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Chemical Information Bulletin

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In This Issue

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Message from the Chair

Dear Colleagues,

The International Year of Chemistry 2011 is more than half over now, but the fun has only just begun! The upcoming CINF technical symposia in Denver will be a perfect complement to the unifying theme of the IYC, **"Chemistry—our life, our future."** These symposia include Chemical Environmental Specific Databases and Searching: Information Related to the Air, Water, and our Environment; Computational Approaches to Spectroscopy Analysis: Battle of the Pocket Protectors! (cosponsored with ANYL, COMP, and PHYS); Cheminformatics Aspects of High Throughput Screening: From Robots to Models: Round Table Discussion. Ding! Ding! (cosponsored with COMP and MEDI); and Chemistry in Mobile Spaces: Chemical Apps for Mobile Devices.

Tuesday will also include the Herman Skolnik Award Symposium, in honor of the winner of the 2011 Skolnik Award, Professor Dr. Alexander (Sandy) Lawson. The lineup for this symposium is most impressive, as is to be expected from someone of Sandy's stature. He is a "gentleman scholar," and I fondly remember meeting him for the first time during a visit to the Beilstein Institute in Frankfurt. The Herman Skolnik Award is the highest honor that CINF can bestow and, in Sandy's case, a well-deserved honor.

An exciting and innovative symposium will take place on Wednesday: the CINFlash symposium, organized by CINF Chair-Elect Rajarshi Guha. CINFlash is a session of "lightning talks," strictly timed talks, no longer than six minutes each, related to cheminformatics and chemical information. As if this were not exciting enough, refreshments will be served during the session (sponsored by Accelrys).

Speaking of refreshments, I would be remiss not to mention the many social networking opportunities that will be available at the Denver meeting. The Sunday Welcoming Reception should be a lovely affair, as will Harry's Party (sponsored exclusively by FIZ CHEMIE Berlin) on Monday. As opposed to the last two CINF luncheon speakers in Boston and Anaheim, who focused on murder (and in the case of Anaheim, included bloody crime scene photos), the speakers for the CINF luncheon in Denver will be decidedly fun; Howard and Sally Peters will speak on "Chocolate, Food of the Gods." Finally, the Skolnik Award Reception in honor of Sandy Lawson will take place Tuesday evening, and, as the one who selected the food for the reception (and as a self-proclaimed foodie), I cannot wait!

Finally, the CINF committee meetings in Denver will start later in the day (much to the delight of non-morning people like me), at 11:30 AM, rather than 7:30 AM. The meetings have been trimmed a bit and are scheduled to be finished by 6:00 PM. They represent an excellent way to network on a much more personal level with CINF colleagues and to "give back" to the chemical information community... and lunch and afternoon snacks will be provided, as well.

I hope that you have had a productive yet relaxing summer, and I look forward to seeing you in Denver!

Warmest regards,

Gregory M. Banik, Ph.D., *Chair*
ACS Division of Chemical Information (CINF)

Letter from the Editor

Greetings from scorching Philadelphia!

Hopefully, the summer is on the wane, although anticipation for and events surrounding the Denver ACS National Meeting are just beginning to heat up. The fall issue of the *Chemical Information Bulletin* has historically focused on the technical program for the meeting, and I fondly recall dashing from session to session, clutching my yellow-covered copy in my hand. I'm delighted that, thanks to the gargantuan efforts of David Martinsen, who assembled the symposium information, and Danielle Dennie, who formatted it, this aspect of the *CIB* is looking better than ever. Readers can get a brief overview of CINF symposia from the "Symposia at a Glance" section or delve deeper, examining the full CINF technical program, with and without abstracts. Of course there is more to an ACS meeting than papers and posters, and, in the "Social Events" section, Graham Douglas and Greg Banik have done a fantastic job of presenting the receptions and networking events. I extend sincere thanks to all of these individuals and my admiration to the Program Committee, chaired by Rachelle Bienstock, without whom we would not have such fascinating sessions to attend.

After perusing the technical program, please cast your eyes over the "Committee Information" section. The CINF committee chairs have submitted agendas for their upcoming meetings in Denver, as well as descriptions of their activities and modes of communication. Many committees are in need of new members, and, if your travel plans have you arriving in Denver on Friday night or Saturday morning, you may be interested in attending one of their open meetings. Contact information for each committee chair appears at the end of his or her piece, as well as in the "CINF 2011 Officers and Functionaries" section of the *CIB*.

In this issue, as well as highlighting the happenings at the upcoming conference, I wanted to include some articles by CINF members, reporting things that they are doing and topics that they find interesting. In the "Interviews and Features" section, you can enjoy Svetla Baykoucheva's excellent interview of Grace Baysinger, become acquainted with some of Fred Stoss's favorite resources for information on the chemistry of climate change, and vicariously "attend" the recent International Council for Scientific and Technical Information and Special Libraries Association meetings with Wendy Warr and Susan Cardinal, respectively. Bob Buntrock has provided another insightful book review, to round out the issue. We have a few other ideas in the hopper for future issues, but we are always looking for content that will interest CINF members; if you have an idea, please do not hesitate to contact us.

This the first issue of the *Chemical Information Bulletin* that I have edited, and I have thoroughly enjoyed working with so many talented, active individuals. I'm extremely grateful to everyone who contributed or assisted with the production of this issue. The new Drupal platform has streamlined the production process and generates an attractive final product, and I hope that you enjoy the results.

Judith N. Currano
Editor, Chemical Information Bulletin
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Awards and Scholarships

CINF Scholarship for Scientific Excellence Sponsored by Accelrys®

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 243rd ACS National Meeting in San Diego, CA, March 25 – 29, 2012. Applicants must be enrolled at a certified college or university and must present a poster during the CINF Welcoming Reception on Sunday evening at the National Meeting. They will also have the option to 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@att.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 22, 2011, and will close on October 17, 2011. 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, 2012. 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 contents, presentation, and relevance of the poster and they will be announced during the reception. The contents should 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
ggrethe@att.net

Chemical Structure Association Trust

Applications Invited for CSA Trust Jacques-Émile Dubois Grants for 2012

The Chemical Structure Association (CSA) Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program, renamed in honor of Professor Jacques-Émile Dubois who made significant contributions to the field of cheminformatics. The Trust is currently inviting the submission of grant applications for 2012.

***Purpose of the Grants*:**
The Grant Program has been created to provide funding for the career development of young researchers who have demonstrated excellence in their education, research or development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and compounds. A Grant will be awarded annually up to a maximum of five thousand U.S. dollars ($5,000). Grants are awarded for specific purposes, and within one year each grantee is required to submit a brief written report detailing how the grant funds were allocated. Grantees are also requested to recognize the support of the Trust in any paper or presentation that is given as a result of that support.

***Who is Eligible*?**

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

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

Application Requirements:
Applications must include the following documentation:

1. A letter that details the work upon which the Grant application is to be evaluated as well as details on research recently completed by the applicant;
2. The amount of Grant funds being requested and the details regarding the purpose for which the Grant will be used (e.g. cost of equipment, travel expenses if the request is for financial support of meeting attendance, etc.). The relevance of the above-stated purpose to the Trust's objectives and the clarity of this statement are essential in the evaluation of the application);
3. A brief biographical sketch, including a statement of academic qualifications;
4. Two reference letters in support of the application. Additional materials may be supplied at the discretion of the applicant only if relevant to the application and if such materials provide information not already included in items 1-4. Three copies of the complete application document must be supplied for distribution to the Grants Committee.

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

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

Other Awards

Wiggins-Roth Award for Outstanding Service
Special Libraries Association Chemistry Division

Ms. Grace Baysinger was the first recipient of the SLA Chemistry Division's Wiggins-Roth Award for Outstanding Service. The Wiggins-Roth Award recognizes outstanding contributions to the field of chemical information, and is named in honor of Gary Wiggins and Dana Roth.

Ms. Baysinger is currently the head librarian at the Swain Library of Chemistry and Chemical Engineering at Stanford University. She is known for her bright outlook, well-thought out opinions, and significant contributions to academic libraries, chemical information, and chemical publishing. Throughout her career, she has developed significant contributions to chemical information reference; these include: Web guides, tutorials, slides, and other materials. She has generously shared these materials with the larger community of chemical information professionals. The entire chemical information community has benefitted from Ms. Baysinger's effectiveness in making the case for changes and improvements in chemistry-related databases, software, and printed products.

Cory Craig
Chair, SLA Chemistry Division Awards Committee

Mike Lynch Award
Chemical Structure Association Trust

Dr. Engelbert Zass received the CSA Trust Mike Lynch Award at the 9th International Conference on Chemical Structures (ICCS), held June 5-9 2011, Noordwijkerhout, The Netherlands. The Mike Lynch Award is presented every three years by the Chemical Structure Association Trust (CSA trust) to acknowledge the lifetime work of an individual with "outstanding accomplishments in education, research and development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and properties" (CSA Trust, 2011).

Dr. Zass is the head of the ETH Zurich Chemistry Biology Pharmacy Information Center. He has been a member of ACS since 1972, and he joined CINF in 1981. He delivered a keynote address at ICCS, entitled "The intermediary reloaded - On the need for a 'Go-Between' to information users and producers," and the slides for this presentation are posted on the ICCS Web site, at http://www.int-conf-chem-structures.org/presentations.html

News Brief: e-CIB migrates to Drupal

As part of our ongoing communication improvement efforts, we are pleased to announce that we have migrated the online version of the *Chemical Information Bulletin*, the *e-CIB*, to a Drupal platform, which will greatly streamline the editing process. The site has been formatted to look similar to the current CINF website. This new platform should give our volunteer *e-CIB* editors the ability to directly upload and update the *e-CIB* without depending solely on the Webmaster. We will now consider applying a similar approach to other areas of the website.

The work of installing Drupal and transferring all *e-CIB* issues from Volume 62, No.1, onward was done thanks to a $5,000 ACS innovation grant given to CINF in order to improve the CINF communications infrastructure. The work was overseen by Webmaster Danielle Dennie and executed by David Pickup, a librarian working at Concordia University in Montreal. The next issue of *e-CIB* will be published using the new Drupal-based system.

Danielle Dennie
CINF Webmaster
Danielle.Dennie@concordia.ca

ACS Chemical Information Division (CINF)
Fall 2011 ACS National Meeting

Denver, CO (August 28 – September 1)

Technical Program Schedule

Rachelle Bienstock, *Program Chair*

OTHER SYMPOSIA OF INTEREST:
Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions *(see* CHAL*, Sun)*
Cheminformatics Aspects of High Throughput Screening: From Robots to Models *(see* COMP*, Sun, Mon)*
Emerging Technologies in Computational Chemistry *(see* COMP*, Sun)*
Mining Protein-Ligand Interaction Space *(see* COMP*, Mon, Tue)*
Predicting and Disrupting Protein Interactions *(see* COMP*, Wed, Thu)*

SUNDAY MORNING

Section A/Colorado Convention Center /Room 110

Chemical Environmental Specific Databases and Searching Information Related to the Air, Water, and our Environment
A. Twiss-Brooks, *Organizer, Presiding*

9:00 Introductory Remarks.
9:05-1. Can a compact means of representing the ionic equilibria of multi-acid/base aqueous solute molecules be devised? **R. D. Wauchope**
9:35-2. USGS National Geochemical Database: Recovering, repackaging, and repurposing 50+ years of historical data. **S. M. Smith**, D. B. Smith
10:05-3. Quality of water resources from the U.S. Geological Syrvey: An introduction. **S. Guo**
10:35 Intermission.
10:50-4. Public access to toxic release data: Exploring TRI and RTKnet.org. **B. Losoff**
11:20-5. CHEMLIST: Chronicling the course of regulated chemistry. **R. J. Schenck**

Computational Approaches to Spectroscopy Analysis:Battle of the Pocket Protectors!
Sponsored by COMP, Cosponsored by ANYL, CINF, and PHYS

Empowering Tomorrow's Science Super Heroes
Sponsored by PRES, Cosponsored by ANYL, BMGT, CHED, CINF, COMSCI, FUEL, GEOC, HIST, I&EC, INOR, MEDI, PHYS, PROF, and YCC

SUNDAY AFTERNOON

Section A/Colorado Convention Center/Room 110

Non-Traditional Careers: What Else Can I Do With a Chemistry Degree?
P. Meindl, *Organizer, Presiding*

1:30 Introductory Remarks.
1:40-6. Aligning scientific expertise and passion through a career path in the chemical sciences. **A. J. Williams**
2:00 Intermission.
2:15 Videos.
2:45 Panel Discussion.

