Baker, N.C.; Hemminger, B. M. Mining connections between chemicals, proteins, and diseases extracted from Medline annotations. *J.*

Biomed. Inform. **2010**, 43(4), 510-519) for establishing new datasets to analyze the relationships between chemical structure and biological activity. Alex' team has transformed assertional metadata into a database for modeling toxicity (Rodgers, A. D. *et al.* Modeling Liver-Related Adverse Effects of Drugs Using kNearest Neighbor Quantitative Structure-Activity Relationship Method. *Chem. Res. Toxicol.* **2010**, 23(4), 724-732).

Data curation, however, is vital (Fourches, D.; Muratov, E.; Tropsha, A. Trust, but Verify: on the Importance of Chemical Structure Curation in Cheminformatics and QSAR Modeling Research *J. Chem. Inf. Model.* **2010**, 50, 1189–1204). Alex illustrated how computational models help in detecting and correcting erroneous data, and he described a study combining QSAR modeling, virtual screening, text mining, and gene expression profiling for identifying novel, experimentally confirmed, high-affinity GPCR ligands as potential anti-Alzheimer drug candidates. He concluded that both chemical and biological data in integrated databases should be carefully curated, that QSAR models have the power of correcting erroneous biological data, and that structural hypothesis fusion and focused experimental validation afford opportunities for drug (re)profiling.

Bobby Glen's talk also covered drug discovery. He first used Zomig to exemplify some of the issues of drug delivery, safety, and efficacy. One is solubility. Both predicting and measuring solubility are difficult problems. Bobby illustrated this fact with literature examples and with some work of his own team using random forest. So, they adopted a reliable, reproducible method to create a "standard" dataset of solubilities. Bobby described the protocol in some detail. This work was so important that they collaborated with *JCIM* to produce a solubility challenge, the results of which were published in Hopfinger, A. J. *et al.* Findings of the Challenge to Predict Aqueous Solubility. *J. Chem. Inf. Model.* **2009**, 49, 1–5.

A second challenge is metabolism. Understanding the pharmacokinetics of drugs is very important. Metabolism can alter activity (for example, from antagonist to agonist), deactivate drugs, convert pro-drugs into active forms, produce toxic compounds, and create environmental toxins. Bobby developed a method (MetaPrint2D, available on the Web) using circular fingerprints to predict the sites and products of metabolism.

Bobby's third topic was new targets. One that interests him is apelin, a GPCR which is a difficult target and has interesting pharmacological effects. The group replaced each of the amino acids by alanine and looked at the changes in the biological activity. They also constructed cyclic peptides and used NMR 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. The group then attempted to make an antagonist by stabilizing the antagonist conformation and they designed linkers to the allosteric binding site. A competitive antagonist is currently being evaluated in disease models.

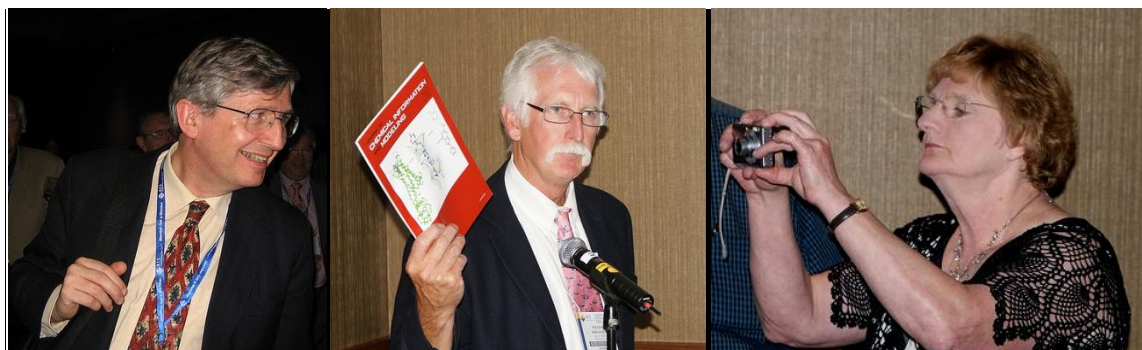
The symposium concluded, appropriately, with a presentation by *JCIM*'s most prolific author Peter Willett (<http://pubs.acs.org/page/jcisd8/anniversary/50/most-prolific.html>). Peter talked about weighting and fusion methods for similarity-based virtual screening. These techniques were used to

search the MDDR and WOMBAT databases. Binary fingerprints work well, but it was hoped that use of fragment frequency information might produce even better results. It is assumed that if two molecules have multiple occurrences of a fragment in common they are more similar than if they have just a single occurrence in common, and if two molecules share a very rare fragment, they are more similar than if they share a very common fragment. Experiments show that the former assumption is correct, but that there is much less evidence for the latter (Arif, S. M.; Holliday, J. D.; Willett, P. Analysis and use of fragment occurrence data in similarity-based virtual screening. *J. Comput.-Aided Mol. Des.* **2009**, *23*, 655-668; Arif, S. M.; Holliday, J. D.; Willett, P. Inverse frequency weighting of fragments for similarity-based virtual screening. *J. Chem. Inf. Model.* **2010**, *50*, 1340–1349).

Experiments in text retrieval show that documents retrieved by multiple search engines are more likely to be relevant to a query than if they are retrieved by a single search engine. To see if this effect also applies in cheminformatics, researchers at Sheffield have carried out extensive virtual screening experiments to investigate whether structures retrieved by multiple virtual screening methods are more likely to be active than if they were retrieved by a single method. Sets of 25 searches for a reference structure were carried out using five different similarity coefficients and five different fingerprints. As the number of searches increases from 1 to 25, there is a rapid decrease in the numbers of molecules retrieved in all of the searches, and a rapid increase in the percentage of those retrieved molecules that are active. This provides an empirical rationale for the use of data fusion, where multiple rankings of a database are combined to give a single, fused ranking. The Sheffield team has experimented with a whole range of different combination rules, some used previously and some novel. Their results show conclusively that one of the new rules, called CombRKP, is by far the most effective in virtual screening, this arising from the rule approximating molecular probabilities of activity (Chen *et al.* Combination rules for group fusion in similarity-based virtual screening. *Molecular Informatics* **2010**, *29*, 533-541).

