

Join us for the  
ACS Fall 2009  
National Meeting  
& Exposition



**Chemistry and  
Global Security:  
Challenges and  
Opportunities**



August 16-20, 2009  
Washington, DC, USA

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## Message from the Chair

Greetings! It is a great honor and pleasure to serve you as CINF Division Chair in 2009. The Division of Chemical Information was very active and had a successful Spring 2009 national meeting in Salt Lake City, Utah. I would like to extend my sincere gratitude to all division functionaries and committee members, symposium organizers and speakers, and to our sponsors for putting together such a memorable event. The dedication and hard work of all the volunteers in the CINF Division made the spring meeting very exciting. It was truly wonderful to see many of you in Salt Lake City!

Let me reflect on some of the notable activities in the CINF Office at the spring meeting. Early on Saturday morning about thirty members attended a Long Range Planning meeting, where we had a lively discussion about the future of division publications, Chemical Information Bulletin and CINF E-News. Bill Town, Publications Chair, wrote an interesting overview of the committee's plans for this issue of CINF E-News. David Martinsen, Nominating Chair, was busy finalizing the slot of candidates for the 2009 CINF Elections. This year we are electing for the positions of Chair-Elect, Secretary, and Councilor/Alternate Councilor. This will be the first time CINF uses electronic balloting and voting. We will use Survey Monkey. Please participate in the 2009 CINF Elections!

To commemorate the outstanding contributions of the late Val Metanomski to the Division the CINF Meritorious Service Award was renamed the Val Metanomski Meritorious Service Award. Eileen Shanbrom was recognized as the 2009 recipient of this prestigious award.

I was very pleased to see several new members joining CINF committees at the spring meeting: Judy Olson – Membership, Philip Heller – Fund raising, and Martin Brandle and Egon Willighagen – Program committee, and Judy Matthews as CINF E-News Editor – Publications committee.

Our next meeting will be in Washington, DC, August 16-20, 2009. The ACS theme for the fall meeting is Chemistry and Global Security. The Division of Chemical Information will feature the Herman Skolnik Award Symposium honoring Yvonne Martin, Best Presentation Award in Chemical Text Mining and Public Molecular Databases symposium, CINF Scholarship for Scientific Excellence, and many more innovative symposia.

- *Svetlana Korolev*

## Report From the ACS Council Meeting Held March 25, 2009

The Council of the American Chemical Society met in Salt Lake City, UT on Wednesday, March 25, 2009 from 8:00am until approximately 12:30pm in the Grand Ballroom B/C of the Grand America Hotel. The meeting opened with a moment of silence in respect for the passing of ACS Past President, Ernest Eliel and several Councilors. The minutes of the Council meeting held in Philadelphia, PA in August 2008 were approved and Dr. Thomas Gilbert was confirmed as the Vice-Chair of the Council. Additional key items from the meeting are as follows.

### Attendance at the Meeting

As of March 25, 2009, the ACS spring national meeting had attracted 10,668 registrants as follows: Regular attendees 5,781; Students 3,439; Exhibitors 780; Exposition only 411; and Guests 257. There were a total of 228 companies that exhibited in 356 booths. The attendance is about 3K less than that at the meetings held in 2008 (both Philadelphia and New Orleans drew numbers in the thirteen thousands). The Committee on Meetings and Expositions (M&E) reported that the meeting locations for the year 2019 are Orlando (3/25/19) and San Diego (8/25/19).

### Nominations and Elections

*President-Elect:* The Committee on Nominations & Elections had identified four nominees for the office of 2010 ACS President-Elect: Berkeley (Buzz) W. Cue, Jr., Nancy B. Jackson, Cheryl A. Martin, and Dorothy J. Phillips. Council **VOTED** to select Dr. Jackson and Dr. Martin as the two candidates who will run for office in the fall of 2009 in addition to any valid petition candidates that may arise. This was the first time that Council used audience response devices to record a vote. This was a test, but it appeared to work quite well. In an informal vote, three hundred and ninety-four councilors present voted to continue the use of the devices, while twenty-eight voted against their use.

### Report of the Chair of the Board of Directors

Judith Benham reported that the six strategic goals of the Society can be accessed at <http://strategy.acs.org>. She noted that CAS has registered more than 44 million substances. She also reported that on March 27, 2008 the jury found against ACS in their lawsuit against some ex-employees (<http://www.bizjournals.com/columbus/stories/2008/03/24/daily32.html>), but that the Society filed an appeal on November 20, 2008. The appeal process is estimated to take about one year and there can be little if any comment made on the subject until the process has been completed. She reminded Councilors that anyone can create a group within the ACS network and encouraged members to sign up.