Cheminformatics Aspects of High Throughput Screening: From Robots to Models; Round Table Discussion. Ding! Ding!
Sponsored by COMP, Cosponsored by CINF and MEDI

Science on the Hollywood Screen
Sponsored by PRES, Cosponsored by ANYL, BMGT, CHED, CINF, COMSCI, FUEL, GEOC, HIST, I&EC, INOR, MEDI, PHYS, PROF, and YCC

SUNDAY EVENING

Section A

CINF Scholarship for Scientific Excellence
G. Grethe, *Organizer*

6:30 - 8:30
7. Development of an open source ELN. **F. Rudolphi**, L. J. Goossen
8. Introduction of InChI to researchers in the Department of Chemistry at Louisiana State University. **K. L. Salazar**, W. W. Armstrong
9. Stochastic search for the structures of small germanium clusters and their anions: Enhanced stability by spherical aromaticity of the Ge_{10} and Ge_{12}^{2-}systems. **T. Ba Tai**
10. SMARTNames: A new framework to organize chemical structural information based on chemically relevant functional groups . **B. Bhhatarai**, S. Schurer

11. Molecular docking and 3D-QSAR studies for design and development of selective aspartate semialdehyde dehydrogenase inhibitors. **A. Luniwal**, A. Pavlovsky, P. W. Erhardt, R. Viola

MONDAY MORNING

Section A/Colorado Convention Center/Room 110

Chemistry in Mobile Spaces: Chemical Apps for Mobile Devices
D. Martinsen, M. Braendle, *Organizers, Presiding*

9:00 Introductory Remarks.
9:05-12. Chemistry in the hand: The delivery of structure databases and spectroscopy gaming on mobile devices. **A. J. Williams**, S. Shevelev, A. S. Lang, J. Bradley, K. Theisen
9:35-13. SciFinder mobile: Innovation for today's chemical researchers. **K. W. Zielenbach**, J. M. Wilson, J. F. Sjostrom
10:05-14. Useful and fun chemistry on the go. **D. A. Evans**, P. Caduff
10:35 Break.
10:45-15. Nature of publishing anytime, anyplace, anywhere. **J. Wilde**
11:15-16. Current and emerging mobile technologies at ACS publications. **D. O'Brien**, Y. Ma

Bioinformatics
Sponsored by COMP, Cosponsored by BIOL, CINF, and MEDI

Cheminformatics Aspects of High Throughput Screening: From Robots to Models
Sponsored by COMP, Cosponsored by CINF and MEDI

MONDAY AFTERNOON

Section A/Colorado Convention Center/Room 110

Chemistry in Mobile Spaces
D. Martinsen, M. Braendle, *Organizers, Presiding*

1:30 Introductory Remarks.
1:35-17. Post-textbook era: What it means for the chemistry classroom. **T. Gray**
2:05-18. Riding the mobile wave. **S. M. Muskal**
2:35-19. ChemWriter: Enabling cross-platform mobile chemistry applications through Web standards. **R. L. Apodaca**
3:05-20. Computer Vision based chemical information extraction from digital images and streaming videos. **M. Karthikeyan**
3:35 Break.
4:25 CINF Open Meeting and the Joint Board-Council Committee on CAS.

TUESDAY MORNING

Section A/Colorado Convention Center/Room 110

Herman Skolnik Award Symposium: Information Services in Chemical Sciences: Perspectives
A. Lawson, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35-21. The Information Century and the Learned Society. **R. J. Massie**
9:15-22. Beyond the journal: Innovation in 21st century publishing. D. A. Evans, R. Sidi, P. Terheggen, **M. Tanke**
9:55 Intermission.
10:10-23. ChemSpider: Does community engagement work to build a quality online resource for chemists? **A. J. Williams**, V. Tkachenko
10:50-24. Riding the wave: TIB`s strategy in the context of non-textual materials. **U. Rosemann**, **I. Sens**

Challenges in Industrial Computational Methods
Sponsored by COMP, Cosponsored by CINF

TUESDAY AFTERNOON

Section A/Colorado Convention Center/Room 110

Herman Skolnik Award Symposium: Information Services in Chemical Sciences: Perspectives
A. Lawson, *Organizer, Presiding*

1:30 Introductory Remarks.
1:35-25. Discovering drugs: Generating pharmacologically relevant leads that target disease. **R. C. Glen**
2:15-26. From data to knowledge capture and retrieval in Medicinal Chemistry – if we only knew what we already know. **T. Hoffmann**
2:55 Intermission.
3:10-27. Enriched research documents at the cutting edge: When research papers no longer make sense on paper. **R. Potenzone**, L. Dirks
3:50-28. Reading the e-leaves. **W. A. Warr**
4:20-29. Challenges and opportunities in preserving the scientific record: Reaxys and beyond. **A. J. Lawson**
4:50 Concluding Remarks.

Challenges in Industrial Computational Methods
Sponsored by COMP, Cosponsored by CINF

Material Science: Look Out POLY. You're Officially on Notice.
Sponsored by COMP, Cosponsored by CINF and PMSE

WEDNESDAY MORNING

Section A/Colorado Convention Center/Room 110

General Papers
R. Bienstock, *Organizer, Presiding*

8:30 Introductory Remarks.
8:35-30. MarVis: An intuitive patent Markush structure visualization tool for medicinal chemists. **W. Deng**, S. J. Berthel, W. V. So
8:55-31. Modeling activity landscapes using multiple representations: Consensus models. A. B. Yongye, K. Byler, R. Santos, K. Martinez-Mayorga, G. M. Maggiora, **J. L. Medina-Franco**
9:15-32. Unique cycle families: A set of unique and chemically meaningful rings. **A. Kolodzik**, S. Urbaczek, M. Rarey
9:35-33. Improved conformational search using a cooperative swarm of simulation replicas. **N. J. Bruce**, R. A. Bryce
9:55-34. System chemical biology studies of endocrine disruptors. O. Taboureau, **T. I. Oprea**
10:15 Break.
10:25-35. Large-scale data analysis of bioactivity information in PubChem using 2D and 3D chemical similarity. **E. Bolton**
10:45-36. Structure representations in public chemistry databases: The challenges of validating the chemical structures for 200 top-selling drugs. **A. J. Williams**, D. Sharpe, A. Tropsha, E. Muratov, D. Fourches, J. Mestres, R. Garcia-Serna, A. Yerin, C. Southan
11:05-37. Merging small molecule compound libraries of Bayer HealthCare AG and Schering AG. **J. F. Schamberger**, M. Grimm, A. Hillisch, A. Steinmeyer
11:25-38. Functional classification of drugs based on their multiphenotype interaction network. **A. C. Palmer**, F. M. Harbinski, F. Nigsch, J. Lehár, C. J. Wilson, J. L. Jenkins, R. Kishony
11:45-39. Flavor landscape: Towards a systematic characterization of a comprehensive flavor database. **K. Martinez-Mayorga**, T. L. Peppard, A. B. Yongye, G. M. Maggiora, J. L. Medina-Franco

Challenges in Industrial Computational Methods
Sponsored by COMP, Cosponsored by CINF

WEDNESDAY AFTERNOON

Section A/Colorado Convention Center/Room 110

General Papers
R. Bienstock, *Organizer, Presiding*

1:30 Introductory Remarks.
1:35-40. RInChIs and reactions. **J. M. Goodman**
1:55-41. CAS learning solutions: Responding to customer needs worldwide. **J. Knoop**
2:15-42. NIST-journals cooperation: Implementation of new tools for editors, reviewers and authors. **J. W. Magee**
2:35 Break.
2:45-43. What has your chemistry librarian been doing? A new science librarian's work report and current trends in chemistry/science librarianship. **S. Guo**
3:05-44. Development and assessment of online SciFinder tutorials toward the promotion of scientific literacy in undergraduates. **D. L. Jacobs**, P. H. Dawson, S. Q. Yang
3:25-45. Check us out: Librarians as departmental PR agents. **D. Wrublewski**, **M. Leonard**
3:45-46. Elements of research misconduct. **D. Wrublewski**, **M. Leonard**

Section B/Colorado Convention Center/Room 112

CINFlash
R. Guha, *Organizer, Presiding*

1:30 Discussion.

Challenges in Industrial Computational Methods
Sponsored by COMP, Cosponsored by CINF

Material Science: Nanoscopic Investigation. Did You Just Makeup A Word? No, Investigation Is A 'Real' Word.
Sponsored by COMP, Cosponsored by CINF and PMSE

THURSDAY AFTERNOON

Material Science: Everyone Studies Materials, but We Do It Better. And We Develop the Methodologies.
Sponsored by COMP, Cosponsored by CINF and PMSE

Social Networking Events at the Fall ACS National Meeting

Please Join Us at these CINF Events!

The ACS Division of Chemical Information is pleased to host the following social networking events at the Fall 2011 ACS National Meeting in Denver, CO.

CINF Sunday Welcoming Reception & CINF Scholarships for Scientific Excellence Posters
6:30-8:30pm, Sunday August 28th – Capitol Ballroom 2/3, Hyatt Regency Denver

Reception co-sponsored by:

- Digital Science
- InfoChem
- OpenEye
- PerkinElmer
- *Journal of Chemical Information and Modeling*
- *Greenhouse Gases: Science and Technology*

Scholarships for Scientific Excellence sponsored exclusively by **FIZ CHEMIE Berlin**.

Harry's Party
5:30-8:00pm Monday, August 29th – Pikes Peak Suite 1921, Westin Tabor Center

Sponsored exclusively by **FIZ CHEMIE Berlin**. *** Use ACS Shuttle #3**

CINF Luncheon *(Ticketed Event – See Greg Banik)*
12:00-1:30pm Tuesday August 30th – Room 201, Colorado Convention Center

Luncheon co-sponsored by:

- Bio-Rad Laboratories
- RSC Publishing.

Speaker: Howard and Sally Peters will speak on "Chocolate, Food of the Gods."

Herman Skolnik Award Reception honoring Dr. Alexander Lawson
6:30-8:30pm Tuesday, August 30 – Centennial Ballroom F/G, Hyatt Regency Denver

Sponsored exclusively by Reaxys®.

CINFlash Symposium – Snacks & Refreshments
1:30-5:00pm Wednesday, August 31 – Room 112, Colorado Convention Center

Sponsored exclusively by Accelrys.

Committee Information

The following CINF committee and governance meetings will occur on Saturday, August 27, 2011, at the Colorado Convention Center. The CINF Executive Committee Meeting is a closed meeting; if you wish to attend it, contact the division chair.

11:30 AM - 1:00 PM	Long Range Planning Luncheon	Room 702/704
1:00 PM - 2:00 PM	Awards Committee Meeting	Room 709
2:00 PM - 3:00 PM	Finance & Fundraising Committee Meetings	Room 709
1:00 PM - 3:00 PM	Education Committee Meeting	Room 706
1:00 PM - 3:00 PM	Communications & Publications Committee Meeting	Room 707
1:00 PM - 4:00 PM	Program Committee Meeting	Room 705
4:00 PM - 6:00 PM	Executive Committee Meeting	Room 702/704

The chairs of several CINF committees, those that are meeting in Denver and some that are not, have included agendas and descriptions of their work. Most are actively recruiting new members; if you are interested in joining a committee, please contact its chair.

Careers Committee

The Careers Committee will not be meeting at the Denver ACS National Meeting.

The Careers Committee is seeking new members, as well as a new chair. Since many of the committee's members do not attend the national meetings, they usually communicate via e-mail. For more information, please contact the current chair, Patricia Meindl, at pmeindl@chem.utoronto.ca

Membership Committee

The Membership Committee will not be meeting at the Denver ACS National Meeting

The Membership Committee is in need of new members! Although they do not have a Saturday meeting scheduled for the Denver conference, they hope soon to discuss their goals for the coming year, how they can recruit new members to the Membership Committee, and how they can encourage new CINF members to become more involved in the Division.

If you would like more information or wish to join the committee, please contact the Membership Committee Chair, Jan Carver, at jbcarv1@email.uky.edu.

Communications & Publications Committee

The following is a preliminary meeting agenda for the Communications & Publications Committee.

1. CINF website and the new e-CIB (Drupal) layout
2. New e-CIB content
    - Committee agendas and reports
    - Soliciting information from CINF members - ideas for features
3. New columns
    - "CINF Reviews," highlights from the chemical information literature
    - Database reviews (like the book review section)
    - "Cool articles I read" wiki - could supply material for CINF Reviews editor
4. ACS meetings information - currently ends up being on both the website and in the e-CIB
5. Editors for the four e-CIB issues in 2012
6. Committee membership - welcome to Song Yu and Carmen Nitsche (both 2011-2014) and search for new members
7. Committee chair (2012-2014)
8. ACS Network and its relationship to the CINF website

If you have questions or comments, please contact the Chair of the Communications & Publications Committee, Bill Town, at bill_town@mac.com.

Education Committee

The Education Committee always welcomes new members and encourages interested parties to attend its meeting, the agenda for which follows.

1. Review of Denver meeting
    - Program
    - CPT meeting (to be arranged)
2. San Diego meeting – March 25 – 29, 2012
    - Program – Symposium: Educational Tools for Chemical Information
    - Other
3. Looking ahead
    - Philadelphia – August 19-23, 2012
    - New Orleans – April 7-11, 2013
4. BCCE 2012 – Penn State (University Park, PA) July 29 – August 2, 2012
5. Workshops – should we resume them at ACS meetings?
6. Information Competencies for Chemical Undergraduates – update on response from CPT (if not covered above)
7. Information Competencies for Chemical Graduates – getting the ball rolling.
8. New business

For more information, please contact the chair, Chuck Huber, at huber@library.ucsb.edu.

Fundraising Committee

After a less than robust fundraising cycle for the spring 2011 meeting in Anaheim, we have had a nice rebound in sponsor interest for the fall 2011 meeting in Denver. We have a record six co-sponsors for the CINF Sunday Welcome Reception, two sponsors for the Tuesday CINF Luncheon, continued funding for the CINF Scholarships for Scientific Excellence and for Harry's Party Monday, snacks and beverages for the Wednesday CINFlash symposium, and a very generous contribution for the Herman Skolnik Award Symposium and Reception.

Please see the CINF Social Networking Events listing for event times, locations and sponsors. CINF thanks all our sponsors for making these great activities possible.

We are always looking for new members and we are specifically looking for an assistant Fundraising Chair who will transition to Chair in 2012. Please contact Graham Douglas at Fundraising@acscinf.org if you would like to join the CINF Fundraising Committee.

Graham C. Douglas
CINF Fundraising Chair
Fundraising@acscinf.org

Program Committee

The Program Committee always welcomes new members and attendees to come and join us at our meeting. Our meetings are always open, and any member is free to come and participate and offer program suggestions for future meetings or even to offer to chair and organize a symposium for a future meeting.

At our meetings, for example, the meeting in Denver, we will review the details and statistics for the current program (i.e. how many symposia, topics of symposia, how many abstracts, etc.) and the proposed program for the upcoming meeting, in this case Spring 2012 in San Diego. We will then open the floor to members to begin to discuss the program for future meetings.

Because the abstract submission deadlines for ACS meetings are extremely early, planning the proposed symposia and programs for the national meetings must occur considerably in advance, and we will begin planning meetings almost 2 years ahead. We want an interesting and diverse program, and it helps to have members of our committee that represent all the diverse topical interests of CINF membership. The proposed programs and symposia for future meetings are stored on a Google doc document that all committee members are given permission to view.