The symposium presented an interesting mixture of history, philosophy, strategy and up-to-date research. Symposia in honor of people or journals can tend to lean towards nostalgia and self-congratulation, so it was a pleasure on this occasion to hear some recent results as well as the historical perspectives. The number of citations to the journal itself was impressive, even allowing for the fact that the speakers would be biased. *JCIM* is the foremost journal in cheminformatics (Willett, P. A bibliometric analysis of the literature of cheminformatics. *Aslib Proceedings*, **2008**, *60*(1), 4-17), and I hope that it will continue in that role for the next 50 years.

Wendy A. Warr, Associate Editor, *JCIM*



2010 HERMAN SKOLNIK AWARD SYMPOSIUM

The Herman Skolnik Award recognized Anton “Tony” J. Hopfinger’s research and service to the field of cheminformatics and computational chemistry and biochemistry. Tony is perhaps best known as the father of multi-dimensional QSAR, including the 4D-QSAR and Molecular Shape Analysis methodologies. More recently Tony introduced a pseudo structure-based method, Membrane-Interaction (MI) QSAR analysis, to estimate ADME-Tox properties involving membrane transport processes.

The Herman Skolnik Award Symposium honoring Tony Hopfinger at the Boston ACS meeting provided a great overview of how Tony’s work – past and present – is shaping the view of QSAR and molecular modeling into a single concentration of ideas instead of them both evolving as separate fields. The morning session of the Symposium focused on the cheminformatics aspects of combining molecular modeling and simulation to extend and refine molecular descriptors used in the QSAR paradigm.

The first speaker was Emilio Xavier Esposito of exeResearch, LLC. Emilio’s talk focused on physico-chemical features of polyphenols with respect to gaining a better understanding of antioxidants. The dominant physical feature of antioxidants is phenols; polyphenols according to Alton Brown. The proposed antioxidant-tyrosinase mechanism, based on a series of experimentally determined mushroom tyrosinase structures, provides insight to the molecular interactions that drive the reaction. While the enzyme structures illustrate the important molecular interactions for tyrosinase inhibition, the enzyme structures do not always facilitate the understanding of what makes a good inhibitor or the mechanism of the reaction. Binary QSAR models were constructed to indicate the important antioxidant molecular features. Exploring models constructed from molecular descriptors based on fingerprints (MACCS keys), traditional molecular descriptors (2D and 2½D), VolSurf-like molecular descriptors (3D) and molecular dynamics (4D-Fingerprints), the relationship between polyphenols' biologically relevant molecular features - as determined by each set of descriptors - and their antioxidant abilities were discussed.

The next speaker was Jürgen Bajorath of the University of Bonn. Even though Jürgen was ill and not able to travel to Boston, he gave his talk via Skype on the “Engineering and 3D protein-ligand interaction scaling of 2D fingerprints.” In this talk he discussed the refinement and advancement of molecular descriptors for SAR analysis. While fingerprints have long been the preferred descriptors for similarity searching and SAR studies, the standard fingerprints typically have a constant bit string format and are used as individual database search tools. However, by applying “engineering” techniques such as “bit silencing,” fingerprint reduction, and “recombination,” standard fingerprints can be tuned in a compound class-directed manner and converted into size-reduced versions with higher search performance. It is also possible to combine preferred bit segments from fingerprints of distinct design and generate “hybrids” that exceed the search performance of their parental fingerprints. Furthermore, effective 2D fingerprint representations can be generated from strongly interacting parts of ligands in complex crystal structures. These “interacting fragment” fingerprints focus search calculations on pharmacophore elements without the need to encode interactions directly. Moreover, 3D protein-ligand interaction information can implicitly be taken into account in 2D similarity searching through fingerprint scaling techniques that emphasize characteristic bit patterns.

The next speaker of the morning session was Y. Jane Tseng of the National Taiwan University. Jane discussed her group's recent work on the development of *in silico* binary QSAR models for the prediction of a compound's potential to block the human ether-a-go-go related gene (hERG) ion channel. The blockage of the hERG potassium ion channel is a major factor related to cardiotoxicity. Hence, binding to this channel has become an important biological endpoint in side effects screening. A structurally diverse hERG data set of 250 compounds was used to construct a set of two-state hERG QSAR models. The descriptor pool used to construct the models consisted of 4D-fingerprints generated from the thermodynamic distribution of conformer states available to a molecule, 204 traditional 2D descriptors, and 76 3D VolSurf-like descriptors computed using the Molecular Operating Environment (MOE) software. One model is a continuous partial least squares (PLS) QSAR hERG binding model. Another related model is an optimized binary QSAR model that classifies compounds as active or inactive. This binary model achieves 91% accuracy over a large range of molecular diversity spanning the training set. An external test set was constructed from the condensed PubChem bioassay database containing 816 compounds and successfully used to validate the binary model. The binary QSAR model permits a structural interpretation of possible sources for hERG activity. In particular, the presence of a polar negative group at a distance of 6 to 8 Å from a hydrogen bond donor in a compound is predicted to be a quite structure-specific pharmacophore that increases hERG blockage.