### Report of the Executive Director – ACS Highlights of 2008

Madeleine Jacobs reported that the ACS highlights of 2008 can be accessed at: <http://www.acs.org/acshighlights>. This is an excellent report and should be of interest to all ACS members. It includes current facts on CAS coverage, the status of ACS publications (ACS journals ranked number one in fifteen of the twenty-six categories in which they are covered by Thomson Reuters, Healthcare and Science business' Impact Factors (formerly ISI), and innumerable ACS initiatives—including the addition of forty-two online business and management skills courses at discounted rates from the Harvard Business School. Madeleine also reported on the new ACS “branding” that can be seen at: <http://www.acs.org/branding>. This is of particular importance to Divisions and Local

Sections for use in the publications and other outreach initiatives as they can download the new ACS logo that bears the tag line “Chemistry for Life” along with other document templates. She noted that web-based tools for promoting chemistry will be available this summer. Information on careers can be accessed at: <http://www.acs.org/careers>.

The Committee on Nominations and Elections also announced the results of the election to select candidates from the list of nominees to represent District I and District V on the Board of Directors for the term 2010-2012. Nominees for District I included: D. Richard Cobb, Neil D. Jespersen, Wayne E. Jones, and James L. Kallmerten. Nominees for District V included Thomas J. Barton, Judith L. Benham, Peter K. Dorhout, and John W. Moore. By mail ballot, the Councilors from these districts selected D. Richard Cobb and Neil D. Jespersen as District I candidates; and as District V candidates, Judith L. Benham and Peter K. Dorhout. Ballots will be mailed on or before October 10, 2009 to all members in District I and District V for election of a Director from each District.

The Committee on Nominations and Elections announced the selection of the following candidates for Directors-at-Large for a 2010 - 2012 term: Dennis Chamot, H. N. Cheng, Ray A. Dickie, and Valerie J. Kuck. The election of two Directors-at-Large will be conducted in the fall. Ballots will be mailed to the Council on or before October 10, 2009.

The Committee on Nominations and Elections presented Roger F. Bartholomew and Roland F. Hirsch to Council as candidates for election to the Committee on Committees (ConC) to fill a vacancy created by a committee member’s resignation. By written ballot, the Council **VOTED** to elect Roland F. Hirsch.

Candidates Carol B. Libby and Robert A. Pribush were presented to Council for election to the Committee on Nominations and Elections (N&E) to fill a vacancy created by a committee member’s resignation. By written ballot, the Council **VOTED** to elect Robert A. Pribush.

### ACS Finances

The Committee on Budget and Finance presented the financial results for 2008 and gave a briefing on the Society’s finances, which showed that in spite of the economic challenges faced in 2008, the Society’s operating performance held up well. Total revenue was approximately \$458.8 million, up just over 3% from 2007. The Society’s Net from Operations was \$9.7 million, and \$563K favorable to budget. This is the fifth consecutive year of positive operating results.

Information Services (CAS and Publications) provided a net of \$49.2 million. Investments provided a net of \$9.8 million and dues provided a net of \$4.3 million. All other activities operated at a net loss.

However, in 2008 ACS was adversely impacted by the historic collapse in the capital markets, which resulted in a sharp decline in the Society’s unrestricted net assets from \$212 million at December 31, 2007, to \$60 million at December 31, 2008. There were two factors driving this decrease, both related to the poor performance in the capital markets. These are substantial investment losses and a sizable increase in pension liability from the Society’s Defined Benefit Pension Plan. For this and other reasons, action was taken in 2007 to close the Defined Benefit Pension Plan, and, in 2008, to freeze benefit accruals for all Defined Benefit Pension Plan participants in 2009. It was noted that the unrestricted net assets from 2004 through 2008

were \$185M, \$211M, \$281M, \$212M, and \$60M, respectively.

It is in this context that the Board received a detailed briefing from management at this meeting on the framework of the 2009 Contingency Plan. In 2006, the Society had the foresight to develop a robust Contingency Plan that contemplated potential threats from many different sources, their probability of occurrence, likely duration and financial impact. The updated 2009 Plan covers all operating and administrative units as well as member programs, and identifies new and emerging threats. ACS management has also updated the mitigation strategies to respond to the threats and ensure the Society's long-term financial sustainability.

Society management and the Board of Directors are closely monitoring financial performance versus the budget. In addition, significant reductions in discretionary spending have already been implemented and additional cost control measures are under consideration. However, despite the adverse impact of the economic downturn, the Society remains highly liquid with more than \$275 million in cash and investments, and limited debt of \$30 million. To see the slides from the Budget and Finance presentation, go to: [http://portal.acs.org/portal/PublicWebSite/about/governance/committees/budget/WPCP\\_012569](http://portal.acs.org/portal/PublicWebSite/about/governance/committees/budget/WPCP_012569).

