

CHEMICAL Information BULLETIN

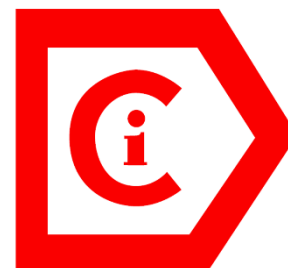


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Chemical Information Bulletin

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Message from the Chair	3
From the Editor	4
CINF Social Networking and Business Events at the Fall 2017 ACS Meeting	5
Tuesday Luncheon Talk	7
Awards and Scholarships	8
Committee Reports	15
Book Review by Robert E. Buntrock	18
Twenty-five Years Ago in Washington by Wendy Warr	21
Notes From Our Sponsors	23
2017 CINF Officers and Functionaries	32
Future ACS Meetings	35

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Chemical Information Bulletin

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Message from the Chair

Hello CINF!

During a recent discussion with ACS videographers, I had to summarize the CINF division, and what made it unique. I reported that we were an eclectic mix of people from a tremendous variety of careers, all focused on the creation, curation and consumption of information. We are all tied together in a great iterative cycle around data.



Data, data, DATA!

It's one of the things I love about any CINF event - everyone there has something they are passionate about in regards to chemical information, and the discussions to be had around them are inspiring. With the National Meeting coming up next week, I'm particularly looking to the in-person CINF events, but a number of the online debates have been just (if not more!) spirited. Excellent stuff!

All of these are nothing without you, the members, involved. So if you are coming to the National Meeting, please do try to join us for the CINF Welcoming Reception, our Tuesday luncheon with special guest speaker Kim Pruitt from the NCBI, and our Skolnik award symposium followed by reception. Or just catch us in the hallway with your latest idea. It's the time to really connect with people.

How to bring the value of the National Meeting to those that can't attend in person is an ongoing challenge, especially to the broader ACS community. ACS has been making some strides, especially with things like Presentations on Demand. Each meeting we seek permission of speakers to collect and share slides from CINF talks. Keep an eye on the website after the meeting!

The most prominent thing on my mind is still how to bring value to CINF members outside of the National Meeting. There have been some great ideas circulating, but there are always more. Hearing from the members themselves is paramount. Please reach out to me if you have any thoughts on the subject, or catch me at the National Meeting if you're attending! I'm always keen to hear from you.

Thanks for being a member!

Erin Davis
CINF Chair
cinfchair@gmail.com

From the Editor

Another summer means another ACS fall meeting approaches.

In this issue, you will find a report from our CINF Councilors, Bob Buntrock's review of *Science and the Law: Analytical Data in Support of Regulation in Health, Food, and the Environment*, Wendy Warr's reflections on the 1992 fall meeting in Washington DC, and a list of the CINF social events. Here's the technical program of CINF symposia and speakers (<http://bit.ly/CINFACSDC>). Unfortunately I will not be able to attend, but I look forward to reading the conference reports in the next issue, especially the talks on professional skills development for undergraduates, graduate students, and post-docs.

I know that summer is "playing catchup" for many of us, or at least that is what we tell ourselves we will have time to do. But I would love to see more features in next summer's issue. My contact information is below if you have ideas about something you would like to write about.

As for my annual update on the best of chemistry, science, and popular culture, I decided to save that for spring *CINF Bulletin*. Comic-Con was last month, and there were more UC San Diego researchers than ever talking about science and science fiction, sometimes sharing the stage with those television and film producers and screenwriters. As the librarian here for the Department of NanoEngineering, I made a special point of attending the nearly packed [Nanotechnology in Sci-Fi: Fact or Fiction](#) panel. The UC San Diego speakers are the ones wearing the [Star Trek uniforms](#). Not only were they impressive speakers, but the questions from the audience were thoughtful and drew some good responses.

Along with thanking our contributors and everyone who assisted with the production and copyediting of this issue, I want to give an additional "thank you" to our generous sponsors, many of whom provided news and updates about their recent chemical information products. So please check their product news and stop by their booths at the meeting to find out more.

And finally: a special congratulations to our 2017 ACS Fellows, Grace Baysinger and Lisa M. Balbes, and to Judith Currano, who has been appointed the 2018 Chair of the ACS Committee on Ethics.

Have a great time in Washington!

Teri M. Vogel
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CINF Social Networking Events at the Fall 2017 ACS Meeting



Please Join Us At These
Division of Chemical Information Events!