Robert D. Clark of Simulations Plus, Inc. in Lancaster, California gave an informative talk that highlighted the challenge of evaluating pharmacophore model performance. He likened the problem to having the ability to tell "the good from the bad and the ugly." Pharmacophore models are useful when they provide qualitative insight into the interactions between ligands and their target macromolecules, and therefore are more akin in many ways to molecular simulations than to quantitative structure activity relationships (QSARs) based on the partition of activity across a set of molecular descriptors. When the performance of a pharmacophore model is assessed quantitatively, it is usually in terms of its ability to recover known ligands or, less often, in terms of how well it distinguishes ligands from non-ligands. This status as a classification technique also sets it apart from more numerical QSAR methods, in part because of fundamental differences in what being "good" means. Carefully defining what "good" classification is, however, can make creative combination with other techniques a productive way to capture the value of their intrinsic complementarity.

The afternoon session moved from the cheminformatics aspects to the molecular modeling and simulation side of the QSAR paradigm. In this session, speakers spoke about how their research efforts are a mixture of molecular modeling and QSAR techniques.

Curt M. Breneman of Rensselaer Polytechnic Institute kicked off the afternoon with an intriguing look at using QSAR approaches to learn from protein crystal structures. In practice, there is no inherent disconnect between the descriptor-based cheminformatics methods commonly used for predicting small molecule properties and those that can be used to understand and predict protein behaviors. Examples of such connections include the development of predictive models of protein/stationary phase binding in HIC and ion-exchange chromatography, protein/ligand binding mode characterization through PROLICSS analysis of crystal structures, and the use of PESD binding site signatures for pose scoring and predicting off-target drug interactions. In all of these cases, models were created using descriptors based on protein electronic and structural features and

modern machine learning methods that include model validation tools and domain of applicability assessment metrics.

William L. Jorgensen of Yale University discussed his research group's success designing novel HIV reverse transcriptase inhibitors. Drug development is being pursued through computer-aided structure-based design. For *de novo* lead generation, the BOMB program builds combinatorial libraries in a protein binding site using a selected core and substituents, and QikProp is applied to filter all designed molecules to ensure that they have drug-like properties. Monte Carlo/free-energy perturbation simulations are then executed to refine the predictions for the best scoring leads including ca. 1000 explicit water molecules and extensive sampling for the protein and ligand. FEP calculations for optimization of substituents on an aromatic ring and for choice of heterocycles are now common. Alternatively, docking with Glide is performed with the large databases of purchasable compounds to provide leads, which are then optimized via the FEP-guided route. Successful application has been achieved for HIV reverse transcriptase, FGFR1 kinase, and macrophage migration inhibitory factor (MIF); micromolar leads have been rapidly advanced to extraordinarily potent inhibitors.

José S. Duca of Novartis provided an overview of the evolution of structure-based drug design (SBDD) and *n*D-QSAR methods while he was doing a postdoc in Tony's lab. José discussed case studies in which QSAR and SBDD have worked in concert during the discovery process of pre-clinical candidates. The importance of incorporating time-dependent sampling to improve the quality of the *n*D-QSAR models ($n=3,4$) was discussed and compared to simplified low dimensional QSAR models.



The Skolnik Award Symposium was concluded with Tony stressing that QSAR analysis and molecular modeling/simulation methods can often be complementary, and when combined in a study yield results greater than the sum of their parts. Modeling and simulation offer the ability to design custom, information-rich trial descriptors for a QSAR analysis. In turn, QSAR analysis is able to discern which of the custom descriptors most fully relate to the behavior of an endpoint of interest. Grid cell occupancy descriptors (GCODs) of 4D-QSAR analysis form one useful set of custom QSAR descriptors from modeling and simulation for describing ligand-receptor interactions. These descriptors characterize the relative spatial occupancy of all the atoms of a molecule over the set of conformations available to the molecule when in a particular environment. GCODs permit the construction of a 4D-QSAR equation for virtual screening, as well as a spatial pharmacophore of the 4D-QSAR equation for exploring mechanistic insight. Applications that can particularly benefit from combining QSAR analysis and modeling/simulation tools are those in which a model chemical system is needed to determine the sought after property. One such application is the transport of molecules through biological compartments, an integral part of many ADMET properties. For example, the reliable estimation and characterization of the diffusion of organic compounds through cellular membranes is greatly enhanced by simulation modeling, and the subsequent extraction of properties from the simulation trajectories as custom descriptors to build a corresponding QSAR-based diffusion model. The key descriptors of the QSAR models, in turn, also permit the investigator to probe and postulate detailed molecular mechanisms of action.

Emilio Exposito, Co-organizer, 2010 Herman Skolnik Award Symposium



**ASSESSING COLLECTIONS & INFORMATION
RESOURCES IN SCIENCE & TECHNOLOGY:
A JOINT EFFORT BY ACS CINF & SLA CHEM**



It is always interesting for chemistry librarians to consider our collections, and we've become skilled at making tough choices over the years as the gap between pricing and budgets has widened. Understanding and leveraging the impact of collections on research is becoming even more critical as scholarly communication trends, information technologies, and librarianship shift as never before. What kinds of measures are available and how can we combine them to inform decisions about budgets and services? Do we need different metrics for different resources - journals, books, databases? How do different stakeholders utilize information about usage? CINF joined forces with the SLA CHEM Division to tackle these questions in a lively symposium in Boston that covered the spectrum from usage of books, journals and databases; user preferences for format, starting place and discovery; to reshaping the functions of libraries in acquiring and using resources. Collection assessment in academic research libraries dominated the discussion, but speakers and audience members included government and corporate attendees whose perspectives indicated that many of the issues are similar, although the paths to solutions may vary.