### ACS Dues for 2010

The Committee on Budget and Finance presented the recommended 2010 membership dues (an increase of \$5.00 – from \$140 to \$145). The increase to ACS dues is based upon an escalator defined in the ACS Bylaws (Bylaw XII, Section 3,a). The dues are calculated by multiplying the base

(current) rate “by a factor which is the ratio of the revised Consumer Price Index for Urban Wage Earners and Clerical Workers (Service Category) for the second year previous to the dues year to the value of the index for the third year previous to the dues year, as published by the United States Department of Labor, with the fractional dollar amounts rounded to the nearest whole dollar”.

Base rate 2009: \$140.00

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

2008 CPI-W Services: 252.176

2007 CPI-W Services: 244.275

Change in CPI-W Index: 3.234%

2010 Dues, fully escalated: \$144.53 ( $\$140.00 \times 1.0323$ )

2108 Dues, Rounded: \$145.00

There was considerable heated discussion regarding the dues increase, but in the end Council **VOTED** to approve the recommended increase. The vast majority of Councilors agreed that this was necessary in light of the current economic situation and, as one Councilor said – it just means giving up a single Starbucks latte during an entire year. Just a reminder that all ACS members in good standing who are unemployed may apply for a dues waiver.

### ACS Membership Statistics

At the close of 2008, Society membership totaled 154,024, compared to 160,052 for year-end 2007. In 2008, ACS completed the transition of its 15 year-old membership fulfillment system to a new, more robust system. The year-end 2008 membership numbers reflect a drop in membership of approximately 2% due to the economy and a correction to the counts of 2,589 Emeritus members whom ACS has not been able to reach for many years. Compared to its sister societies, ACS experienced a smaller loss of members in 2008.

55b-6bfe-40e1-8a4c-3b976f237b43. The Council **VOTED** to approve the Professional Employment Guidelines, as submitted by the Committee on Economic and Professional Affairs.

CEPA noted that there were 611 job seekers at the Salt Lake Meeting. There were 32 employers offering a total of 176 jobs – the lowest in recent years.

### Special Discussion Item

A special discussion item was again put on the Council agenda for this meeting. ACS President Thomas H. Lane invited the Chair of the Committee on Membership Affairs to present the results of a Councilor survey as a preface to the discussion on what can ACS do to attract new members while better serving our membership during these challenging economic times. Following the presentation, President Lane led Councilors in a lively discussion that focused on the value of ACS membership and on growth opportunities among students, international scientists, high school teachers, technicians, diverse ethnic groups and others.

### Bylaw Changes for Action

There were no Bylaw changes on the agenda for Council Action.

### Bylaw Changes for Consideration

There was one Bylaw change included in the Agenda book for consideration only. Action will be scheduled for Washington DC in the fall of 2009. The bylaw being requested to be changed by the Committee on Nominations and Elections (N&E) is Bylaw V – the Manner of Election (national elections). The potential change is to the timeline for elections as candidates have complained about the length of the election process and the

### Committee on Committees (ConC)

The Committee on Committees reported that the Committee on Chemistry and Public Affairs (CCPA) wished to change its charter to include policies that impact science education funding. The first point of their charter currently reads: “Identify and analyze legislative, regulatory, research and other science policy issues that impact upon the chemical sciences and technologies.” They are requesting that Council approve the following to replace it: “Identify and analyze legislative; regulatory; research; **Science, Technology, Engineering, and Math (STEM) education funding**; and other science policy issues that impact upon the chemical sciences and technologies.” CCPA is already active in efforts to increase federal funding for STEM education at NNF, DOE, and the Department of Education. They believe that their efforts will only increase due to their involvement in the pilot State Government Affairs Program as the state program will be focused on science education. Council **VOTED** to approve the request.

### Committee on Economic and Professional Affairs

The Committee on Economic and Professional Affairs (CEPA) requested that Council approve the Eighth Edition of the Professional Employment Guidelines (PEG). It contains revisions to make the document consistent with “The Academic Professional Guidelines (APG)” and “The Chemical Professional’s Code of Conduct.” It also updates the document with new issues. It was submitted for consideration at the Philadelphia National meeting in August 2008 and has been approved by ACS legal Counsel. The documents noted above can be accessed at: [http://portal.acs.org/portal/acs/corg/content?\\_nfpb=true&\\_pageLabel=PP\\_TRANSITIONMAIN&node\\_id=1095&use\\_sec=false&sec\\_url\\_var=region1&\\_\\_uuid=c0eb1](http://portal.acs.org/portal/acs/corg/content?_nfpb=true&_pageLabel=PP_TRANSITIONMAIN&node_id=1095&use_sec=false&sec_url_var=region1&__uuid=c0eb1)

exclusion of petitioners from the full election/vetting process. The proposed timeframe will make the campaign process less onerous and allow full participation of candidates in the Council review process. With this change, N&E would submit the names of nominees by March 1 rather than by January 15. Petition candidates would be identified by June 15 rather than July 15. Council would select candidates for President-elect at a meeting to be held no later than October 1 (rather than May 1). The selection would no longer be limited to two candidates, but would be limited to half of the number of nominees (the sum of those chosen by N&E and by member petitioners). If an odd number of nominees is on the Council ballot, then the number of candidates to be selected to the next higher integer. The financial impact of this petition is still being assessed.