Please feel free to attend our meeting in Denver and offer your program suggestions or volunteer to organize a symposium on your favorite topic (related to CINF interests, of course!), or contact me with your suggestions at rachelleb1@gmail.com.

Rachelle Bienstock
CINF Program Committee Chair
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Report on the Council Agenda for August 31, 2011

The Council of the American Chemical Society will meet in Denver, CO on Wednesday, August 31, 2011, from 8:00am until approximately 12:00pm in the Centennial Ballroom A - E of the Hyatt Regency Convention Center Hotel. All ACS members are welcome to attend, although only Councilors are permitted to vote. A continental breakfast is usually available at 7:00am for all attendees.

There are a number of items for Council Action, but the majority is routine and not major. The action items are summarized below.

Nominations and Elections

Council Policy Committee
Council will vote to fill four slots on the Council Policy Committee. There are eight nominees as follows: Spiro D. Alexandratos, Lawrence Barton, Michael J. Brownfield, John W. Finley, Mark D. Frishberg, Peter C. Jurs, Mamie W. Moy, and Eleanor D. Siebert.

Committee on Committees
Council will vote to fill five slots on the Committee on Committees. There are ten nominees as follows: Matthew K. Chan, Richard S. Danchik, Rigoberto Hernandez, Roland F. Hirsch, James. M. Landis, Jr., Bonnie Lawlor, Zaida C. Morales-Martinez, Howard M. Peters, Sara J. Risch, and Jason E. Ritchie.

Committee on Nominations and Elections
Council will vote to fill five slots on the Committee on Nominations and Elections. There are ten nominees as follows: R. Gerald Bass, Cherlynvaughn Bradley, William H. (Jack) Breazeale, Jr., Catherine C. Feneslau, Lydia E. M. Hines, Robert L. Lichter, Anne T. O'Brien, Robert A. Pribush, Andrea B. Twiss-Brooks, and Steven W. Yates

Town Hall Meeting
A Town Hall meeting organized by the Committee on Nominations and Elections is scheduled for Sunday, August 27, 2011 in the Hyatt Regency Convention Center Hotel, Centennial Ballroom F/G, from 4:45pm - 5:45pm. It will highlight a Q&A session with the candidates for Directors-at-large. All ACS members are encouraged to attend. It is a great way to gather first-hand information and decide for whom you might want to vote in the fall election.

Change in Committees

The Committee on Committees (ConC) will put forth a recommendation for the continuation and/or dissolution of the committees that have been reviewed as required by the Committee Sunset Laws. The committees were not named in the Agenda Book. ConC will also honor all committee chairs and members who have reached their statutory limit of service and will recognize Councilors who reached the milestones of 15, 20, 25, 30, 35 and 40 years of service.

Division Dissolution and Division Creation

The Division of Fuel Chemistry and the Division of Petroleum Chemistry wish to combine effective year-end 2011. In June, the Committee on Divisional Activities (DAC) voted to support the following motion: "The Committee on Divisional Activities recommends to Council that the Division of Petroleum Chemistry be dissolved, and that its assets and members be combined with those of the Division of Fuel Chemistry, under the new name of the Division of Energy and Fuels, effective December 31, 2011." DAC will bring this recommendation to Council for a vote in Denver.

DAC will also recommend that the probationary Division of Catalysis Science and Technology (CATL) be granted full Division status. CATL's bylaws have been approved by the Committee on Constitution and Bylaws (C&B), and C&B will recommend that Council approve the Bylaws as part of their being recommended for full Division status.

Special Discussion Item

On occasion, an ACS President will request that a special discussion item be placed on the Council agenda. In Denver, the topic "How can ACS best cultivate a culture of safety in U.S. universities and colleges?" will be discussed in response to devastating incidents in academic laboratories and observations by many that graduates do not have strong safety skills.

In June 2011, the Safety Culture Task Force (SCTF) held a retreat to discuss and begin efforts to prepare publications that might assist academia in strengthening its safety cultures. Specifically, SCTF seeks to identify the best elements and best practices of a good safety culture, identify academic institutions that are currently using these best practices, identify specific recommendations that could be used by universities and colleges to strengthen their safety culture, and identify tools and resources that could be beneficial in these efforts.

Elements that SCTF believe to be critical to strengthening safety cultures are: leadership; teaching basic laboratory and chemical safety; safety ethic/attitude/safety awareness; learning lessons from laboratory incidents; collaborative interactions; promoting and communicating safety; and encouraging institutional support of safety by budgeting for safety programs and supplies.

SCTF seeks: 1) input, suggestions, and recommendations for strengthening the safety culture in academia; 2) "bright spots" – those places within academia that provide exemplary examples of one or more of the above mentioned safety culture elements; and 3) good resources and instructional materials that can be used to build strong safety cultures. Send your comments and suggestions to Marta Gmurczyk, ACS Staff Liaison to the Committee on Chemical Safety at M_Gmurczyk@acs.org

Bylaw Changes for Council Vote

Petition on Position Statements
(adapted from the Council Agenda Book)

The ACS Constitution makes it clear that any position statement that expresses the position of the Society as a whole requires the approval of the Board of Directors. ACS Bylaws (Bylaw IX) regulate the issuance of position statements by any "Society Body" other than the Board. Theses bodies include Local Sections, Divisions and, presumably, ACS Committees.

As currently written, Bylaw IX could potentially conflict with the Board Regulations governing position statement development. This petition is intended to allow for a clear and consistent position statement development process for the Society.

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

The Budget and Finance Committee has examined the petition and concludes that it will have no financial impact on the Society. The Committee on Constitution and Bylaws (C&B) has prepared a revised version of the petition, making editorial changes to clarify the wording and to remove wording that was not necessary, and to include additional new language from petitioners that addressed C&B's concerns. C&B finds the petition to be legal and consistent with other provisions of the Society's documents. A two-thirds vote of Council is required for approval. If approved by Council, the amendment will become effective upon confirmation by the Board of Directors.

Bylaw Changes for Consideration Only

Petition on Market Data Collection
(reproduced from the Council Agenda Book)

In March 2010, the ACS Board and President established the ACS Board-Presidential Task Force on Society Services and Associated Dues Pricing Models. The Task Force was charged with reviewing and making recommendations based upon member input related to any concerns, questions, and/or suggestions that they had in these areas. In seeking member input, the Task Force relied on three main sources:

- Actual input from Divisions, Committees, Local Sections and individual members
- Results from the 2010 ACS Membership Satisfaction Survey and,
- Information as to why the Society loses over 20,000 members per year – almost 11.5%

Based upon the findings from these sources, the Task Force proposed the following recommendations:

- Allow for test marketing of membership concepts
- Review the dues escalator
- Minimize dues category information within the Society Bylaws
- Consider permitting institutional memberships

The Society has historically changed bylaws without the benefit of test data. This petition seeks to add a provision to allow for the recommended controlled market testing to collect data before the Society changes benefits, dues, or membership categories.

The financial impact of this petition is still being assessed. The Committee on Constitution and Bylaws (C&B) has reviewed the petition and finds it to be legal and consistent with other provisions of the Society's documents. However, C&B is concerned that there are no stated limits to market testing, either in scope or duration. There appears to be no precedent in the Society's documents for allowing a Council Committee to override the Bylaws by setting dues and other member benefits without stated limits. There is also no provision to report to the Board on a yearly or other stated time period.

Comments and suggestions from committees, petitioners and other interested members on the

substance of the petition should be directed to the Committee on Membership Affairs, which has primary substantive responsibility for the petition. Other comments and suggestions may be directed to C&B.

Petition to Amend Recorded Vote Request Procedure
(reproduced from the Council Agenda Book)

Since March 2009, the Council has routinely used a clicker system for voting and surveys. While only numerical results have been reported, the computer that totals the votes can list votes by clicker number from which it can be determined how each Councilor voted.

Because the new technology can facilitate recorded votes without the need to put all business on hold while signed ballots are collected and counted, Bylaw III, Sec.4, d, was recently amended to permit clicker voting, or any other method from which it can be determined how each Councilor voted, to be used for recorded votes.

This recent change in the Bylaws raises secondary issues. Can a call for a recorded vote come after a clicker vote, and if so, should there be a second clicker vote or should the record from the first clicker vote be the one published in *Chemical & Engineering News?* Clarification is necessary.

To address this issue, the Council Policy Committee (CPC), which has the authority to set the Council's agenda and procedures, issued guidelines for first use at the Spring 2011 ACS National Meeting. The guidelines provide that "Whenever the Chair chooses a clicker vote, Councilors should be asked if there is a request for a recorded vote." The guidelines also provide that there will be only one clicker vote on any one issue. In addition, at its spring 2011 meeting, CPC agreed to prepare a petition to clarify the Society Bylaws on this issue in collaboration with the Committee on Nominations and Elections and with the advice of the Committee on Constitution and Bylaws.

The proposed Bylaws change makes it clear that there will be only one recorded vote possible on any one issue. It also makes it clear that other voting, such as a voice or show of hands, can precede the recorded vote. However, a call for a recorded vote after clicker voting has commenced will be out order as would a call for a recorded voted after the initial clicker voting has taken place. A variation of the phrase "a voting method from which it shall be determined how each Councilor voted" already in this Bylaw has been added to the first sentence of the Bylaw. Although apparently redundant language, the first phrase clarifies procedure; the second defines a recorded vote.

Clicker voting is referenced in this explanation because it is the specific technology that has raised the issue. The more inclusive language in the proposed Bylaw, "a method from which it can be determined how each Councilor voted" has been chosen to allow for other technology that Council may use in the future. Council's traditional method of signed ballots is also covered by the inclusive language should Council ever wish to return to that method for a recorded vote.

The financial implications of this petition are still being assessed. The Committee on Constitution and Bylaws has reviewed the petition and finds it to be legal and consistent with other provisions of the Society's documents.

Comments and suggestions from committees, petitioners and other interested members on the substance of the petition should be directed to the Council Policy Committee, which has primary substantive responsibility for the petition. Other comments and suggestions may be directed to C&B.

Respectfully submitted July 25, 2011

CINF Councilors

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A New Reality for Academic Chemistry Librarians:

An Interview with Grace Baysinger

By Svetla Baykoucheva

Grace Baysinger is the Head Librarian and Bibliographer of the Swain Chemistry and Chemical Engineering Library at Stanford University (http://lib.stanford.edu/swain). She served as Head of Stanford's Science and Engineering Libraries from 1999-2005. Prior to coming to Stanford, she worked at the University of Michigan Libraries. Her professional interests include collection development and management, scholarly communication and publishing issues, online searching and interface design, and user instruction. She is currently a member of the American Chemical Society (ACS) Committee on Chemical Abstracts Service, ACS Chemical Information Division–German Chemical Society's Computer in Chemistry Collaborative Working Group, Chemical Structure Association Trust, *CRC Handbook of Chemistry and Physics* Advisory Committee, Thieme's *Science of Synthesis* Advisory Board, and the *Journal of Chemical Education* Advisory Board. Previous professional activities include serving as a member of the Royal Society of Chemistry's Journals Committee, a member and the Chair of the ACS Publications Committee and Copyright Subcommittees, and Chair of an ACS Task Force on the Electronic Dissemination of Meeting Content. Grace has a B.S. in Botany and an M.S. in Library Science from the University of Michigan, and an A.S. in Science from Kalamazoo Valley Community College in Michigan. Grace was awarded the Stanford University Marshall D. O'Neill Award in 1996, the Stanford University Libraries' Distinguished Service Award in 1997, the ACS CINF Meritorious Service Award in 2004, and the SLA Chemistry Division's Wiggins-Roth Award for Outstanding Service in 2011.

Svetla Baykoucheva: You have been a fixture for members of the Chemical Information Division (CINF) of the American Chemical Society (ACS) for many years. Is there at least one ACS national meeting that you have missed in the last 15 years? Which are your favorite cities to go to for an ACS national meeting?

Grace Baysinger: I've been to all of the ACS national meetings in the past 15 years. I don't really have any favorite cities and I have enjoyed going to all of them. Being able to visit different parts of the country is great. My favorite part of attending ACS meetings is seeing colleagues! Learning new things, having in-depth conversations, participating in team efforts, and lobbying to help shape the information landscape are other reasons why I think it is essential to attend every ACS national meeting.

SB: During the years, you have been able to see many developments at ACS, in general, and CINF, in particular. Could you name some of the important ones which, in your opinion, have brought significant changes to ACS and/or CINF?

GB: Technical sessions have remained a strong, core benefit for CINF members and across ACS. The knowledge and experience of people involved in CINF and ACS activities is impressive. Strategic planning has grown in importance both as a roadmap and as a foundation for evaluating effectiveness of activities. Fostering the next generation of leaders within CINF and ACS has become more purposeful. As it has been throughout society, technology has been an important factor driving change. Celebrating its 20th birthday, CHMINF-L has enabled a global community of chemical information professionals to communicate quickly and easily with one another. Web sites provide an easy way to share information and distribute publications. Debbie Molina and Barden Shimbo, from Stanford's Swain Library, digitized CINF documents such as the Procedures Manual, Education Committee workshops, and the booklet celebrating CINF's 50th Anniversary (https://lib.stanford.edu/swain/projects). In 1999, when I was the

Chair of CINF, I spearheaded efforts to launch CINF E-News. CINF has always been a leader and early adopter within ACS, providing access to CINF presentations given at ACS national meetings. ACS has made great strides in the past couple of years and now provides access to hundreds of presentations from these meetings. ACS plans to hold a career fair at the upcoming meeting that will include forums for virtual participants. Task forces, committees, and other governance work often include virtual meetings. The ability to work, play, and communicate using mobile devices is becoming ubiquitous. While technology tools have changed the way we all do business, the talent and expertise in CINF and ACS have resulted in creative, thoughtful deployment that helps catalyze our activities.

SB: The nature of the work chemistry librarians are doing today has changed and many chemistry libraries closed in the last 10 years. How does this affect the morale and self-esteem of chemistry librarians professionally?