Assessing journals in the face of cancellation in tight budgets is an age - old, but still elusive challenge to remain as locally relevant as possible. Grace Baysinger (Stanford University) gave an excellent overview of various approaches to looking at journals such as benchmarking. Excellent national data on science and engineering can be had from nsf.gov/statistics, including data on academic article/patent output and statistics showing the relative focus on the physical sciences in the United States and Europe (falling) compared to Asia (rising). Hone local collections to local needs through gap analysis on publication activity and monitoring requests for full text not available through link resolvers.

Luti Salisbury (University of Arkansas) used citation analysis within her institution to consider allocations across discipline collections, identify collection strengths, zero in on large publishers to manage impact of package subscriptions, and identify key journals. Just 100 titles covered half of publishing in sciences, and roughly 80% of cited references were to less than 20% of titles. Repeated studies indicated some improvements in the selections, increased cancellations from budget pressures, and changes in the local research emphasis.

A numeric comparison can be helpful in considering a range of journals, talking with stakeholders and making cancellation choices. Matthew Willmott (Massachusetts Institute of Technology) presented on a points system constructed with colleagues built on cost-per-use, impact factor, local publication and citation metrics. Targets can be dynamically set for various measures to assist librarians with professional collection decisions. Further enrichment of the tool is being considered through incorporation of additional measures such as trend analysis and the Eigenfactor.

Book metrics are less familiar to many of us, but as more statistics become available and books make the transition to electronic format, assessment becomes more critical in this area. Michelle Foss and Stephanie Haas (University of Florida) considered a range of data collection techniques, including circulation, shelving, and usage from a patron - driven e-book acquisition pilot. The

authors sliced the analysis by call number subclass and visualized the results as a TagCloud to zero in on subjects and specialized areas for increased collecting.

What the potential utility is in investing in large packages of e-books is the question Norah Xiao (University of Southern California) tackled. What can the usage data tell us about user behavior and what is user interest in these new collections? Usage data drove the questions of a survey to determine how people were finding the books and also serve to raise awareness of the resources. Keys to discovery were multiple discovery points, such as a library e-books lists, Google, and publisher links.

Teri Vogel (University of California San Diego) sought user input from focus groups, often expensive and yielding complicated results. But nothing beats live dialogue to learn more about how faculty and students find and use resources from their own perspectives and determine where to put energy into promotion and instruction of resources. Students and faculty both indicated a preference for Google for locating known items and specialized databases for general browsing for articles, although some concern was expressed about the need to evaluate material found through Google.

Publishers also consider usage statistics and other measures of their resources to target needs of both users and authors of their material. Melissa Blaney and Sara Rouhi (ACS Publications) discussed several approaches, including web hits, COUNTER reports, mobile app hits and surveys. Qualitative inputs is also sought through a visitation program to institutions, ACS on Campus, converging around a variety of timely themes such as scholarly publishing, peer review, ethics and alternate careers.

Susan Makar and Stacy Bruss (National Institute of Standards and Technology) also brought a new perspective to the academic librarians in the audience with their work on SciFinder usage in a government lab. Database usage in this setting is characterized by comprehensive searching and significant index browsing. Scientists and librarians were challenged with the change in format and complex pricing for the new web version and looked to statistics help inform the transition. Multiple metrics enabled analysis by type of searching, temporal trends and labs from various disciplines, and framed the case for improved funding and development support.

Assessing current and future roles of library collections was Leah Solla's goal (Cornell University), using a variety of analyses to convert an entire collection from print to electronic. Several examples were presented including historic trends, usage, circulation, requests, and user feedback. General trends indicated most use was online, and that print acquisitions were drastically reduced from budget pressures, but there was still an active print core collection. Deeper analysis was conducted on journals and books to inform where to relocate these print materials for continued access and how to expand electronic access.

A lively discussion ensued among the panel and audience members with several emergent themes: broadening the scope of metrics and improving collection and analysis metrics; e-only/virtual libraries (are we ready?), corporate perspective where most libraries as places have already disappeared and information professionals are still trying to figure out how best to access resources and make them easier to find; managing in-house source materials; and return-on-investment type studies. Clearly this is a topic that resonates across the information profession and grows richer in

complexity as it ages. Any of these themes would be a compelling future symposium and CINF and SLA-DCHE are well poised to bring together the critical voices. I look forward to the next joint symposium hosted by SLA-DCHE, tentatively scheduled for 2012.

Leah Solla, Co-organizer, Assessing Collections and Information Resources...Symposium



NEWS FROM THE MULTIDISCIPLINARY PROGRAM PLANNING GROUP (MPPG)



After a very successful program at the 240th National ACS Meeting in Boston, with 20 Divisions programming in 168 sessions, including CINF with three, under the theme of “Combating and Preventing Disease,” MPPG is now working with the Divisions and Theme Organizers on the themes for the next three years.

The programs promise to be very exciting at the two meetings in 2011. The theme for the 241th meeting in Anaheim is “Chemistry of Natural Resources” and the theme organizer is Prof. Ann-Christine Albertsson, KTH Stockholm.

Her programming ideas for Divisional Program Chairs are summarized in the following synopsis:

“Nature holds a vast treasury of inorganic and organic chemicals, covering the entire span from very small to gigantic in molecular weight, and from simple to complex in structure and formulation. Since ancient times we have been using the chemicals and materials provided by Nature, and as societal awareness of the climate situation increases, we look upon Nature’s pantry with renewed interest. Finding and isolating natural resources can help us develop renewable chemicals and materials. Identifying and understanding their chemistry can help us use them more wisely. Refining our knowledge of the chemistry of natural resources can help us to use them in a more sustainable way. A sound platform of insights about the chemistry of natural resources also supports our mimicking of the chemistry in Nature.

Within this theme, emphasis will be on the various aspects of understanding, creating and using the chemicals of Nature. This includes the recovery, utilization and production of chemicals from by-products and waste within the forestry, mining and agricultural processing industries, the production of functional materials and fuels from renewable resources, the environmental interaction of

renewable materials, new approaches to synthetic photosynthesis and the chemistry of natural products.”