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

### **Committee Actions**

The Board received reports from its Executive Committee, Committees on Grants and Awards (G&A), the Committee on Planning, and the Committee on Professional and Member Relations (P&MR). On the recommendation of the Committee on Grants and Awards, the Board **VOTED** to delegate oversight authority for the new ACS Fellows Program to G&A. G&A also presented the Board with a screened list of nominees for the 2010 Priestley Medal and the Volunteer Service Award. The Board **VOTED** to accept the committee's lists and agreed to announce the winners of the 2010 Priestley Medal and the Volunteer Service Award after its June meeting. On the recommendation of the Committee on Professional and Member Relations, the Board **VOTED** to amend its Regulations to reflect P&MR's responsibility to review and approve requests for international alliances under delegated authority from the Board. The Board also **VOTED** to

eliminate the requirement that an individual have a Pubs/CAS subscription authentication in order to be eligible for participation in the Network as an ACS global partner.

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

The Executive Director/CEO, along with several of her direct reports, updated the Board on the activities of Chemical Abstracts Service, the Publications Division, and the Society's General Counsel. The Board **VOTED** to approve a co-editor appointment and two reappointments of journal editors.

### **Compensation of Society Staff**

On the recommendation of the Committee on Executive Compensation, the Board **VOTED** to approve several actions relative to compensation for the Society's executive staff. The compensation of the Society's executive staff receives regular review from the Board.

### **Other Society Issues**

The Board was briefed by its working group monitoring the 2009 Plan for Continuous Improvement. This plan, which currently includes four broad topic areas and subtopics, is designed to enhance overall Board effectiveness.

Respectfully submitted April 20, 2009

— **CINF Councilors**

**Bonnie Lawlor**

**Andrea Twiss-Brooks**

## Technical Programming — Past, Present and Future

Technical programming is one of the key features of any National Meeting (apart from the receptions!). The diverse interests of the CINF membership, make technical programming both challenging and extremely interesting. I'd like to provide a brief summary of the programming for the past meeting in Salt Lake City, an overview of the upcoming meeting in Washington, D.C. this Fall and a taste of things being planned for San Francisco in the Spring of 2010.

### Salt Lake City, Spring

The past National Meeting in Salt Lake City was a little low in attendance—but it didn't seem like it from the crowded talks in CINF! There was a total of nine symposia made up of 17 sessions. The meeting started off with a full day symposium on the adoption and use of the InChI identifier, organized by Steve Heller. A variety of talks from academia and industry gave the audience some insight in to the variety and extent of usage of this identifier. Concurrently, there was a symposium on libraries and information issues focusing on engineers, organized by Patricia Kirkwood and a symposium on nomenclature for nanotechnology, organized by Peter Rusch. Sunday evening saw the CINF Scholarship for Scientific Excellence poster session. This meeting saw five excellent posters from students, ranging from reaction modeling to docking studies. Monday saw a symposium on fragment based drug design, organized by Rachelle Bienstock and Alex Tropsha. Given the buzz surrounding this topic, this was a very timely symposium – three sessions with packed audiences. The popularity of this symposium suggested a replay and we plan to hold it again in San Francisco (Spring 2010). In parallel, we had a symposium, organized by Erja Kajosalu and Meghan Lafferty, on current issues affecting chemical information professionals. Topics covered in this symposium ranged from the changing roles of librarians in today's connected world to data curation and Open Access policies. The Spring meeting is when CINF co-organizes a

symposium with the CSA Trust. This year we had Dimitris Agrafiotis and Eric Martin organize the symposium on the topic of adaptive scoring functions. Three sessions covered a variety of topics in the area of 3D structure based design. Tuesday saw a full day symposium, organized by Bill Town and Frank Allen on the use of crystal structure information in pharmaceutical applications – ranging from computational methods to regulatory issues. On Wednesday we had a very interesting symposium on genealogy, organized by Chuck Huber, in which the talks covered some intriguing topics such as the use of forensic genealogy to identify remains from an airplane crash to the use of genealogy in historical epidemiology. Last but not least, the meeting closed with a very healthy General Papers with 13 papers, including one given from a ski lodge via Skype.

So while, Salt Lake City might have been a bit cold and blustery, I like to think that the technical program helped to keep everybody's intellectual engines at high revs. I'd like to thank the symposia organizers, for their time and effort in helping put together an excellent program, as well as the various sponsors for their generous contributions to various symposia.