GB: Budget reductions, space competition, deferred facilities maintenance, and rapidly expanding digital collections have resulted in a number of branch libraries being closed, consolidated, or downsized. These radical changes may include a profound sense of loss but also offer a range of new opportunities and possibilities. No longer working to keep daily operations on an even keel, chemistry librarians can focus on collections and services. While the format of materials has changed from print to electronic, the need to acquire content to meet programmatic needs has not diminished. Financial crises offer the perfect opportunity to do an in-depth analysis of collection use to help ensure you get the biggest bang for your buck. Developing sustainable models to provide instruction and develop course/research guides offer ways chemistry librarians keep in sync with users' needs. Systematic communication to keep the dialogue open is essential. Digital collections and powerful, yet intuitive, discovery tools provide a foundation for a 21st century library but don't just happen by themselves. They need input from specialists like chemistry librarians, who are used to dealing with large, complex resources. Point-of-use needs should be addressed through online self-service so that staffing resources may be used for complex information needs. Through digital collections and services, we have the opportunity to act locally but think globally!

SB: How do we move from reference to eScience? What are the plans at Stanford with respect to this new area for librarians, and in what way are you involved in it?

GB: Librarian colleagues in the life sciences, earth sciences, social sciences, and government documents have dealt with data for a number of years. Having conversations with these colleagues could provide insight into practices that might be adopted in chemistry. Deposition of crystallographic data associated with research papers is the norm. Chemistry librarians have in-depth experience searching numeric databases, such as Reaxys and CHEMnetBASE resources. So, I feel like we are doing eScience already. The aspect that is new is to become involved much earlier in the process: trying to understand practices used by researchers when data are being generated, being involved in metadata creation for these data, working with our colleagues who manage our institutional repositories to help ensure methods area viable for our researchers, etc. This will be followed later on by requests to locate multiple data sets that contain *x* type of information that were generated under *y* conditions, requests that are common in the GIS realm. So support for researchers is going to be interesting in ways that will require new skill sets for chemistry librarians.

Regarding eScience activities at Stanford, about a year and a half ago Lynn Yarmey was hired in a new Data Science Librarian position (*First Science Data Librarian Named*, ReMix, November 18, 2010, Issue 34. http://hosted.verticalresponse.com/260487/cde16e8198/TESTTEST#Four). Data will be deposited into Stanford's Digital Repository (http://lib.stanford.edu/sdr). Last summer, Lynn and Joe Wible, Head Librarian at Stanford's Hopkins Marine Station, did a pilot project to learn more about data needs (*Science Data and Libraries*, ReMix, May 21, 2010, Issue 28 http://hosted.verticalresponse.com/260487/4f8510f69b/TESTTEST#1). More recent efforts have included

doing faculty interviews. I'm still in the learning phase and will be working closely with Lynn as things move ahead to address data curation needs for the chemists and chemical engineers.

SB: You have been involved in many initiatives at ACS. Which of these you have found to be particularly interesting, challenging, and/or rewarding?

GB: ACS is a large and interesting organization. I thoroughly enjoyed being on the Joint Board-Council Committee on Publications (JBCCP). I was Chair of JBCCP (the first librarian to be appointed to this position; the JBCCP Chair is also the Chair of the *Chemical & Engineering News* (*C&EN*) Editorial Board, whose members include the Chair of the ACS Board of Directors and the President of ACS). Both of these meetings were always interesting, challenging, and rewarding. In January, the JBCCP Chair is invited to attend an ACS Editors Conference whose attendees include the Editor-in-Chief for each of the ACS journals. Listening to their comments and learning more about scholarly publishing issues from their perspective was wonderful and thought-provoking. I'm currently a member of the Joint Board-Council Committee on Chemical Abstracts, which also deals with an array of interesting topics and issues. Being on the ACS Committee on Community Activities was a lot of fun. I've been on three ACS task forces, two as a member and one as a Chair. When Chairing the Electronic Dissemination of ACS National Content Group (http://www.acs.org/meetingcontent), I had the opportunity to work with a different cross-section of the organization, to benchmark what other organizations were doing, and to learn more about the impact sharing meeting content online has on prior publication. Richard Love, along with ACS staff, did a wonderful job of implementing a pilot program that has subsequently grown into a library of about 500 presentations per meeting (http://www.acs.org/meetingcontent).

At the CINF Level, one of the most interesting and rewarding initiatives I've been involved in is the CIC-CINF Working Group, the first division-to-division collaboration between ACS and GDCh (Gesellschaft Deutscher Chemiker). Led by Guenter Grethe and René Deplanque, we developed XCITR (http://www.xcitr.org) which stands for eXplore Chemical Information Teaching Resources, a repository of instructional materials, and have co-organized symposia. We meet at ACS national meetings and have met in Germany several times.

SB: You are also very involved in scholarly publishing. How do you see the developments in this area in the near future? How does scholarly publishing relate to eScience?

GB: In the near future, digitization of older materials, along with born digital materials, will provide a vast online library to scholars. Structured databases, complemented by semantic web technologies in full-text resources, will aid discovery. Visualization tools of content and search results will help provide users a bird's eye view of results and will aid them in identifying areas of deeper inquiry. Interdisciplinary research will continue to grow, as addressing complex problems will require researchers from different domains. While new forms of publications will grow and old ones will be mashed up in new ways, I don't see the traditional journal going away in the sciences or publishers being replaced by institutional repositories. Instead, we will have both the traditional and new forms of scholarly communication.

Regarding eScience and focusing on data, knowing the provenance of the data will be important. Being able to compare data sets or interpret a particular data set requires knowing a broad array of information about that data. Having more "raw" data for research linked to a published article would be helpful in a number of ways. For example, it would help readers who want to look at data from a different perspective than the author did or who want to replicate an experiment. As part of the publishing process, I expect automated methods to grow that will help in detecting error, fraud, or plagiarism. If formatted properly, live data could be the foundation for more specialized databases, as there is now for crystallographic data. For authors, eScience data offer an opportunity to be recognized and cited in new ways. To promote data

deposition, a reward system needs to be built in for authors. So stay tuned for adventure as eScience activities move forward!

SB: What is the most pleasant thing you enjoy doing at work? Tell us about something that even people like me who have known you for a long time don't know about you.

GB: Helping people find what they need is very rewarding. Building collections and understanding the ecosystems of the collections themselves is a close second. Because interface design and discovery, as well as licensing and pricing, impact access and delivery of the content, I am interested in those aspects of collection building, too.

Regarding something most people don't know about me, one of my earliest volunteer efforts some 30 years ago was volunteering with another University of Michigan librarian colleague at a women's prison in Michigan. While legal libraries are required in prisons, no requirements existed for educational or recreational reading. The non-legal materials had all been donated and were sitting on shelves unorganized. There were probably 10 linear feet of math textbooks sitting on the shelves (talk about being punished!). During our weekly visits over three years, we weeded, organized, labeled, and cataloged materials so that the collection could be used more effectively and efficiently. It was a memorable experience about an underserved population in our society.

Academically, I have a B.S. in Botany and you may wonder how I ended up being a Chemistry Librarian. My interests have always been broad. As an undergraduate I took a number of graduate level classes because I enjoyed doing library research. I was curious about the history of the earth and how plant populations have changed and evolved over time. Coursework included a number of paleobotany classes as well as geology classes in geomorphology and sedimentology. One prominent method for studying what kind of plants existed in a geographic region was studying what pollen was preserved from these plants (palynology). Learning about life during the Ice Age was fascinating! I considered becoming a palynologist but decided that I liked working with people too much and didn't want to spend my days in front of a microscope. Most jobs for palynologists were either working for an oil company analyzing cores or becoming an academic. I decided neither option was appealing. While I was thinking about what career path to choose, I took a paraprofessional job at the University of Michigan's Natural Sciences Library and subsequently attended library school and was hired as a reference librarian in the same library. Some of my most intriguing and challenging reference questions were biochemistry ones. My interest in chemistry continued to grow and when the Head of the Chemistry Library position at the University of Michigan became available, I decided to apply for it, and, as they say, the rest is history. Patricia Yocum was a strong mentor during my entire decade at the University of Michigan Libraries. Patricia helped me build a strong foundation that has served me well throughout my career. In 1989, I was recruited to apply for the Head of Stanford's Swain Chemistry and Chemical Engineering Library. It has been a wonderful place to work. The people are great and there's never a dull moment!

SB: Thanks, Grace, for this information-rich interview and congratulations on your SLA Award.

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Chemistry Resources for Changing Climates

By Fred Stoss

The topic of global climate change is complex and controversial. There is a large and rapidly growing body of data and information generated by regional, national, and international research; modeling; monitoring; development programs; and campaigns. The physical and life sciences serve as the scientific and technical core and the basis for our understanding of climatic changes. Chemistry provides the greatest contribution to that understanding, as we examine the dynamic nature of abiotic and biotic interactions in the atmosphere, oceans, and landmasses. Look at the number of results you get with a SciFinder search on concepts related to global climate change and greenhouse gases (carbon dioxide and other radiatively active so-called greenhouse gases). Good science and good access to scientific data and information, much of it in the field of chemistry, are driving good policies and decision-making processes. There are tens of thousands of Web-based resources where the chemistry of climate change takes center court. Here are several personal favorites.

Carbon Dioxide Information Analysis Center and World Data Center (WDC) for Atmospheric Trace Gases at Oak Ridge National Laboratory provides chemistry-related data to glaciology, physiochemical geology (land and marine), meteorology, and other climate-related disciplines involving human interactions in our environment. Look for CO_2, CH_4 and other atmospheric concentrations, one of the most comprehensive CO_2 emission inventories, and ocean chemistry data. (Other highly relevant WDCs are at http://www.ngdc.noaa.gov/wdc/wdcmain.html.)
http://cdiac.ornl.gov

The Royal Society of Chemistry's "The Chemistry of Climate Change" resources site for students in age groups of 14-16 years and 16-18 years and their teachers, including a rather special PowerPoint presentation and full text documents.
http://www.rsc.org/Education/Teachers/ClimateChange/index.asp

The National Science Digital Library, the National Science Foundation's online library of resources and collections, including images, video, audio, animations, software, datasets, and text documents, such as lesson plans and journal articles. Results can be filtered by K-12 grade level, higher education, and user groups of teachers, educators, and librarians.
http://nsdl.org/

America's Climate Choices, a 2011 report (free PDF downloads) of America's Climate Choices project, the National Research Council's most comprehensive study of climate change to date, including links to other National Academies reports and videos on climate change.
http://www.nap.edu/catalog.php?record_id=12781

ARM - Education: Teachers' Lounge from the U.S. Department of Energy's Atmospheric Resources Monitoring Program provides strong links to the sciences supporting atmospheric chemistry and physics as they relate to the Earth's climate.
http://education.arm.gov/teacherslounge/lessons/global.stm

Lesson Plan: Global Warming, produced by the Public Broadcast System with NOW Classroom standards-linked resources for students and teachers in "social studies, debate, language arts, government/citizenship, and current events, grades 9-12," with links to other NOW Classroom resources. (NOW is a production of JumpStart Productions, LLC, in association with Thirteen/WNET New York)
http://www.pbs.org/now/classroom/globalwarming.html

The U.S. Global Change Research Program, an overview of the 21-year old, integrated and coordinated, 13 inter-agency research programs bringing a scientific understanding of global change phenomenon, including climate change, through research, education, communication, information, and decision-making.
http://www.globalchange.gov/

Global Change Master Directory is NASA's comprehensive "finding tool" for data and information resources from among more than 25,000 earth and environmental sciences datasets and inventories. The GCMD has a very robust search capability and serves as a major resource for finding scientific and technical data.
http://gcmd.nasa.gov/

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CINF Members Confer

Members of ACS CINF are very active, not only in local and national ACS activities, but also in other professional societies. Dr. Wendy Warr and Susan Cardinal responded to an open call to report the happenings at recent meetings that they attended.

International Council for Scientific and Technical Information

by Wendy A. Warr

ICSTI's winter meeting consists of ICSTI committee meetings, for members only, plus a one-day workshop open to the public; the summer meeting involves the General Assembly and committee meetings for ICSTI members, plus a more major conference than the winter one. The ICSTI 2011 Winter Meeting was held on February 6-7, 2011, and was followed on February 8 by a workshop, the theme for which was "Multimedia and Visualization Innovations for Science." Both events were hosted by Microsoft, an ICSTI member, on their Redmond campus, Washington. The program is at http://www.icsti.org/spip.php?article213, and PowerPoint presentations can be accessed from that page. The videos are password-protected on the ICSTI members' pages. The official meeting overview states:

Multimedia and visualization tools and technology offer tremendous opportunity for accelerating scientific discovery. Where science was once limited to text and two-dimensional graphs and charts for communications purposes, multiple factors have contributed to a rise in the use and availability of multimedia and visualization as tools to augment and enhance more rapid uptake of science. This workshop featured leading-edge innovations in science-oriented web multimedia, large-scale data exploration and visualization, speech and object recognition, image indexing and analysis, human/computer interaction and virtual environments, among other topics. Presentations were made by technology, science, and information professionals across the broad spectrum of academia, government, business, and industry. *(http://www.icsu.org/events/scientific-associate-events/multimedia-and-visualisation-innovations-for-science, accessed August, 2011)*

ICSTI's 2011 Annual Conference was held June 7-8 in Beijing. It was hosted by ISTIC, the Institute of Scientific and Technical Information of China, and the theme of the Conference was "Upgrading Information to Knowledge." About 400 people attended. The conference program and the presentations are at http://www.icsti2011.org/eng/download_information.html. The full text of "submitted papers" (not presented orally, but published in a prestigious Chinese journal) can be accessed from http://www.icsti.org/. The Conference was followed by ICSTI's General Assembly and committee meetings from June 8-9.