The theme for the Fall meeting in Denver is “Chemistry of Air, Space and Water” organized by Prof. Ron Cohen, Director of the Berkeley Atmospheric Science Center, University of California, Berkeley. He provided the following synopsis to help Divisions with programming under the theme:

“Chemistry on Earth is mediated by air and water. The two interact - rainfall removes soluble gases from the atmosphere. Ocean circulation transports heat from equatorial regions poleward. Clouds are water droplets suspended in air and their formation affects the Earth’s radiative balance and the availability of fresh water on the planet. With the discovery of more than 100 planets orbiting distant stars, one wonders what chemistries control their atmospheres and oceans.

This theme will focus on the chemistry of air and water. This includes characterization of the natural state on Earth and elsewhere, understanding perturbations to that state, and evaluating ideas for deliberate engineering of air and water composition in the future. This includes chemistry affecting the exposure and response of humans to toxins in their air and water, chemistry affecting the climate and chemical strategies for removing greenhouse gases from the atmosphere (or reducing their emissions to it), and chemistry for enhancing the availability of clean drinking water. It includes the chemistry of atmospheres and clouds on other planets—especially as these provide insight into thinking about our own planet.”

The approved themes for the 2012 meetings in San Diego (Spring) and Philadelphia (Fall) are “Chemistry of Life” and “Materials for Health and Medicine,” respectively. In 2013, the ACS meetings are scheduled to take place in New Orleans (Spring) and Indianapolis (Fall). The themes for these meetings, “Chemistry of Energy and Food” and “Chemistry in Motion,” respectively, have been selected by MPPG and await approval by the Divisions.

Over the last few years, selecting a general theme for ACS National Meetings and programming by Divisions under the theme has proven to be quite successful. It is strongly supported by ACS as evidenced by the planned cover of a forthcoming C&EN issue for the preliminary program for Anaheim.

Guenter Grethe, Chair, Multidisciplinary Program Planning Group

SCHEDULE OF FUTURE ACS NATIONAL MEETINGS

241 st	Spring 2011	March 27 - 31	Anaheim, California
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

REPORTS FROM THE 2010 FALL ACS NATIONAL MEETING

YOUR ACS NETWORK JUST GOT BETTER

Sometime in the early morning hours of July 22, ACS put the final pieces in place for the most significant upgrade of the ACS Network to date. However, efforts to improve the ACS Network began long before that. Since its initial launch in August of 2008, the ACS Network has steadily evolved into the premier social/professional network for ACS members and the chemical enterprise.

The most recent effort to improve the ACS Network included a consolidation of the primary functionality of the Network to a single software system, a major upgrade of the software, and the implementation of a data hub to synchronize ACS Network profiles with the ACS member database records.


With these changes in place, ACS is positioned to take full advantage of the new software's functionality and improve with subsequent software releases. As a result, state-of-the-art social networking tools such as email digests, bookmarking, status updates, in-system messaging, private discussions and document sharing have been added to the existing cache of ACS Network tools. The Network now supports enhanced profile-building tools and "friending" capabilities to assist Network members in the building of their professional networks.

The software upgrade and data migration represent just one aspect of how the ACS Network is being improved. Earlier this summer, all ACS Members were informed about a recent ACS Board of Directors action to create an online member directory within the ACS Network. As a result, approximately 120,000 new members will be added into the Network this fall, bringing the total number of Network member to approximately 150,000 members.

It has taken time, and the dedication of early adopters, for the ACS Network to take hold, as is to be expected of any new technology. In its first 24 months the ACS Network has matured and become a vital tool for ACS members, governance, staff, and the global chemistry community to connect with one another as never before.







The ACS Network is a powerful tool, but is remarkably easy to use and can be leveraged in as many possible ways as it has members. It's an ideal place to collaborate on projects, convene groups, plan activities and discuss topics within private or open forums. If you have not joined the ACS Network, login at www.acs.org/network. If you're not sure where to begin check <https://communities.acs.org> for details (no login required).

Mark O'Brien and Christine Schmidt, ACS Staff



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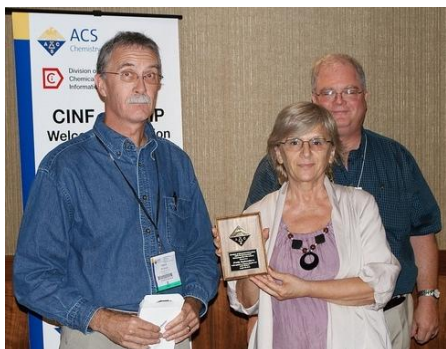
American Chemical Society

REPORT OF THE CINF COMMUNICATIONS AND PUBLICATIONS COMMITTEE

CINF e-Publications

During the Long Range Planning meeting we sought feedback for Communications and Publications Committee on the new *e-CIB* and obtained the following comments and questions:

- Many people are still printing the whole or parts; it prints very nicely from PDF.
- HTML is also very nicely linked.
- HTML and PDF content are not currently matched; sometimes there is more in the HTML version and sometimes less.
- The CINF program is much better represented in *e-CIB* than on the ACS website. PACS makes a mess of abstracts.
- What are the Google analytics on usage?
- *e-CIB* is in a transition period; the webmaster is planning a stable architecture going forward.
- What is the version of record? This version of record question may be included in the survey below. We need more discussion and will continue the PDF quarterly snapshot in the meantime.



Svetla Baykoucheva has stepped down as *e-CIB* editor and was thanked for her contribution. She was presented with the CINF Metanomski Meritorious Service Award at the Boston meeting. Svetla will continue with her series of interviews of CINF personalities

In 2011, Svetlana Korolev will cover post-meeting issues of *e-CIB*, Judith Currano will serve as editor of the pre - 2011 fall meeting *e-CIB*, Dave Martinsen will serve as editor of the pre - 2011 spring meeting *e-CIB*, using ACS Network as a test case.