### Washington, D.C., Fall 2009

The Fall 2009 meeting is coming up in August at Washington, D.C. and I'm pretty excited about the

program. The meeting starts with a symposium on chemical text mining and databases organized by Alex Tropsha and Antony Williams. This will be a full day symposium, with speakers from academia, industry and government. The symposium will focus both on public databases themselves as well as new technologies to enhance individual databases and interesting approaches to managing distributed information. As before, the CINF Scholarship for Scientific Excellence poster session will be held on Sunday evening concurrently with the CINF welcoming reception and this meeting sees six student submissions. On Monday and Wednesday we stay with the database theme and have a symposium on the topic of federated searching organized by Wendy Warr, that will address issues and challenges in integrating multiple databases, likely containing very different data types. Speakers in this symposium will address a variety of topics ranging from cases studies of chemical and biological databases, to new approaches for distributed indexing and content delivery. Monday sees a symposium organized by Grace Baysinger on the topic of chemistry handbooks. Since 2009 is the 100<sup>th</sup> anniversary of Houben-Weyl, this is a very timely symposium. Given the venue of this meeting, we will have a number of topics related to intellectual property rights. Andrea-Twiss Brooks and Leah Solla are organizing a symposium on copyright and author rights on Sunday followed by another symposium (co-organized with Pamela Scott) on Wednesday that address educational issues in the field of intellectual property. The Fall meeting is when we

hold the Herman Skolnik Award symposium. This year's awardee is Yvonne Martin, and she has organized a great symposium on Tuesday that will cover various aspects of structure-activity modeling, ranging from data sources to cheminformatics methodologies. Yvonne has been part of the SAR modeling field since its early days and has put together an impressive speaker list of luminaries from the molecular modeling field. This is one symposium you don't want to miss. On Wednesday, we have a symposium on crystallography, organized by Bill Town, Gary Battle, Frank Allen and George Ferrence. In contrast to the crystallography sessions in Salt Lake City, this meeting's symposium will address the use of crystallographic information in education. This looks to be an interesting symposia for both educators as well technologists as there will be talks addressing the use of well known databases for teaching as well as software for crystallographic education. Finally, we again have a healthy General Papers with thirteen papers. In contrast to previous meetings, this one will be arranged a little differently – one session will be on Monday afternoon and one will be on Thursday morning.

The Fall meeting will be the first to see the Best Presentation Award symposia. For this meeting, the "Chemical Text Mining and Public Molecular Databases" symposium has been selected as the award symposium. A panel of judges will assess speakers and the winner will receive an invitation to the CINF luncheon, a plaque, and \$1000 toward registration and expenses.

**Selected 2009 CINF Symposia and  
Co-sponsored Symposia are available at:**

[http://acscinf.org/dbx/mtgs/  
cinfsymposia.asp?nth=237](http://acscinf.org/dbx/mtgs/cinfsymposia.asp?nth=237)

Finally, I'd like to point out that the program lists a number of symposia in other divisions (COMP, CHED, HIST and so on) that may be of interest to members. These include symposia on SAR databases, scripting and programming, virtual

screening for anti-infectious agents, classic books in chemistry and visualization for chemical education.

### San Francisco, Spring 2010

It's always a pleasure to visit San Francisco and the planned programming for the meeting in 2010 makes it more so. While the program is still not fully finalized, we have a really broad range of symposia coming up, including visualization of chemical information (ranging from SAR data to patents and literature), cheminformatics for

materials chemistry, library spaces (both virtual and real), and developments in online journals and global publishing. However, the program is still in flux and the next newsletter will provide a more detailed look at the Spring 2010 program.

Reading about symposia is obviously much less fun than attending them. So I'll stop here and I hope to see many of you at the Fall meeting in Washington, D.C.

— Rajarshi Guha, *CINF Program Chair*



Scenes from the ACS 2009  
SciMix event in Salt Lake City

(photos courtesy of Svetla Baykoucheva)



## The Future of the CINF Division publications

During the recent Salt Lake City ACS meeting, the CINF division focused on the future of its publications. The topic was discussed during the CINF Long Range Planning meeting, the CINF Publications Committee meeting and the CINF Executive Committee meeting. In this brief article I will attempt to summarize the conclusions from these discussions.

At the previous ACS meeting in Philadelphia, the CINF Executive Committee had taken the decision in principle that the Chemical Information Bulletin (CIB) should become fully electronic and the print version should cease. The purpose of these discussions was to formulate a plan for achieving this transition by 2010 and to identify action points.

During the discussions there emerged a consensus that changing to a completely electronic publication strategy provides opportunities for innovation. In consequence, we envisage that the CIB will become a dedicated area of the CINF website with its own home page that will serve as a portal to other sections of the website holding all the content normally expected to be found in the print CIB. We will still need to generate original content which will be linked to the home page. These will include interviews, profiles of CINF members, news stories, etc. The frequency of update of the CIB will increase but we will still continue the concept of 'CIB issues' and periodically we will automatically generate PDF snapshots of the CIB which can be downloaded and archived.