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Teaching, Networking, and Learning at SLA 2011 in Philadelphia, Pennsylvania

by Susan K. Cardinal

As I drove into Philadelphia on a sunny June day, I was very optimistic about the value of the SLA meeting to me. I was a little nervous also, because, for the first time, I would be co-teaching "Chemistry for the Non-Chemist Librarian" with Judith Currano.

Early Saturday morning, we met eight science librarians and information professionals, both from corporations and from academia, who wanted a crash course in chemistry to help them communicate better with their patrons. Judith and I delivered a full day of history, stories, hands-on activities, and lectures that defined the vocabulary and nomenclature of chemistry. We were all pleased when the fear left our participants' eyes and some of the terminology that earlier had confused them became clear.

Our reward was a tasty meal at the No-Host dinner at the "Palace at the Ben." I enjoyed meeting several Royal Society of Chemistry staff members.

On Sunday, I was a participant in Judith's and Denise Callihan's Extreme Structure Searching. Although I was familiar with substructure searching, I picked up more nuances, especially setting points of attachment on R/G Groups. For the first time I realized that patents in a family can have more differences than just language.

In the evening, Thomas Friedman, columnist for the *New York Times*, told us about globalization and that being average is no longer safe since everyone in the world could potentially be a candidate for our jobs. Visit http://www.theconferencecircuit.com/2011/06/12/1708/ for a summary of his talk.

The next morning, at the Academic Round Table, each table picked one or two topics to discuss. At my table, we discussed "What roles do discovery platforms play in chemistry research?" After defining a discovery platform as the next generation metasearch engine for articles and more, the conclusion was that these interfaces are mostly geared towards the general undergraduate as Google competition. Other topics discussed were:

- How can you facilitate partnerships with chemistry faculty to successfully promote library resources?
- What role will InChI play in a chemical semantic Web?
- Now that so much information is online, how might we embed ourselves physically, virtually or both into chemistry departments?
- What are the budget predictions for next year, and how will we cope?
- How do we react to the illegal distribution of scientific e-books when we can't (or don't) pay for the e-book packages? What are the ethical implications?
- How can we use mobile technology to its fullest advantage when working with our patrons?
- What role does data curation play in your liaison activities? Do you envision this role changing in the future?

Later in the morning, I listened, as Lutishoor Salisbury from the University of Arkansas described a 1-credit seminar class that helped undergraduates get involved in research earlier in their studies. In one assignment, a small group of students picked three faculty members to study and then selected one to interview about his or her research. The class included a library instructional session, during which the students learned about the library, the databases, and Boolean searching, applying their knowledge to the task of finding and understand their professor's publications.

That afternoon, at "So They Say You Have to Publish," I received lots of advice on how to find ideas and write. The core message was to read and write regularly and to start small. It is okay to contact editors when you think you have a concrete idea for a paper to see if it will fit the journal. Editors may even be willing to be consulted by potential authors, regarding research and analysis methodology.

The next day, during the Chemistry Division Business Meeting and Breakfast, I was very pleased to witness Grace Baysinger receiving the first Wiggins-Roth Award for Outstanding Service, sponsored by Elsevier/Reaxys. We elected Susan Makar from National Institute of Standards and Technology (NIST) to be the Chair-Elect for 2012 and Lee Pedersen from Brown University to be the Secretary for 2012-2013. During lunch, Judith Currano showed me two cool widgets on the University of Pennsylvania Chemistry Library's home page, one for book renewals and one for signing up for training sessions.

Louise Deis from Princeton told me that, at the "International Year of Chemistry: Perils and Promises of Modern Communication" session, Dr. Lawrence Souder and Dr. Jean-Claude Bradley from Drexel spoke about how scientific "knowledge rests on the trust in ethics and morals of those practicing" (Souder, 2011). The truth is twisted to serve purposes; sometimes, reported information is not accurate, and the peer review system fails us. Blogs are taking a more prominent role in evaluating research and presenting science. Dr Bradley's students compared melting points for 24 compounds from trusted sources, and their faith in these sources was shaken due to errors found. He suggested that science will make faster progress if research results are posted openly and are easily found.

In the evening, I attended the poster session and was overwhelmed with interesting posters. I'm checking with the Chair, Bill Armstrong, to see if there will be an online poster session later in the year as I'd like to study them at a slower pace.

During the course of the meeting, I also met with several publishers and vendors. What a valuable and fabulous 2011 Philadelphia SLA meeting! As usual, there wasn't enough time in the week to take it all in.

If you'd like to learn more, please visit the SLA Chemistry Division website at http://units.sla.org/division/dche/index.htm.

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Book Review

Special Topics in Intellectual Property; Twiss-Brooks, A., Ed.; ACS Symposium Series 1055; American Chemical Society: Washington, DC, 2010, $150.00 (Hardcover). 128 pages. ISBN: 9780841225947.

(Disclaimer: the reviewer wrote one chapter of this book and reviewed, pre-publication, one of the other chapters. His pre-publication knowledge of the remainder of the book was limited to article titles.)

This book is based on the symposium, "IP to IP: Intellectual Property for Information Professionals," organized by Leah Solla, Andrea Twiss-Brooks, and Pamela J. Scott and presented at the 238th National Meeting of the American Chemical Society, Wed. Aug. 19, 2009, Washington, DC. Of the six papers presented in the symposium, five appear as chapters in this book, and five additional chapters on related topics have been added. The book includes an index and contact information for authors of chapters.

In the introduction, Pamela Scott outlines the scope of the symposium (and therefore, the book) as the intersection of the fields of intellectual property (IP) and information science, in which the key players are lawyers, other IP specialists, educators, searchers, librarians, and consultants. Readers of this book, as well as most of those in attendance at the symposium, are likely acquainted with the authors and editors.

Renate Chancellor leads off with "Copyright in the Information Age," describing copyright from the viewpoint of librarians, who often find themselves squeezed between the needs of publishers and those of their clients. Lawrence Robins follows with a chapter, "Copyright Basics," an excellent primer on copyright from the legal standpoint, including ownership, rights, and things that can and cannot be copyrighted. Although both authors cover Fair Use, neither seems to discuss the recent and often contentious issues surrounding Open Publishing and Open Access. The next chapter, also by Robins is entitled, "A Guide to Trademark Selection, Clearance, and Use" and discusses a number of topics, including registration, priorities, and searching. These three chapters provide valuable information and background on those aspects of IP not covered nearly as well as patents.

Robert Buntrock follows with "Careers in Intellectual Property." In this chapter he expands his contribution to Chapter 20 in the Chemical Information Sources Wiki ("Careers in Chemistry," http://en.wikibooks.org/wiki/Chemical_Information_Sources/Careers_in_Che...) and stresses the need for educational background in chemistry and other sciences for these careers. Pat Newcombe then presents a chapter, "Interviews with Professionals in the Field." She interviews eight IP professionals: three patent attorneys, two patent educators, a patent agent, a patent searcher, and a technology specialist. Via Q&A, they recount the nature of their work, applicability of their education, methods of maintaining their skills, advantages/disadvantages, and future developments.

The book closes with four chapters on educational aspects of intellectual property. Lucy Akers describes "Continuous Learning," including mentoring, online services, universities, libraries, associations, patent offices, and certification. John Calvert writes "Educating the Inventor Community" from the viewpoint of the US Patent and Trademark Office (USPTO). Edlyn Simmons describes "The PERI Patent Information Course," with which she has long been associated. PERI (PMA Education and Research Institute) provides courses sponsored by the Pharmaceutical Manufacturers Association, and Simmons describes the course's background and curriculum. Robert Stembridge concludes with "Education and Certification of Patent Information Professionals in Europe."

This book should be a resource for IP professionals, especially those dealing with the information and education aspects of the related fields. Those new to or contemplating entering the field will find this book especially valuable. At $1.17 per page, this book is an expensive purchase, especially for non-subsidized individuals, but it is a good product and could be valuable to a wider audience. However, one should question the impact of very expensive symposium books, which are so highly priced as to limit the market. In all fairness, the price will make the book less attractive for individual, as opposed to library, purchase.

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News from Our Sponsors

The American Chemical Society Division of Chemical Information (CINF) is very fortunate to receive generous financial support from our sponsors to maintain the high quality of the Division's programming and to promote communication between members at social functions at the ACS Fall 2011 National Meeting in Denver, CO, and to support other divisional activities during the year, including scholarships to graduate students in Chemical Information.

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Bio-Rad Announces Advances in Spectral Searching and Database Building in Its KnowItAll Software

HERCULES, CA – August 9, 2011 – Bio-Rad Laboratories, Inc. (NYSE: BIO and BIOb), a multinational manufacturer and distributor of life science research and clinical diagnostic products, today announced an unlimited spectral range and resolution feature in version 9.0 of its award-winning KnowItAll® software.

KnowItAll 9.0 allows users to store spectra in a user database at the precise range and resolution at which each spectrum was measured rather than being forced to conform to a fixed range and resolution for the entire database. As a result, users have more control over their data and can perform more accurate spectral searches that compare experimental spectra to reference databases.

"Technological advances have changed disk space and computational time limitations of computer search methods, making possible major advances in spectroscopic computing," explained Gregory M. Banik, Ph.D., General Manager, Bio-Rad Informatics. "Removing constraints on spectral data is critical to those who perform spectral searches or store spectral data, since altering an original spectrum's resolution has a significant impact on search results. With KnowItAll 9.0, researchers can preserve the integrity of their spectral databases. In addition, they have access to search software that follows best practices defined by the most recent research conducted by spectral search experts at Bio-Rad Laboratories as well as American Society for Testing and Materials standards."

Additional features in the KnowItAll 9.0 release include:

- Independent management of properties from multiple analytical techniques in user databases
- User database creation simplified
- New structure drawing tools to comply with IUPAC structure drawing guidelines
- Higher resolution spectra in HaveItAll® IR, NIR, Raman database subscriptions
- Spectra added to HaveItAll IR, UV-Vis, and NMR database subscriptions

Additional information on the KnowItAll 9.0 release is available at www.knowitall.com/literature

About Spectral Searching
Researchers use spectral search software to identify unknown substances and verify the composition of synthesized materials in a number of applications and industries. First, precision instruments measure a substance and produce a spectrum, which is expressed as a graph showing a series of peaks and valleys that is specific to the sample material. That spectrum is then compared with a database of the measured spectra of known substances. If a matching spectrum is found, the material in question can be identified. Bio-Rad's KnowItAll solutions provide search software tools, as well as the world's most extensive collection of reference spectra used in this type of analysis.

About KnowItAll Informatics Software
Bio-Rad's KnowItAll Informatics System is a fully integrated chemistry software and database package that provides scientific researchers multiple tools, including database building and management, search, analysis, structure drawing, and reporting all within a single user interface. The company's award-winning KnowItAll Informatics System offers fully flexible and expandable solutions for Infrared (IR), Raman, Near IR (NIR), Nuclear Magnetic Resonance (NMR), Mass Spectrometry (MS), Ultraviolet-Visible (UV-Vis) spectroscopy, chromatography, chemometrics, and metabolomics.

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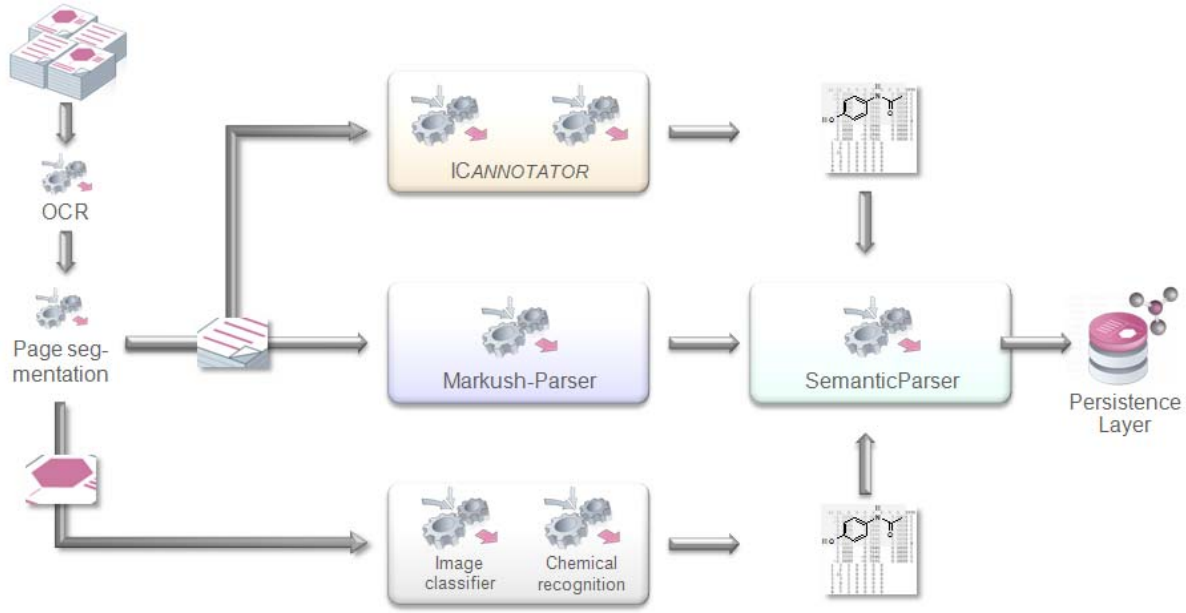
Developments in the ChemProspector research project
Automatic extraction of generic structures from patent documents

InfoChem has presented new achievements of the research project "ChemProspector - Intelligent search of chemical structures in documents" at the THESEUS-SME Congress, which took place in the THESEUS Innovation Center in Berlin on June, 28. The main goals of the project are the automatic abstraction of Markush-structures from patents and the creation of a structure searchable integrated search platform to access the abstracted information.



With a live demonstration Dr. Josef Eiblmaier illustrated how a database containing 10,000 patents and 280,000 chemical compounds could be built automatically with the Markush extraction algorithm of ChemProspector. Over 80 representatives from politics, research institutions and of small and medium size enterprises followed the presentation with great interest.