CINF website

We recorded our thanks for Rick Williams' many years of service as CINF Webmaster. Danielle Dennie will be our new CINF webmaster starting in 2011. Rick will be supporting the transition. We have received an ACS Innovation grant, which gives us opportunities to do new and different things with our publications and the website.

During the Long Range Planning meeting we sought feedback for the Communications and Publications Committee on the CINF website and obtained the following suggestions:

- We need a search box on the CINF website.
- We should move away from Sharepoint use.
- We need more dynamic, instant update, not waiting for the Webmaster.
- There should be scope for more collaborative work, e.g., the editorial work for *CIB* should be enabled.

ACS has a new mechanism for hosting division websites, using webs.com, currently at no cost to divisions. We will investigate if this is an option for the new CINF website - it may not have database support underneath. We will perform a survey to get input on the CINF website using an open ended questionnaire.

ACS Network

(see article by Christine Schmidt and Mark O'Brian for an update in this issue)

CINF currently has many communication channels through which we communicate and work. How do they relate?

- The ACS Network should be the main channel for CINF members and committees to communicate with each other in the future. We will need 3 levels in the ACS Network: 1) open to all interested, 2) private for functionaries, 3) private committee groups.
- ACS Network staff presented during the Long Range Planning meeting. They will set up a webinar for CINF members and we will publicize this when details are known.
- CHMINF-L will be continued - it has a different audience and a different purpose.
- The CINF Yahoo! group will be closed and we will encourage members to switch to the ACS Network.
- Sharepoint currently contains 150Mb of documents; we will all need to review the contents before this service is closed down.
- As regards the LinkedIn CINF group, we should encourage people to join the ACS Network; we will only use LinkedIn for job advertising.

Bill Town, Chair, CINF Communications and Publications Committee

REPORT OF JOINT BOARD-COUNCIL COMMITTEE ON CHEMICAL ABSTRACTS SERVICE: CCAS SEEKS FEEDBACK

Adapted from text by Michael Filosa, CCAS Associate Member 2010

The Committee on Chemical Abstracts Service (CCAS) met at the Fall meeting in Boston under the leadership of the new Chair, Spiro Alexandratos of Hunter College. CCAS meets twice annually in conjunction with the Spring and Fall National ACS Meetings. The CCAS meetings are attended by committee members, associates, liaisons and key CAS staff led by CAS President, Bob Massie. The mission of the committee is to act as an information conduit between ACS members and CAS management and vice versa. The committee wishes to solicit the opinions of ACS members on Chemical Abstracts Service so that it can evaluate those opinions and concerns and present them to CAS management. Similarly, CCAS will also help CAS communicate with ACS members.

Since the Spring Meeting in San Francisco, CCAS has established a group on the ACS Network, thanks to the efforts of CCAS member, Grace Baysinger, of Stanford University. There, ACS members and other interested parties can read about current activities of the committee, as well as questions presented by ACS members and answered by CAS staff, led by marketing Vice-President, Chris McCue. The CCAS Group is open to guest access at <https://communities.acs.org/groups/chemical-abstracts-service-committee>. ACS Network registration is not necessary to access this resource.

You are free to contact any member of CCAS with any of your questions or concerns, including the CCAS Chair, Prof. Alexandratos at alexsd@hunter.cuny.edu. A complete listing of current CCAS members is available at the CCAS Group on the ACS Network. To quote Prof. Alexandratos from his most recent report from the Fall CCAS meeting, "I can assure you that CAS president Bob Massie and his entire staff are committed to being responsive to the issues you raise. Each query will be addressed. CAS operates for the benefit of the scientific community and CCAS can be your first point of contact if there is an issue that concerns you."

For the full text of Prof. Alexandratos' report to Council, as well as other information from the fall session of the committee, please visit the CCAS Group on the ACS Network.

Judith Currano, Member, Committee on Chemical Abstracts Service

CINF SOCIAL NETWORKING EVENTS AND SPONSORED SYMPOSIA

The ACS Division of Chemical Information (CINF) hosts focal social networking events at each ACS national meeting and secures support for CINF symposia speakers to assure successful programming and social gatherings. The Division depends on our generous sponsors to support these important activities.

The co-hosted CINF-COMP Welcoming Reception on Sunday blended members and guests from both divisions for a wonderful networking mixer attended by over 200. Sponsored exclusively by **ACS Publications**, the reception and the symposium on Monday celebrated the **50th Anniversary of the Journal of Chemical Information and Modeling**. The venue also provided a backdrop for the **CINF Scholarships for Scientific Excellence** poster session and the three \$1,000 scholarship presentations to the scholarship winners by sponsor **FIZ CHEMIE Berlin**.





The re-energized Harry's Party in the Presidential Suite of the Westin Boston Waterfront on Monday was sponsored by **FIZ CHEMIE Berlin**. Old friends and new acquaintances of CINF crowded the suite shoulder-to-shoulder as usual to enjoy some snacks, drinks and especially the company.

The CINF Tuesday Luncheon provided fare and entertainment to 75 attendees who were very fortunate to hear our special speaker, Michael Capuzzo, who illuminated his recent best selling publication, *The Murder Room*, and hosted a book signing. **Bio-Rad Laboratories**, **CambridgeSoft** and **Thieme** were very generous to support this special event.



Over 100 guests braved the rain to attend the Herman Skolnik Award Reception honoring Dr. Anton Hopfinger on Tuesday. Our sponsors, **ElsevierReaxys**, **Procter & Gamble**, **InfoChem** and **RSC Publishing** are to be thanked for providing support for Dr. Hopfinger's symposium and reception, and for providing the attendees with the opportunity to network and enjoy the fare.