*“During the discussions there emerged a consensus that changing to a completely electronic publication strategy provides opportunities for innovation.”*

CINF E-News will increasingly become the method for driving use of the CIB content on the website. It will be redesigned as an attractive HTML newsletter with short excerpts of articles, etc. with hyperlinks giving access to the content on the CINF website. The redesign may be funded by an Innovation Project grant from ACS. We should aim to move to a monthly publication cycle although it may take some time to achieve this publication frequency.

Both the CIB and the CINF E-News will need to be managed by a dedicated editor whose role will be to oversee the publication process. In addition, we will need a Content Editor or Features Editor (who will be responsible for generating original content), a Copy Editor (who will ensure the accuracy of new content), a Web Editor and possibly Education Liaison and Software Reviews Editors but the roles of Business Manager and Subscription Manager will disappear. The CINF E-News will carry advertising but this advertising will be part of the new CINF sponsorship package. CINF E-news will be a benefit of CINF membership but the CIB content will be accessible to everyone.

To oversee these changes the CINF Publications committee will be expanded. I am pleased to announce that Bonnie Lawlor, David Martinsen, and Judith Currano have agreed to help and I welcome them to membership of the committee which currently also includes Svetla Baykoucheva, Richard Williams, Bruce Slutsky, Brian Lynch and Graham Douglas as members.

— Bill Town, CINF Publications Chair

## CINF Scholarship for Scientific Excellence Sponsored by Symyx

At the 237<sup>th</sup> ACS National Meeting in Salt Lake City, March 22-26, 2009, the Division of Chemical Information (CINF) announced the winners of the CINF-Symyx Scholarship for Scientific Excellence. Five scholarships valued at \$1,000 each were awarded at the CINF divisional luncheon by Carmen Nitsche of Symyx to Chloe-Agathe Azencott and Jonathan H. Chen of UC Irvine, N.J. Maximilian Macaluso of the University of Cambridge, and Richard Martin and Iain Mott of the University of Sheffield. The scholarship recipients presented posters of their work at the CINF reception on Sunday evening.

The titles of their presentations were *Learning Adaptive Scoring Functions for Chemical Expert Systems* (Azencott), *Reaction simulation expert system for synthetic organic chemistry* (Chen), *Where does the tetrazole ring belong? Insight to the binding pose of AT1 atagonists using homology modeling, molecular dynamics, and docking* (Macaluso), *Wavelet compression of GRID*

*fields for similarity searching and virtual screening* (Martin), and *Multiobjective approach to optimizing scoring functions for docking* (Mott).

The international scholarship program of CINF 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. The scholarship program was initiated in 2005 and the awards funded by different organizations are given out at each ACS National Meeting: and scholarship winners receive a year's complimentary membership in CINF.

— Phil McHale, Chair, CINF Awards Committee



Carmen Nitsche (Symyx), Max Macalusa, Iain Mott, Jonathan Chen, Chloe-Agathe Azencott, Richard Martin, Phil McHale (CINF Awards Chair) - photo courtesy of Guenter Grethe

## 2009 Val Metanomski Meritorious Service Award to Eileen Shanbrom

On behalf of the Awards Committee of the Division of Chemical Information (CINF) of ACS I am delighted to congratulate Eileen Shanbrom as the recipient of the prestigious Val Metanomski Meritorious Service Award. This award is given to members who have made outstanding contributions to the division, and this is just the eighth time this award has been given in the history of the division. The announcement was made at the Executive Committee meeting at the Spring ACS meeting in Salt Lake City, and the award will be presented to Eileen at the CINF divisional luncheon at the 238th National ACS Meeting in Washington DC.



Eileen joined ACS as a chemistry student in 1967, and she has been a member of CINF since 1983. During her more than twenty five years of service to CINF, she has been active on committees, providing leadership and mentoring, and she has been instrumental in shaping the strategic direction and vision for the division. Eileen served on the CINF Program Committee (2002-3), CINF Division Chair Office 2004-6, CINF Membership Committee (2006-8), and CINF Taskforce on Branding and Mission Statement (2007-8). While serving as CINF Chair in 2005, Eileen revised the CINF mission statement to reflect the expansion of the division's programs and memberships; and she wrote a division self-nomination for the ACS ChemLuminary Award, which was received for the first time in CINF history.

Eileen has also organized, chaired, co-authored and presented at a number of CINF symposiums at the ACS national meetings, including "Expanding horizons of the STM information landscape" 8/27/2001, "Genomics gorilla...handling sequence overload" 8/22/2002, "Integration Continuum...different strokes for different folks" 8/18/2002, "New Developments in Electronic Publishing" 4/8/2002, "Fishing for the Right Scientific Information in the Information Sea" 9/8/03, "Forging Leadership Pathways for Women in Science" 8/22/04.