“Thanks to the ChemProspector project we are developing new technologies for the automatic abstraction of chemical information from documents concentrating in particular on generic information, so called Markush-structures. This is very important for our customers, who take great advantage of these developments.” says Dr. Josef Eiblmaier, responsible project manager for ChemProspector.

More information about the ChemProspector project can be found at http://infochem.de/news/projectdisplay.shtml?chemprospector.shtml or in the flyer to download under http://infochem.de/content/downloads/chemprospector.pdf.

ChemProspector is part of the THESEUS research program, initiated by the German Federal Ministry of Economy and Technology (BMWi).

Greenhouse Gases: Science and Technology

Wiley and Society of Chemical Industry (SCI) announce the launch of a new online-only journal dedicated to the management of greenhouse gases.

Launched in February 2011, ***Greenhouse Gases: Science and Technology*** *(GHG)* provides an important resource exploring:

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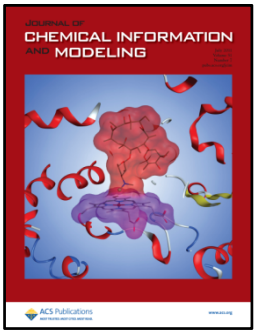

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ACS Chemical Information Division (CINF)
Fall 2011 ACS National Meeting
Denver, CO (August 28 – September 1)

Abstracts

CINF 1 Can a compact means of representing the ionic equilibria of multi-acid/base aqueous solute molecules be devised?

R. Don Wauchope[(1)]*, don_wauchope@citcom.net, 3801 Cascade Lake Rd., Pisgah Forest NC 28768, United States . (1) Agricultural Research Service, US Department of Agriculture, United States*

A number of important databases exist created to tabulate the chemical and physical properties of compounds of environmental interest. Many such compounds are Brönsted acids or bases and some contain multiple acid-base sites. If such sites are "weak", i.e. their degree of ionization varies within the range of *pH* found in environmental waters, this profoundly effects and complicates the molecule's behavior in all environmental compartments. The representation of such acid-base properties in these databases is poor because (a) no conventions for representation are well established (b) for more complex molecules representation requires a disproportionate amount of space in the database. An approach to a compact representation for such molecules will be proposed.

CINF 2 USGS National Geochemical Database: Recovering, repackaging, and repurposing 50+ years of historical data

Steven M Smith[(1)]*, smsmith@usgs.gov, MS 973, P.O. Box 25046, DFC, Denver Colorado 80225, United States ; David B Smith*[(1)]*. (1) Mineral and Environmental Resources Science Center, U.S. Geological Survey, Denver Colorado 80225, United States*

The U.S. Geological Survey's (USGS) National Geochemical Database (NGDB) contains inorganic analyses for approximately 1.4 million samples of rocks, sediments, soils, plants, water, minerals, and other materials collected since the early 1960s. Additionally, the NGDB project has recovered and compiled data from the U.S. Department of Energy's National Uranium Resource Evaluation (NURE) Hydrogeochemical and Stream Sediment Reconnaissance (HSSR) Program conducted during the late 1970s and early 1980s. The NURE HSSR databases contain analyses from about 398,000 sediment/soil and 335,000 groundwater/surface-water samples. All data are being repackaged into searchable and downloadable datasets on the USGS Mineral Resources On-Line Spatial Data website (http://mrdata.usgs.gov).

Although samples were collected to support geologic research and mineral exploration, the historical geochemical data and archived samples are increasingly being repurposed to identify hazards to the environment, to human and animal health, and to provide benchmarks for detecting temporal changes in the chemical environment.

CINF 3 Quality of water resources from the U.S. Geological Syrvey: An introduction

Shu Guo[(1)]*, guo1s@cmich.edu, Park Library 231, Mt. Pleasant Michigan 48859, United States . (1) Reference Department, Central Michigan University, Mt. Pleasant Michigan 48859, United States*

The U.S. Geological Survey (USGS) collects and analyzes chemical, physical, and biological properties of water resources from sites across the Nation. The rich collection of data, assessments, publications, reports and maps on quality of water resources is a non-replaceable information resource for chemical environmental research. USGS provides specific data on: water quality (real-time, daily and statistics); contamination and pollution (trace elements, medication, pesticides, nutrients, petroleum, viruses); contaminants in groundwater, aquifers, surface and other water resources. USGS's National Water-Quality Assessment (NAWQA) program provides datasets and reports on: water-quality status and trends for surface and ground water; National-Synthesis assessments; contaminants in lake sediments, public and domestic wells etc. The NAWQA Mapper allow users to view chemical concentrations found in streams, lakes, wells and other water resources in the US, which are generated directly from the 17 million water quality results stored in NAWQA Data Warehouse. Techniques methods and modeling are also provided.

CINF 4 Public access to toxic release data: Exploring TRI and RTKnet.org

Barbara Losoff[(1)], *Barbara.Losoff@colorado.edu, 184 UCB, 1720 Pleasant Street, Boulder CO 80309-0184, United States . (1) Science Library, University of Colorado Boulder, Boulder CO 80309, United States*

In response to one of the world's worst industrial accidents, the 1984 Bhopal tragedy, the United States Congress established the Toxic Release Inventory (TRI) in 1986. The TRI, under the jurisdiction of the Environmental Protection Agency (EPA), provides access to toxic release data for entire country. The TRI site is publicly available providing users the ability to investigate toxic release data in their communities. TRI data is also mined by other organizations. One such site is the Right-to-Know Network (RTKnet.org) which strives to empower citizens in the government decision-making process. This talk will compare TRI and RTKnet.og as tools for presenting environmental data to the non-practitioner including: ease of navigation, facility in both understanding and using the data, and level of site support.

CINF 5 CHEMLIST: Chronicling the course of regulated chemistry

Roger J Schenck[(1)], *rschenck@cas.org, 2540 Olentangy River Road, Columbus Ohio 43202, United States . (1) Department of Content Planning, Chemical Abstracts Service, Columbus Ohio 43202, United States*

CAS has long been associated with collecting and making publicly available the data about substances in commerce. With the inception of the US Toxic Substances Control Act in 1976 to the present, CAS scientists have been closely associated with the registration of substances in commerce and regulations about their use, transport, and environmental fate. Updated weekly, the CHEMLIST regulated chemicals database is a single place to locate regulatory requirements, inventory status, summaries of regulatory information, and other compliance requirements. In addition to describing the inventories and listings available in CHEMLIST, this presentation will cover the challenges in uniquely representing the wide range of substances typically found in national inventories. From polymers and polymer blends to materials and complex biological entities, CAS techniques for representing these commercial substances in the CAS REGISTRY database will be described.

CINF 6 Aligning scientific expertise and passion through a career path in the chemical sciences

Antony John Williams[(1)], *williamsa@rsc.org, 904 Tamaras Circle, Wake Forest NC 27587, United States . (1) ChemSpider, Royal Society of Chemistry, Wake Forest NC 27587, United States*

Antony Williams is the Vice President of Strategic Development for ChemSpider at the Royal Society of Chemistry. ChemSpider is one of the world's primary online resources serving the chemistry community. Antony has a PhD in Chemistry specializing in NMR spectroscopy and has worked in a government laboratory, in academia, for a Fortune 500 company (Eastman Kodak), for a small start-up organization and has started two of his own companies prior to joining the Royal Society of Chemistry. During his career path he has experienced multiple work cultures. Antony will provide a short overview of his career path and discuss the various decisions that helped motivate his change in career from professional spectroscopist to website host and innovator to working for one of the world's foremost scientific societies.

CINF 7 Development of an open source ELN

Felix Rudolphi[(1)(2)], *rudolphi@mpi-muelheim.mpg.de, Kaiser-Wilhelm-Platz 1, Muelheim an der Ruhr NRW 45470, Germany ; Lukas J. Goossen*[(1)]*. (1) Department of Chemistry, TU Kaiserslautern, Kaiserslautern 67663, Germany (2) IT department, MPI für Kohlenforschung, Kaiserslautern 67663, Germany*

The use of Electronic Laboratory Notebooks (ELN) has many advantages over traditional documentation of experiments. We have developed *open enventory*, a web-based open source ELN with integrated inventory database that facilitates planning and documentation of chemical reactions, as well as further analysis of the collected data. When planning a reaction, the inventory database provides information on availability of chemicals, physical and safety data. Tools to create and analyze series of reactions have proven to be useful in high throughput applications. Analytical data with preview images is attached to the reaction, providing a complete overview over all relevant information. Researchers can search the reaction database by keywords, numeric parameters, chemical substructures or combinations of criteria. They can access their own data, open data created by colleagues and data of former group members, making the ELN a valuable tool for collaboration and knowledge exchange.

CINF 8 Introduction of InChI to researchers in the Department of Chemistry at Louisiana State University

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As chemical information has transitioned from print to electronic format, a universal, non-proprietary method of identifying chemical compounds has been needed in order to take full advantage of new communication and search technologies offered via electronic databases and the web. To this end, InChI was developed by IUPAC, in collaboration with NIST, for identifying well-defined chemical substances. The resulting identification scheme converts chemical structures into machine-readable strings that allow data mining of the web and linking of relevant chemical information. In order to be effective, this new electronic identification system must be understood and used by researchers, educators, and publishers on a large scale. The authors will introduce InChI to researchers in the Department of Chemistry at Louisiana State University through a systematic approach that can be implemented at other similar institutions. This presentation will document our progress.

CINF 9 Stochastic search for the structures of small germanium clusters and their anions: Enhanced stability by spherical aromaticity of the Ge_{10} and Ge_{12}^{2-}systems

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Investigations on germanium clusters in the neutral, anionic and dianion states Ge_n^x (n = 2 – 12, x = 0, -1, -2) are performed using quantum chemical calculations with the B3LYP functional and coupled-cluster CCSD(T) methods. An improved stochastic method is implemented for searching the low-lying isomers of clusters. Comparison of our results with previous reports on germanium clusters shows the efficiency of the search method. The Ge_8 system is presented in detail. The anionic clusters $Ge_n^{-/2-}$ are studied theoretically and systematically for the first time, and their energetics are in good agreement with available experiments. The clusters Ge_{10}, Ge_{10}^{2-} and $Ge_{12}^{2-}$are, in their ground state, characterized by large HOMO-LUMO gaps, high vertical and adiabatic detachment energies and substantial average binding energies. The enhanced stability of these magic clusters can consistently be rationalized using the jellium electron shell model and the spherical aromatic character.

CINF 10 SMARTNames: A new framework to organize chemical structural information based on chemically relevant functional groups

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We developed a new framework to describe chemical information based on chemical functional groups (CFGs). For the first time we rigorously associate common CFG names with chemical structural representations. CFGs were defined using the SMARTS query language and extensively validated. Names, structures, and relationships among CFGs were modeled in an ontology leveraging the web ontology language (OWL 2.0). CFGs were organized into four hierarchies: (i) major chemical bonds, (ii) common functional groups, (iii) chemical reactivity, and (iv) undesired properties. Each class is further sub-classified based on atom and bond level descriptions into a formal subsumption hierarchy. This ontological description of CFGs allows the definition of novel CFG classes by combining existing CFGs. Further, CFGs can be part of multiple hierarchies depending on the intended use of the framework. The SMARTNames framework was used to analyze several database providing new insights that are founded in the chemically meaningful definitions of CGFs.

CINF 11 Molecular docking and 3D-QSAR studies for design and development of selective aspartate semialdehyde dehydrogenase inhibitors

Amarjit Luniwal[(1)]*, aamarji@rockets.utoledo.edu, 2801 W. Bancroft St., Toledo Ohio 43606, United States ; Alexander Pavlovsky*[(1)]*; Paul W. Erhardt*[(2)]*; Ronald Viola*[(1)]*. (1) Department of Chemistry, University of Toledo, Toledo Ohio 43606, United States (2) Center for Drug Design and Development, University of Toledo, Toledo Ohio 43606, United States*

Development of microbial resistance against many antibiotics is a major emerging challenge to human health. Targeting of key enzymes that play an important role in the biosynthesis of essential amino acids can be

a effective way to counter antimicrobial drug resistance. We have focused on the discovery and development of selective inhibitors against aspartate semialdehyde dehydrogenase (ASADH). This enzyme constitutes an early branch point in a microbial biosynthetic pathway for both essential amino acids and quruorum sensing molecules. We have carried out a series of docking and 3D-QSAR studies to design and develop new classes of selective inhibitors against ASADH. Our promising preliminary results will be described in the presentation. This work is supported by a grant from the NIH (AI077720).

CINF 12 Chemistry in the hand: The delivery of structure databases and spectroscopy gaming on mobile devices

Antony J Williams[(1)]*, williamsa@rsc.org, 904 Tamaras Circle, Wake Forest NC 27587, United States ; Sergey Shevelev*[(1)]*; Andrew S.I.D Lang*[(2)]*; Jean-Claude Bradley*[(3)]*; Kevin Theisen*[(4)]*. (1) ChemSpider, Royal Society of Chemistry, Wake Forest NC 27587, United States (2) Department of Computer Science and Mathematics, Oral Roberts University, Tulsa Oklahoma 74171, United States (3) Department of Chemistry, Drexel University, Philadelphia PA 19104, United States (4) iChemLabs, Piscataway NJ 08854, United States*

The proliferation of mobile devices in the form of smartphones and tablet devices has put into our hands computational power and capability previously limited to desktop until recently. Couple this with the connectivity of these devices to the internet and the trend of increased capability and accessibility in smaller devices continues. This presentation will provide an overview of our efforts to provide access on mobile devices to a large chemistry database, ChemSpider, containing over 25 million unique chemical compounds and associated data including patents, publications, properties and analytical data. We will also discuss how, by providing programming interfaces and Open Data, it has been possible to produce a Spectral Game (www.spectralgame.com) for scientists and students to practice their spectral interpretation skills. We will discuss some of the technology hurdles associated with delivering such capabilities to the various mobile platforms and how modern technologies can significantly enhance the user experience.