The CINF Division would not be able to host these social networking events without the generous support of our sponsors to whom we extend our sincere thanks. The Division was also very fortunate to have **ACS Publications** sponsor speaker travel for the joint CINF-COMP symposium celebrating the 50th Anniversary of the *JCIM*, and to have the help of ACS Corporate Associates to support speakers at the CINF symposium, *Semantic Web in Chemistry*.

Graham Douglas, Chair, CINF Fundraising Committee



CINF Division Chairs: Carmen Nitsche 2010, Gregory Banik 2011, Rajarshi Guha 2012 (from right to left)

Photos from the 2010 Fall ACS National Meeting by Gregory Banik, Bonnie Lawlor and Wendy Warr are available at the CINF Flickr site at <http://www.flickr.com/photos/cinf>

SPONSOR ANNOUNCEMENTS

CambridgeSoft and KNIME.com Execute Commercial Collaboration Agreement

At the CambridgeSoft User Meeting and Conference, August 24-25, 2010,

CambridgeSoft
www.cambridgesoft.com

CambridgeSoft, a leading provider of software and services for discovery, analysis, and



collaboration to the life sciences, and KNIME.com, the company behind the professional open source workflow tool KNIME, announced the execution of a wide-ranging collaboration agreement. Under the agreement, CambridgeSoft will sell, support, and service the KNIME platform in enterprise R&D environments, and both companies will work to tighten the integration of KNIME.com and CambridgeSoft products.

“I am looking very much forward to this collaboration between KNIME and CambridgeSoft - it is exciting to see that one of the prime life-science solution vendors is able to support and service KNIME in a global context. We are also looking forward to the addition of CambridgeSoft’s core technology to the open KNIME platform,” said Professor Michael Berthold, CEO of KNIME.com. “The KNIME server allows direct calling of KNIME workflows as a web service, so this is already in place for linking to CambridgeSoft’s E-Notebook, as an example.”

“It is a natural fit between our organizations,” said Michael G. Tomasic, President and CEO of CambridgeSoft. “CambridgeSoft’s depth of service and support can provide global, multi-language and multi-timezone support for KNIME deployments in mission-critical environments. Our large professional service staff is experienced with KNIME, and is already using it to deploy novel applications with our customers. Further, with this agreement, we are ensuring that our customers benefit by being able to integrate CambridgeSoft’s leading Chem & Bio Office cloud, enterprise and desktop products with the KNIME platform’s workflow, analysis, and reporting ability in ways that will drive customers’ interactive in-process collaborations and decision support to higher levels of efficiency.”

For more information, please visit

<http://www.cambridgesoft.com/news/details/?News=157>

McGraw-Hill Integrates Industry-Leading Chemistry Tool ChemDraw Into Digital Teaching and Learning Platform

For professional chemists, drawing chemical structures can be done with the click of a mouse. For students of organic chemistry, however, practicing this essential skill is much more complicated, as the limitations of electronic homework platforms make it difficult to draw chemical structures in a digital environment. To solve this problem,



McGraw-Hill Higher Education has partnered with CambridgeSoft to integrate ChemDraw – the molecular editor used by today’s chemistry

CambridgeSoft
www.cambridgesoft.com

professionals – into McGraw-Hill Connect Chemistry. Connect Chemistry is a unique web-based assignment and assessment platform designed for organic chemistry courses.

McGraw-Hill Connect is a research-based, interactive assignment and assessment platform that incorporates cognitive science to customize the learning process. The online platform is based on McGraw-Hill's extensive, ongoing research of professors' instructional processes and students' study habits and includes a variety of digital learning tools that enable professors to easily customize courses and allow students to learn and master content and succeed in the course.

ChemDraw will be available for classroom use as a component of McGraw-Hill Connect Chemistry in the spring of 2011. It will initially be offered with three McGraw-Hill texts: *Organic Chemistry*, 3rd edition, by Janice Smith, *Organic Chemistry*, 8th edition, by Frank Carey and Robert Giuliano and *Chemistry: The Molecular Nature of Matter & Change*, 6th edition, by Martin Silberberg.

For more information, please visit

<http://www.cambridgesoft.com/news/details/?News=158>

RSC Publishing

The Royal Society of Chemistry (RSC) originated in 1841 and is the largest European organization for advancing the chemical sciences. We are a not-for-profit society and are supported by our global network of members and publishing, offering education, conferences, science policy and the promotion of chemistry to the public. Our publishing division, RSC Publishing, provides various resources such as journals, books/e-books, databases, and magazines, in a wide range of subjects: biology, biophysics, chemical sciences, materials, medicinal drug discovery, and physics.

In the past few years, we've seen an increase in international contributions:

- ✓ Significant article submissions growth from scientists all over the world allowing our resources' content to be more diverse and internationally applicable, specifically from China, France, Germany, India, Japan, UK and USA.
- ✓ 86% growth in published articles in 2007 to 2009.
- ✓ Significant growth in articles published from USA, China, UK, Germany, Japan, France and Spain.
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We have now launched our new RSC Publishing platform – <http://pubs.rsc.org>

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For more information, please email sales@rsc.org quoting reference code P10142



***Science of Synthesis* Completes Two More Categories With More Updates Scheduled for the Future**

Thieme Publishing Group has announced the launch of *Science of Synthesis Version 3.10*. *Science of Synthesis* is a comprehensive online resource providing users with convenient access to highly evaluated chemical information from leading experts in the field. With this most recent upgrade, *Science of Synthesis* now covers all fields of organic chemistry from organometallics to alkanes. Covered topics will be continuously updated and additional content will be added to this electronic reference through multiple releases per year.