To quote one endorser of this award: "Eileen serves as an excellent role model for leadership—participating in candid discussions about difficult topics while maintaining a professional and courteous attitude"; and "Her commitment to CINF has been steadfast and inspiring."

Congratulations Eileen!

And just a reminder, the deadline for nominations for the 2010 award is March 1, 2010.

—Phil McHale, *Chair, CINF Awards Committee*

## 2009 Lucille M. Wert Scholarship to Kristin Whitman



The scholarship administered by the Division of Chemical Information of the American Chemical Society consists of a \$1,500 grant and a complimentary one-year CINF membership. It is designed to help persons with an interest in the field of Chemical Information to pursue graduate studies in Library Information or Computer Science. The 2009 award will be presented to Kristin Whitman.

Kristin has a BS in Chemistry from the College of William and Mary, and she is currently a first year student in the Master of Library and Information Science course at Rutgers University.

Kristin has worked for the professional patent searching company Landon IP, Inc. since 2005, and she is currently a senior content editor with a special interest in chemical patent information retrieval, including Markush structures. Her expertise led her to contribute a chapter to a book on patent searching (*Patent Searching: Tools and Techniques*, John Wiley & Sons, 2007.) The challenges of patent searching encouraged her to want to gain a greater understanding of this complex area through post-graduate study.

Congratulations Kristin and good luck with your studies.

The deadline for nominations for the 2010 award is February 1, 2010.

— Phil McHale, *Chair, CINF Awards Committee*



### Scenes from Salt Lake City

Left — Salt Convention Center (photo courtesy of Salt Lake Convention and Visitors Bureau)

Below — city skyline view (photo courtesy of [www.go-utah.com](http://www.go-utah.com))



## Vendor Announcements—2 new journals from Chemistry Central

### *Journal of Cheminformatics* publishes launch papers

We are delighted to announce that *Journal of Cheminformatics* has published its launch articles. *Journal of Cheminformatics* is a new open access journal from Chemistry Central publishing peer-reviewed research in all aspects of cheminformatics and molecular modeling. It is run by Editors-in-Chief Christoph Steinbeck (European Bioinformatics Institute) and David J. Wild (Indiana University). Amongst the launch articles is an insightful Editorial by David Wild on Grand challenges for cheminformatics, and a thought-provoking Commentary by Steven Bachrach on Chemistry publication—making the revolution. Also, Antony Williams and colleagues present their work on Computer-assisted methods for molecular structure elucidation. Please share this information with your colleagues working in the field of chemical information who may be interested in the new journal. You can view articles and submit your manuscripts at [www.jcheminf.com](http://www.jcheminf.com).

### *Journal of Systems Chemistry* is inviting submissions

*Journal of Systems Chemistry* is a new peer-reviewed open access journal from Chemistry Central covering all aspects of systems chemistry, including (but not limited to): experimental and theoretical studies of complex molecular networks and emergent phenomena; catalytic and autocatalytic systems; self-replicating and self-reproducing chemical systems; dynamic combinatorial chemistry; and bottom up approaches to synthetic biology and chemical evolution. The Editors-in-Chief are: Günter von Kiedrowski (Ruhr-Universität Bochum, Germany), Sijbren Otto (University of Groningen, Netherlands), and Piet Herdewijn (Katholieke Universiteit Leuven, Belgium); supported by a prestigious international Editorial Board. Submissions are invited and more details are available at [www.jsystchem.com](http://www.jsystchem.com). Please let your colleagues working in this exciting, emerging field know about our new journal.

### Science in the Service of Genealogy

A paper presented at the CINF symposium, "Science in the Service of Genealogy" at the 237th ACS National Meeting in Salt Lake City on March 25, 2009, prompted an article in the "60-Second Science" blog on Scientific American's website. The paper, by Dr. Colleen Fitzpatrick and Odile Loreille, was entitled "Identification of the remains found at the crash site of Northwest Flight 4422 using forensic genealogy and DNA analysis". The presentation by Dr. Fitzpatrick detailed an investigation into a sixty-one year old mystery frozen into a glacier on Alaska's Mount Sanford. To read the news item see:

<http://www.sciam.com/blog/60-second-science/post.cfm?id=csi-alaska-air-crash-victim-identif-2009-03-26>

## Applications Invited for CSA Trust Jacques-Émile Dubois Grants for 2010

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 2010.



### ***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 three thousand U.S. dollars (\$3,000). 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.