CINF 13 SciFinder mobile: Innovation for today's chemical researchers

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SciFinder is widely accepted as the leading research tool for chemists and related scientists, and now SciFinder Mobile is available for research anytime, anywhere. SciFinder's popularity is due not only to its search, retrieval and analysis tools expressly designed by CAS chemists for chemical research, but to the fact that it provides the most direct access to CAS' databases, including the CAS Registry. The world's largest and highest quality collection of information on small molecules, the Registry has been called the "gold standard' for chemical research. Since launching CAS Online in 1980, CAS has been committed to taking advantage of evolving technologies to meet chemists' research needs. CAS pioneered mobile access to substance information six years ago, with the first ever mobile transmission of structure information to the BlackBerry. In 2011, CAS launched SciFinder Mobile, the latest iteration of its mobile technology. SciFinder Mobile is optimized for a range of mobile standards and equipment. It enables scientists to use some of SciFinder's most popular features including researching subject areas, looking up information on chemical substances, and reviewing results of alerts from anywhere. This presentation will detail the operating features of SciFinder Mobile and demonstrate how convenient access to chemical information helps researchers' productivity.

CINF 14 Useful and fun chemistry on the go

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Mobile apps present a new opportunity for delivering chemical information while on the move. We will discuss the development of mobile chemistry applications. Working with the 2010 Reaxys PhD Prize Finalists and with Prof. Carreira's group at ETH Zürich we identified and refined ideas for today's mobile chemistry world that serve specific scientific needs and novel experiences for targeted communities.

Applications were developed in an iterative, collaborative and agile process with a continuous,

strong involvement from the target user population. We will outline all phases from idea generation to product delivery highlighting the key factors that make the mobile environment unique for product development as well as the successes and challenges encountered in bringing chemistry to this medium.

CINF 15 Nature of publishing anytime, anyplace, anywhere

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With the proliferation of mobile devices scientists have the ability to access information anytime, anyplace and anywhere they have a connection to the internet. This provides many challenges to publishers who, invariably, are used to providing information in a rather static format i.e. print, HTML etc...

Nature Publishing Group has spent the last 24 months (the iPhone application launched February 2010 and the iPad application was released January 2011) experimenting with the delivery of scientific content on mobile platforms for both Nature publications, Scientific American and as eBooks.

This talk will focus on the lessons learned - technical, editorial and marketing - in developing these applications and a vision for future developments.

CINF 16 Current and emerging mobile technologies at ACS publications

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The Publications Division of the American Chemical Society is taking steps into the mobile space.

This talk will explore what we have done recently with the ACS Mobile app for Apple and Android devices, plus look forward a bit to other mobile technologies that are under consideration by ACS Publications. In our review of the ACS Mobile app, we will cover some of the product and design decisions that were made along the way as well as some of the challenges and success we experienced. Design considerations range from the construction of the mobile app itself, through the back-end services that support the app, and finally to the content and data that feed the app.

Next, we will look at some mobile technologies under evaluation by ACS Publications. The EPUB format is one of these technologies, and has seen recent improvements that may allow it to better handle the rich scientific content produced by ACS Publications. We will briefly delve into some of the production and delivery considerations involved with potentially producing and supporting these mobile technologies.

CINF 17 Post-textbook era: What it means for the chemistry classroom

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The textbook is broken, both in content and business model. Students don't want to read something that looks like it's been put through a blender (a result of the need to revise it every year to avoid used book sales), and they certainly don't want to pay $200 for it. Fortunately the high price of textbooks makes replacing them with electronic readers like the iPad an attractive proposition both educationally and financially. Touch Press is working closely with educators and hardware companies to explore and define the future of educational materials.

CINF 18 Riding the mobile wave

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We now live in the post-PC era. The growth of mobile computing devices from smart-phones to tablets has been simply explosive - updating the older vision of a "computer on every desktop" to a "connected touch screen device in every pocket." Indeed, mobile devices have enabled 24x7x365 connectivity and thus access into workflows previously constrained to the office. Coupled with cloud computing environments (e.g. Amazon's EC2 and RDS environments), mobile platforms represent very important growth areas in scientific computing and communication. We will describe both technical and business challenges as well as lessons learned over the last two years after having developed and deployed several mobile apps including

iKinase, iKinasePro, iProtein, MobileReagents, and Reaction101.

CINF 19 ChemWriter: Enabling cross-platform mobile chemistry applications through Web standards

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The tablet computer market, created by Apple, now shows increasing signs of competition from devices running Android and Windows operating systems. While this shift offers choices for buyers, it presents a dilemma for product and service providers.

HTML5 and the remarkable array of new Web technologies around it offer a solution that can work both today and tomorrow.

Recently, we introduced ChemWriter, the chemical structure editor designed to run on all common Web browsers, ranging from Microsoft's legacy Internet Explorer releases to the most recently-introduced tablet devices - including iPad. Our decision to implement ChemWriter with standard browser technologies was influenced by growing fragmentation in the tablet computer market.

This presentation will describe the kinds of mobile chemistry applications ChemWriter can enable. In this context, we'll discuss the advantages of HTML5 mobile applications compared to platform-specific alternatives for scholarly publishing, electronic lab notebooks, and laboratory information management systems.

CINF 20 Computer Vision based chemical information extraction from digital images and streaming videos

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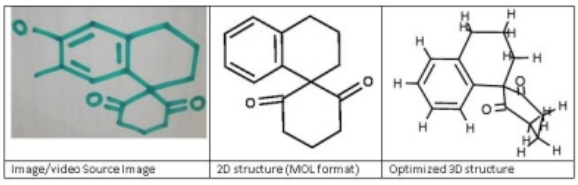
Chemical structures are the perfect examples to test the power of robotic vision to recognize and translate them into truly three dimensional chemical structures. Here we present a open-source based computer program to use digital video devices to capture and analyze rapidly hand drawn or computer generated molecular structures from plain papers. The computer program is capable of extracting molecular images from live streaming digital video signals and pre-recorded chemistry oriented educational videos. The images captured from these sources are further transformed into vector graphics for edge detection, node detection, Optical Character Recognition (OCR) and interpret them into bonds, atoms in molecular context. The molecular information generated is further transformed into re-usable data formats (MOL, SMILES, InCHI, SDF) for modeling and simulation studies. The connection table and atomic co-ordinates (2D) generated through this automatic process can be further used for generation of IUPAC names of the molecules and also for searching the chemical data from public and commercial chemical databases. Applying this software the digital webcams, camcorders can be used for recognition of molecular structure from hand-drawn or computer generated chemical images. The method and algorithms can be further used to harvest chemical structures from other digital documents or images such as PDF, JPEG formats. Effective implementation of this program can be further used for automatic translation of chemical images into common names or IUPAC names for chemical education and research.The performance and efficiency of this workflow can be extended to mobile devices (smart phones) with wi-fi and camera capabilities.

Fig.1: IUPACName (3',4'-dihydro-2'H-spiro[cyclohexane-1,1'-naphthalene]-2,6-dione) generated from hand drawn picture captured by digital video/image devices



CINF 21 The Information Century and the Learned Society

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Learned Societies such as the ACS developed, of course, in the era of print and paper. So, naturally, did the various structures and organizing principles of those societies. Consequently, the meetings, major publications (both primary and secondary), bulletins, reports, magazines, seminars -- in fact every aspect of the life of the Society developed during, and were influenced by, the relatively stable and known world of print communications. That world began slowly to change in the 1970's and 1980's, with change truly

exploding in the last fifteen years. What might be the full, long-term implications for learned Societies now that they truly inhabit the digital age? It has been said that, "If it can be digitized, it will be," with reference to everything from traditional forms of information to personal health information or information in the home never before captured, transmitted and analyzed. Closer to our home, with chemical information now completely electronic and rapidly evolving, what will the impact be on the Societies that have, in the past, organized themselves around the publication of that information in print? This presentation will reflect on the implications and changes already seen and that may be contemplated in the coming years from this ongoing digitization of chemical information.

CINF 22 Beyond the journal: Innovation in 21st century publishing

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Publishing is a balance between the needs of authors and those of the reader. This paper explores how the enormous changes in information technologies are having a profound impact on the way scientific research is disseminated, explored and understood. Today's publishing processes are enriching and enabling content in order to provide researchers and research institutions with far greater insights into the scientific literature. This is a new paradigm for the discovery, use, and sharing of research information to accelerate science and deliver better outcomes.

CINF 23 ChemSpider: Does community engagement work to build a quality online resource for chemists?

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With an intention to provide a high quality free internet resource of chemistry related data for the community, ChemSpider has aggregated almost 25 million compounds linked out to over 400 data sources and provided a platform for the community to both deposit and curate data. This experiment in crowdsourcing for chemistry has now been running for over three years. This presentation will review a number of aspects of the project including (a) the level of community participation in depositing and curating data; (b) the nature of data and content supplied by the community; (c) how ChemSpider is used by the community; (d) using game-based systems to assist in data curation; (e) algorithmic-based approaches to data validation and filtering; and (f) sharing data curation efforts with other online databases.

CINF 24 Riding the wave: TIB`s strategy in the context of non-textual materials

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The European High Level Expert Group on Scientific data (2010) has formulated the challenges for a scientific infrastructure to be reached by 2030: "Our vision is a scientific e-infrastructure that supports seamless access, use, re-use, and trust of data. In a sense, the physical and technical infrastructure becomes invisible and the data themselves become the infrastructure – a valuable asset, on which science, technology, the economy and society can advance".

Here, "data" is not restricted to primary data but also includes all non-textual material (graphs, spectra, videos, 3D-objects etc.). The German National Library of Science and Technology (TIB) must now rise to these challenges: developing solutions together with the chemical community to make such data available, citable, sharable and usable, including visual search tools and enhanced content-based retrieval. With solutions such as DataCite and modular development for extraction, indexing and visual searching of new chemical metadata, TIB will ride this wave.

CINF 25 Discovering drugs: Generating pharmacologically relevant leads that target disease

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Much of early drug discovery depended on leads from natural sources e.g. willow bark yielded aspirin, which led to numerous non-steroidal anti-inflammatory drugs. However, when presented with a newfound biological target, with no small molecule leads, where do we start? How do we probe the target without suitable pharmaceutically active molecules? One approach is to model the receptor and associated endogenous ligands

to understand the criteria for binding (and mechanism of action) combined with compound selection to optimize chemical structures for ADME and the avoidance of toxicity. Using this approach, we are currently investigating a GPCR (Apelin) which is a potent vasoconstrictor and using rational design approaches we have discovered novel agonists, antagonists and small molecule leads. We have combined this approach with access to ethically sourced human tissue, an approach which eliminates many of the problems associated with animal testing and which also allows investigation of not only healthy, but diseased tissue. Drugs can then be targeted at the diseased state, which is more relevant in a clinical setting.

CINF 26 From data to knowledge capture and retrieval in Medicinal Chemistry – if we only knew what we already know

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Medicinal Chemistry is a complex and central science in Pharmaceutical R&D. The successful design and synthesis of drug candidate molecules requires a firm knowledge and understanding of various interfacing disciplines, such as, for example, pharmacokinetics, physicochemical properties, pharmacology, toxicology, as well as modeling and simulation.

Medicinal chemists are constantly challenged with an overwhelming amount of data from both, in-house research as well as literature. Improved software tools are needed, to rapidly access and visualize such data, to retrieve information that can be put into context of chemical structure and ultimately turned into sub-structure based knowledge of molecular function in Medicinal Chemistry.

This talk will outline some basic thoughts about the requirements of such advanced software tools and will also offer suggestions for a step change of how sub-structure based knowledge might be used to enable Medicinal Chemists for further improved design of drug candidate molecules.

CINF 27 Enriched research documents at the cutting edge: When research papers no longer make sense on paper

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Research papers have long enjoyed the ability to exist not only on paper but in enriched electronic form. The ability to embed figures helped, but incorporating chemical structures that included full bonding and structural information brought significant utility to the electronic form over the printed page. Now we are at the edge of a major revolution of recording not only more elaborate versions of results of research, but capturing the very METHODS used, full data and workflows and documenting completely reproducible results. The implications are wide from helping to improve the quality of science, the intellectual transfer of the core discoveries, and preserving the knowledge learned. Several different electronic prototypes will be discussed and their potential impact on the future of science reviewed.

CINF 28 Reading the e-leaves

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Award symposia frequently celebrate the achievements of the past. In contrast this symposium looks to the future, with an underlying theme of change. The publishing industry is at a crossroads: the concepts of "journal" and "database" are changing and the journal article is now at the center, integrated with, for example, the literature in SciVerse ScienceDirect and chemistry in Reaxys. The Web and the open access movement, plus the growth in social networking, have made possible innovative new models such as that of ChemSpider, complementary, but not yet alternative, to the "gold standard" of the CAS databases and SciFinder. Change has also impacted libraries and their role in the long term preservation of the scientific record and securing access to data. Chemistry, the central science, reaches out into biology, with an impact on the use of chemical structures in drug discovery. The final talks in the symposium examine future horizons. The present one will draw together some underlying threads from earlier talks and make some personal

observations about vision, and Professor Lawson's own contributions.

CINF 29 Challenges and opportunities in preserving the scientific record: Reaxys and beyond

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The need for accurate, concise and relevant information has always been of fundamental importance to researchers in industry and academe since the earliest days of scientific method. In view of the accelerating growth in the amount of accumulated recorded data, this basic requirement has always been in conflict with the time constraints that limit scientists in finding the detail most relevant to their immediate needs. The present paper will discuss the evolution of responses to this dilemma, not only from the standpoint of suppliers of chemical information, but also from the user community itself.

CINF 30 MarVis: An intuitive patent Markush structure visualization tool for medicinal chemists

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Reviewing chemical patents is essential for drug discovery project decision making, but can be time-consuming and tedious. A cheminformatics application, called MarVis (Markush Visualization), has been developed for patent Markush structure visualization and analysis. MarVis can show a graphical table of all possible R-groups described in a patent. If a query substructure matches an R-group, MarVis will expand the Markush structure displaying the query substructure. There is also a unique interactive interface that allows chemists to explore Markush structures and zoom in the chemical space of a patent to find a subset of interest. It is especially helpful in cases where the patent Markush structure is very complex with heavily nested R groups. MarVis can significantly reduce time for manual step of patent analysis from days to minutes. The graphical R-group table also facilitates a more efficient subsequent patent analysis.