This latest release encompasses 14,452 new reactions, with over 68,000 structures. Detailed preparative expertise is provided on: nitro, nitroso, azo, azoxy, and diazonium compounds, azides, triazenes, and tetrazenes (Volume 41); alkenes (Volume 47); and alkanes (Volume 48).

"All of the *Science of Synthesis* volumes published to date are now available online, which means that over 265,000 expert-evaluated reactions as well as more than 29,000 selected methods are easily accessible. This release includes a variety of topics, including compounds containing nitrogen functionalities such as *N*-nitroamines - used as propellants, fuels and explosives; carbon - carbon double bond - containing functionalities, i.e. alkenes--important for the petrochemical industry; and last but not least acyclic as well as cyclic alkanes, which are found in nature, and hydrocarbon polymers - used for plastic materials," says Dr. M. Fiona Shortt de Hernandez, Managing Editor *Science of Synthesis*.

Science of Synthesis presents a critical treatment of synthetic organic chemistry from the early 1800s to the present and has been developed in cooperation with InfoChem.

From 2010 onwards the existing volumes in this resource will be complemented by a variety of organic synthesis specialist topic reference works. A modular approach will be used to build this *Science of Synthesis Reference Library*, developed in conjunction with members of the *Science of Synthesis* Editorial Board.

For more information, please visit

<http://www.thieme.de/connect/en/services/press-release/>

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Ms. Carmen Nitsche
Accelrys, Inc.
254 Rockhill Drive
San Antonio, TX 78209
510-589-3555 (mobile phone)
210-820-3459 (office and fax)
Carmen.Nitsche@accelrys.com

Chair Elect:

Dr. Gregory Banik
Bio-Rad Laboratories, Inc.
Informatics Division
2 Penn Center Plaza, Suite 800
1500 John F Kennedy Blvd
Philadelphia, PA 19102-1721
267-322-6952(voice)
267-322-6953 (fax)
gregory_banik@bio-rad.com

Past Chair/Nominating Chair:

Ms. Svetlana Korolev
University of Wisconsin, Milwaukee
2311 E. Hartford Avenue
Milwaukee, WI 53211
414-229-5045(voice);
414-229-6791(fax)
skorolev@uwm.edu

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Ms. Leah Solla
Cornell University
Physical Sciences Library
283 Clark Hall
Ithaca, NY 14853-2501
607-255-1361 (voice)
607-255-5288 (fax)
lrml@cornell.edu

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Science & Engineering Library
108 Walter Library
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Minneapolis MN 55455
612-624-9399 (voice)
612-625-5583 (fax)
mlaffert@umn.edu

Councilor:

Ms. Bonnie Lawlor
National Federation of Advanced Information
Services (NFAIS)
276 Upper Gulph Road
Radnor, PA 19087-2400
215-893-1561 (voice)
215-893-1564 (fax)
blawlor@nfais.org

Councilor:

Ms. Andrea B. Twiss-Brooks
4824 S Dorchester Avenue, Apt 2
Chicago, IL 60615-2034
773-702-8777 (voice)
773-702-3317 (fax)
atbrooks@uchicago.edu

Alternate Councilor:

Mr. Charles F. Huber
University of California, Santa Barbara
Davidson Library
Santa Barbara, CA 93106
805-893-2762 (voice)
805-893-8620 (fax)
huber@library.ucsb.edu

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Dr. Guenter Grethe
352 Channing Way
Alameda, CA 94502-7409
510-865-5152 (voice and fax)
ggrethe@comcast.net

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Dr. Rajarshi Guha
NIH Chemical Genomics Center
9800 Medical Center Drive
Rockville, MD 20852
814- 404- 5449 (voice)
812-856-3825 (fax)
rajarshi.guha@gmail.com

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University of Kentucky
Chemistry Physics Library
150 Chem Phys Bldg
Lexington, KY 40506-0001
859-257-4074 (voice)
859-323-4988 (fax)
jbarv1@email.uky.edu

Archivist/Historian:

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117 Pleasant St SE
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CambridgeSoft Corporation
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Menlo Park, CA 94025-1713
650-235-6169 (voice)
650-362-2104 (fax)
pmchale@cambridgesoft.com

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A. D. Allen Chemistry Library
80 St George Street, Rm 480
Toronto, ON, Canada M5S 3H6
416-978-3587 (voice)
416-946-8059 (fax)
pmeindl@chem.utoronto.ca

Chemical Information Bulletin Editor:

Dr. Svetla Baykoucheva
White Memorial Chemistry Library
University of Maryland
College Park, MD 20742
301-405-9080 (voice)
301-314-5910 (fax)
sbaykouc@umd.edu

**Communications and Publications
Committee Chair:**

Dr. William Town
Kilmorie Consulting
24A Elsinore Road
London SE23 2SL
United Kingdom
+44 20 8699 9764 (voice)
bill.town@kilmorie.com

Constitution, Bylaws & Procedures:

Ms. Susanne Redalje
University of Washington
Chemistry Library
BOX 351700
Seattle, WA 98195
206-543-2070 (voice)
curie@u.washington.edu

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Fund Raising Committee Chair:

Mr. Graham Douglas
Scientific Information Consulting
1804 Chula Vista Drive
Belmont, CA 94002
510-407-0769 (voice)
510-217-3853 (fax)
Graham_C_Douglas@hotmail.com

Tellers Committee Chair:

Ms. Susan K. Cardinal
University of Rochester
Carlson Library
Rochester, NY 14627
585-275-9007 (voice)
585-273-4656 (fax)
scardinal@library.rochester.edu

Webmaster:

Mr. Richard Williams
Vertex Pharmaceuticals
P.O. Box 290718
Boston, MA 02129
617-444-6325 (voice)
webmaster@acscinf.org