### ***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.

### ***What Activities are Eligible?***

Grants may be awarded to acquire the tools necessary to support research activities, or 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:

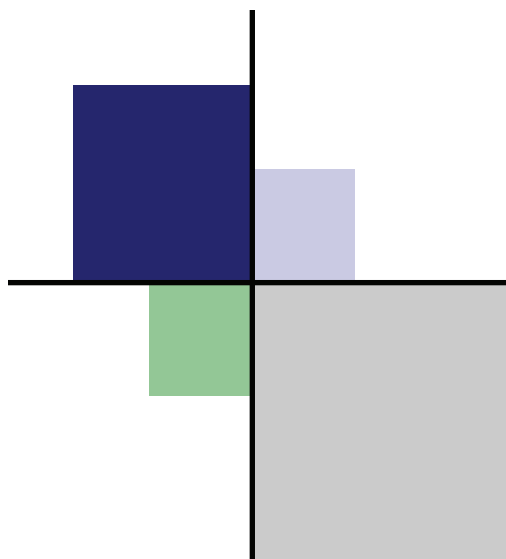
1. A letter that details the work upon which the Grant application is to be evaluated as well as details on research recently completed by the applicant;
2. The amount of Grant funds being requested and the details regarding the purpose for which the Grant will be used (e.g. cost of equipment, travel 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 15, 2010. Successful applicants will be notified no later than May 1, 2010.

### ***Address for Submission of Applications:***

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



## **Funding Aid for CINF Functionaries to Attend National Meetings**

### ***Aim***

Assist functionaries, younger members in particular, to get involved in divisional activities at national meetings by providing financial support for travel when no other funding resources exist.

### ***Who is eligible?***

- Members of executive committee and committee chairs (max \$600/meeting) .
- Symposium organizers - case by case basis
- Others asked to be present in a committee meeting - case by case basis
- Max 2-3 people/conference; any person may get funding only once a year

### ***How much?***

- Max \$300 for travel
- Max \$300 for hotel: \$150/night for 2 nights
- Registration - none
- Will have to submit receipts to the treasurer for refund.

### ***How to apply?***

- Send an application letter stating the need to the CINF chair : Svetlana Korolev (skorolev@uwm.edu) by June 15, 2009.
- Approval committee members: Chair (Svetlana Korolev), Chair-elect (Carmen Nitsche), Past Chair (David Martinsen) , Treasurer (Meghan Lafferty).

You will be notified by July 13 of the status of your request.

## Free Access to Selected ACS Nano Presentations from American Chemical Society National Meeting in March 2009



**ACS**  
Chemistry for Life™

The theme for the just-concluded Salt Lake City

national meeting was *Nanoscience: Challenges for the Future*. Many of the world's foremost nano experts gave talks, and permitted the American Chemical Society to record and post these presentations on [www.acs.org](http://www.acs.org). In all, over 30 nano presentations (audio and slides) can be found by visiting [www.acs.org](http://www.acs.org) (click on 'Nanoscience' box in right margin).

Among others, you'll find the following presentations:

**Raymond Astumian**, Generalized Fluctuation-Dissipation Relations for Brownian Sieves and Molecular Machines

**Ashleigh Baber**, Thermal and Mechanical Activation of Single-Molecule Thioether Rotors

**Angela Belcher**, From Nature and Back Again: Giving New Life to Materials for Energy

**Roman Boulatov**, Maximum Force Obtainable from a Molecular Photoactuator

**Vicki Colvin**, Nanotechnology in the Environment: Safety by Design

**Miguel Garcia-Garibay**, Crystalline Arrays of Molecular Gyroscopes: Toward the Limit of Barrierless Rotation in Solid State Materials

**Mark Haidekker**, Molecular Rotors: TICT Fluorophores with Mechanosensitive Properties

**James Hutchison**, Greener Nanoscience: A Proactive Approach to Advancing Applications and Reducing Implications of Nanotechnology

**Heather Kalish**, Microchip Analysis of Neuronal Secretions by Immunoaffinity Capillary Electrophoresis

**Anatoly Kolomeisky**, Thermally-Driven Nanocars and Molecular Rotors: What Can We Learn from Molecular Dynamics Simulations

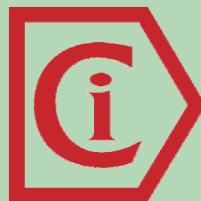
**Josef Michl**, Toward Designed Surface Ferroelectricity

**John Rogers**, Techniques for Molecular Scale and 3-D Nanofabrication

**Mehmet Sarikaya**, Biohesion: Coupling Synthetic and Biological Entities Using Genetically Engineered Peptides

**George Whitesides**, Nanotechnology in Adolescence

Please take our 30 second survey and let us know what you think about ACS making content like this available on-line. The survey can be found on the pages hosting the presentations.



### Our Mission

The ACS Division of Chemical Information (CINF) is committed to promoting the generation of, access to, and use of the world's knowledgebase in chemistry and the related sciences. The Division fosters the sharing of expertise in science informatics, information technology, and librarianship to ensure members benefit from the experience of others and are able to improve the dissemination and utilization of scientific information. We do this through innovative, high quality programming, education, career mentoring, collaboration and outreach, and recognition of excellence.

**We're on the web!**

<http://www.acscinf.org>