(A manuscript of this work has been accepted by Journal of Chemical Information and Modeling, and published online http://pubs.acs.org/doi/full/10.1021/ci100261u)

CINF 31 Modeling activity landscapes using multiple representations: Consensus models

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Activity landscape modeling is a powerful approach to characterizing structure-activity relationships (SAR) including the characterization of activity cliffs.[1] For an *N*-dimensional activity landscape, (*N-1*)-dimensions comprise the chemical space, while the N^{th} dimension is composed of the activity space. Since chemical space is largely influenced by molecular representation, using multiple representations has been proposed for SAR modeling.[2] Herein, we present an example of consensus modeling of activity landscape using 54 compounds with available activities towards three biological targets.[3] 2D and 3D representations are employed to represent chemical space. The effects of 3D conformation on activity landscape are also explored. In addition physico-chemical properties representing drug-likeness are utilized. The overall results highlight the benefits of using multiple representations in characterizing SAR. [1] Maggiora, G. M., *J. Chem. Inf. Model.* **2006,** 46, 1535. [2] Medina-Franco, J. L. et al. *J. Chem. Inf. Model.* **2009,** 49, 477. [3] Yongye, A. B. et al. *J. Chem. Inf. Model.* **2011** (submitted).

CINF 32 Unique cycle families: A set of unique and chemically meaningful rings

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The perception of unique and chemically meaningful rings is fundamental for many chemoinformatic applications like molecular descriptor calculation, substructure (SMARTS) matching, and the generation of 2D and 3D coordinates. This problem

is frequently addressed by calculating a Smallest-Set-of-Smallest-Rings (SSSR) cycle base. Unfortunately, SSSRs are not unique resulting in atom order dependent calculations. Relevant Cycles (RC) as described by Vismara are an alternative to SSSRs but exponential in number for complex ringsystems.

We introduce Unique Cycle Families (UCFs) as an extension of RCs. UCFs represent an intuitive and chemically meaningful description of the rings in a molecular graph. They are unique and only polynomial in number. Therefore, UCFs are a valuable alternative to the commonly used concepts of the SSSR and RCs.

We provide an efficient implementation for the calculation of UCFs and we demonstrate their applicability for real time applications, by showing computing time benchmarks for the PubChem Database.

CINF 33 Improved conformational search using a cooperative swarm of simulation replicas

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The ability to predict molecular conformation is central to structure-based drug design. A range of effective techniques exist for the conformational analysis of small molecules (up to ~500 g/mol). However, for medium-sized to large molecules, there remains a need for robust approaches to accurate prediction of conformation. While molecular dynamics simulations provide some ability to explore and predict the conformation of molecules of this size, the rugged nature of the molecular free energy surface means that only local minima are often identified.

A number of MD-based techniques exist that seek to facilitate conformational analysis, smoothing the free energy surface while maintaining its representative features. One such approach, inspired by the artificial intelligence method of particle swarm optimisation, is SWARM-MD (1). This method attempts to smooth the surface of the system through the use of a swarm of multiple interacting simulation replicas that are driven towards the average conformation of the swarm members. We have recently implemented a version of SWARM-MD in the AMBER molecular dynamics package and for the first time applied this approach to prediction of native states of peptides (2), including Trp-cage miniprotein in aqueous solvent. In each case, the cooperation between swarm replicas was found to improve convergence of the simulations towards the native conformation. Future prospects for this approach will be discussed.

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CINF 34 System chemical biology studies of endocrine disruptors

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Endocrine disrupting chemicals (EDCs) alter hormonal balance and other physiological systems through inappropriate developmental or adult exposure, perturbing the reproductive function of further generations. While disruption of key receptors (e.g., estrogen, androgen, and thyroid) at the ligand binding domain (LBD) has been associated with EDCs, a significant number of EDCs do not appear to influence the LBDs of these receptors. Therefore, we evaluated the potential biological effects of EDCs in humans with the aim to rationalize the etiology of certain disorders associated with the reproductive function. We compiled 675 (known or suspected) EDCs and examined chemical-protein associations via ChemProt [http://www.cbs.dtu.dk/services/ChemProt/]. Over 1000 proteins susceptible to perturbation by one or more EDCs were subject to a protein-protein interaction network evaluation. Synergistic EDC effects resulting in the perturbation of different proteins associated to particular diseases (e.g., cryptorchidism) were evaluated.

CINF 35 Large-scale data analysis of bioactivity information in PubChem using 2D and 3D chemical similarity

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With over 120 million biological assay outcomes from 1.6 million small molecules tested against 3,500 protein targets, PubChem is a massive resource for the bioactivities of substances. Ways to enable effective navigation of these results need to be devised. A proven method is to relate substances by their chemical similarity. Efforts to systematically analyze this data can help one identify chemical similarity motifs and bioactivity patterns across assays and protein targets. Discussed here are efforts to devise the means to navigate biological activity as a function of 2-D and 3-D similarity. While a continual work in progress, these efforts may help researchers rapidly locate bioactivity profiles of interest or help identify cross-target indications.

CINF 36 Structure representations in public chemistry databases: The challenges of validating the chemical structures for 200 top-selling drugs

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Internet-based public domain databases containing chemical compounds have grown in number, capability and content in recent years. There are now many databases containing millions of chemical compounds associated with different types of data including chemical names, properties, analytical data, and with associated mapping to proteins, assay data, clinical information and so on. These disparate data sources suffer from one common issue – quality of data. This presentation will provide an overview of our efforts to source the appropriate structural representations for 200 top-selling drugs from public domain sources. This intra- and inter-laboratory comparison of approaches, processes and necessary agreements exposed the challenges associated with aggregating structure-based data. The project also provided data regarding the distribution of quality issues associated with many of the community's popular databases.

CINF 37 Merging smallmolecule compound libraries of Bayer HealthCare AG and Schering AG

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High throughput screening of in-house libraries is the method of choice for lead identification at Bayer HealthCare AG. Quality and diversity of the compound library is essential for successful generation of leads for drug discovery projects in all relevant indications.The recent merger of Bayer HealthCare AG and Schering AG led to the merging of the pharmaceutical corporate compound collections of both companies. One of the largest compound libraries in pharmaceutical industry was built. Characteristics of a state-of-the-art multi-million screening library are reported by describing the individual compound collections as well as the newly combined collection. in terms of structural identity, similarities and physico-chemical properties.

CINF 38 Functional classification of drugs based on their multiphenotype interaction network

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High throughput cellular assays often yield many positive hits, but the classification of these compounds by mechanism of action remains challenging. Measuring the interaction network of synergy and antagonism among pairwise combinations of compounds can allow their functional classification. However, it is unclear how to implement this conceptual approach in the case of high content screening, where many different phenotypes are measured, making a simple definition of synergy and antagonism elusive. Here, we provide a new framework for analyzing drug interaction networks in multi-dimensional phenotypic space. Defining a 'phenotypic signature' for each drug in this space enables synergistic or antagonistic interactions to be understood as directed interactions whereby each drug modulates the effective concentration of the other. We apply this approach to a high content screen of 29 bioactive compounds (406 pairs) spanning 15,000 combined concentrations. The analysis demonstrates the classification of these compounds by their known mechanisms of action.

CINF 39 Flavor landscape: Towards a systematic characterization of a comprehensive flavor database

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Flavor perception challenges our ability to both predict and design new flavor entities. Previously, we analyzed the pattern of flavor descriptions utilized in the commercially available Leffingwell & Associates Flavor-Base Pro© 2010 database, referenced to the ASTM sensory lexicon. In this work, we use a systematic approach to navigate through the structure-property relationships of this comprehensive flavor database and propose the concept of 'flavor landscapes'. The approach is derived as a natural extension of the emerging concept of 'activity landscapes' used in drug discovery. As such, we introduce structure-flavor similarity (SFS) maps and structure-structure similarity (SSS) maps. The SSS maps are derived from the fact that there are two types of molecular similarity, one based on the flavor characteristics of the molecules being compared, and the "standard" one based on molecular fingerprints. These tools can be used by expert and non-expert flavor chemists alike.

CINF 40 RInChIs and reactions

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InChIs encode molecular structures. How can we best use InChIs to develop a description of chemical reactions? A draft protocol is available and is being tested: http://www-rinchi.ch.cam.ac.uk/. The information, challenges, opportunities and future directions that will arise from these tests before the end of August 2011 will be outlined.

CINF 41 CAS learning solutions: Responding to customer needs worldwide

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CAS information resources are widely seen as "best in class," with the CAS Registry recognized as the gold standard for substance collections. CAS' global input centers speed the world's publicly disclosed chemical information into CAS' comprehensive databases, which are customized for rapid and convenient retrieval and analysis through SciFinder and STN. CAS has recently developed a suite of online training resources that we hope will match our services in quality and leadership. The new CAS Learning Solutions resource center is the most extensive of its kind in the chemical information sector, with more information and more interactive features to suit the evolving web generation's learning styles, as well as the preferences of seasoned searchers. This presentation will explore the rationale and key elements of CAS Learning Solutions.

CINF 42 NIST-journals cooperation: Implementation of new tools for editors, reviewers and authors

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New tools have been recently implemented in support of the ongoing NIST-Journals cooperation. These tools offer enhanced benefits to Editors, reviewers and authors of manuscripts that are submitted to the *Journal*

of Chemical and Engineering Data, *Fluid Phase Equilibria*, *The Journal of Chemical Thermodynamics*, *International Journal of Thermophysics*, and *Thermochimica Acta*. When an author has submitted a new manuscript to these journals, it will be reviewed by NIST in two stages. The first stage provides to Editors a *NIST Literature Report* and the second stage provides a *NIST Data Report*. These two reports are generated on demand by new tools that NIST recently incorporated into *ThermoData Engine* (TDE) software. The *literature report* assists Editors and reviewers with their assessment of the manuscript's scientific contribution, the degree of overlap with published data, and the need for comparison with those published data. The second stage of NIST review occurs just after peer review is completed and prior to an Editors' final decision. The *data report* provides provides a complete assessment of data quality, their underlying uncertainties, their sample descriptions, and their descriptions of experimental methods. Specialized consistency tests, based on requirements of the Gibbs-Duhem equation, are run on vapor-liquid equilibrium (VLE) data, and the final results are summarized with an overall VLE data quality factor. This information is compiled into a data report that is submitted to the Editor. Details of the implementation of these new tools at NIST will be described with examples that illustrate the functionality of the tools. These tools have been part of operations for the five journals for less than one year. A review of the successes and challenges in using the new tools will be presented, together with planned developments.

CINF 43 What has your chemistry librarian been doing? A new science librarian's work report and current trends in chemistry/science librarianship

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Chemistry is a unique science discipline which requires special searching techniques to locate its enormous and fast growing collection of information. Chemistry/Science Librarian plays a critical and indispensable role to bridge existing and potential library resources and information users together in helping our patrons to obtain better results. For the past decade, Case Western Reserve University (CWRU) has not had a librarian with science degree and/or education background to cover Chemistry and other science subjects. As the new science librarian, in the past two years I have made great progresses in the areas of collection development, library instruction, reference services, outreach activities and technology education involved in searching chemistry related information. I will present my working experiences at CWRU library mainly in the subject of Chemistry and also summarize the current trends in Chemistry/Science librarianship in academic libraries servicing in the corresponding areas mentioned above.

CINF 44 Development and assessment of online SciFinder tutorials toward the promotion of scientific literacy in undergraduates

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As recommended by the ACS Committee on Professional Training, students should exhibit proficiency in scientific literacy before entering into a professional atmosphere. In Fall 2008, Organic Chemistry I students at Rider University were required to write a report regarding a relevant societal issue rooted in chemistry. While students reported increased engagement in the material, communication and literacy skills were poor. To address this fundamental deficiency, a collaboration with Rider Libraries evolved, resulting in a semester-long literature project for Organic Chemistry II. The research process is facilitated by online Adobe® Flash® tutorials for SciFinder®, specifically designed to be relevant to Rider's undergraduate population. Herein is reported the ongoing tutorial development process, as well as the results of a two-year comprehensive assessment of their impact on students' scientific literacy. These measurements are crucial in continuing to identify the needs of Chemistry undergraduates, as dictated by the needs of their future employers.

CINF 45 Check us out: Librarians as departmental PR agents

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In these days of competition and rankings, every department is vying for the best graduate students. The Chemistry department at the University of Florida has been taking steps to increase its web presence and advertise the research of its graduate department. This

talk will discuss the role of the science librarian as advisor to this process, including compiling publication lists, negotiating publication restrictions to provide access to published research, and streamlining the collection and dissemination of department achievements. At UF, a local implementation of the VIVO Network, which enables the discovery of research and scholarship across disciplines, is being implemented to achieve these goals. The Marston Science Library has been heavily involved in promoting VIVO across its departments, focusing on how it can be used to expand collaborative opportunities and advertise professional expertise. Some observations on the effectiveness of this strategy will be discussed.

CINF 46 Elements of research misconduct

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What do scientists, educators, librarians, and game designers all have in common? In the fall of 2010, this team at the University of Florida was awarded a grant from the the NSF to support Gaming Against Plagiarism (GAP). The purpose is to develop a self-directed, interactive, online game to educate STEM graduate students to recognize and avoid plagiarism, including falsification and fabrication of data. GAP's intellectual merit lies in its goal of training these students in U.S. institutions to function effectively and ethically as authors within multinational research teams. This talk will discuss the four phases of the game: preliminary content development, design and development, usability, and evaluation. The team conducted a survey to elucidate students' perceptions of plagiarism and research misconduct. The overall results, including Chemistry-specific concerns, will be discussed. This grant project highlights the role that subject librarians can "play" in plagiarism and research misconduct awareness campus-wide.

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