Division of
Chemical
Information

The ACS Division of Chemical Information is pleased to host the following social networking events at the Fall 2017 ACS National Meeting in Washington, DC.

Sunday Welcoming Reception & Scholarships for Scientific Excellence Posters

6:30-8:30 pm, Sunday, August 20th – Farragut Square/Lafayette Park – Grand Hyatt Washington

Reception co-sponsored by: **Journal of Chemical Information & Modeling (ACS Publications)**,
Journal of Cheminformatics (Springer Nature), **InfoChem**,
PerkinElmer and **Simulations Plus**.

Scholarships for Scientific Excellence

Sponsored exclusively by **ACS Publications**.

Tuesday Luncheon (Ticketed Event – Contact Division Chair, Erin Davis)

12:00-1:30 pm Tuesday, August 22nd – Constitution Ballroom B – Grand Hyatt Washington

Sponsored exclusively by the **Royal Society of Chemistry**.

Speaker: Kim D. Pruitt, Ph.D,

Acting Chief, Information Engineering Branch

Director, Data Services Division

National Center for Biotechnology Information, NLM, NIH, DHHS

Presentation:

Managing ~~Terabytes~~ Petabytes of Data to Support Connecting Data to Knowledge.

Herman Skolnik Award Symposium & Reception Honoring

Prof. Dave Winkler, CSIRO, Australia

Symposium:

1:45 pm-5:20 pm Tuesday, August 22nd – Junior Ballroom 1 – Washington Marriott at Metro Center

Reception:

6:30pm-8:30pm Tues. August 22nd – Independence Ballroom A – Grand Hyatt Washington

Sponsored by: **ACS Division of Chemical Information**.

CINF Business Meetings

Saturday, August 19: 12:30-2:30 PM

- o Education Committee – Constitution E – Grand Hyatt Washington
- o Awards Committee – Arlington – Grand Hyatt Washington

Saturday, August 19: 12:30-6:00 PM

- o Program and Executive Committees – Constitution B – Grand Hyatt Washington

Sunday, August 20: 12:00-2:00 PM

- o Chemical Structure Association Trust – Franklin Square-GH – Grand Hyatt Washington

Tuesday Luncheon Talk

Kim D. Pruitt, Ph.D.

Acting Chief, Information Engineering Branch

Director, Data Services Division

National Center for Biotechnology Information, NLM, NIH, DHHS

Managing Terabytes Petabytes of Data to Support Connecting Data to Knowledge

12:00-1:30 pm Tuesday, August 22nd

Constitution Ballroom B – Grand Hyatt Washington

Sponsored exclusively by the [Royal Society of Chemistry](#)

The National Center for Biotechnology Information (NCBI) was established in 1988 to manage and process molecular biology information. Over the course of three decades, NCBI established sequence, literature, and chemical databases that contain petabytes of data and represents an essential infrastructure supporting research, clinical, and education communities. NCBI manages GenBank, the Nation's sequence database archive, PubMed and other literature databases, PubChem, and a suite of additional data types, resources and tools that relate to these three central activities. In this presentation, I will provide an overview of these data and their value, process management practices, and activities to maintain and enhance 'data to knowledge' connections.



Chemical Structure Association Trust

Applications Invited for CSA Trust Grant for 2018

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 and is now inviting the submission of grant applications for 2018.



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. One or more Grants will be awarded annually up to a total combined maximum of ten thousand U.S. dollars (\$10,000). Grantees have the option of payments being made in U.S. dollars or in British Pounds equivalent to the U.S. dollar amount. 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, for example, for travel to collaborate with research groups, to attend a conference relevant to one's area of research (including the presentation of an already accepted research paper), 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. A copy of the completed application document must be supplied for distribution to the Grants Committee and can be submitted via regular mail or e-mail to the Committee Chair (see contact information below).

Deadline for Applications

The application deadline for the 2018 Grant is March 31, 2018. Successful applicants will be notified no later than May 9, 2018.

Address for Submission of Applications

The application documentation can be mailed via post or emailed 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 chescot@aol.com prior to submission so that she can contact you if the e-mail does not arrive.

Chemical Structure Association Trust: Recent Grant Awardees

2017

Jesus Calvo-Castro: University of Hertfordshire, England, was awarded a grant to cover travel to present his work at the Fifth International Conference on Novel Psychoactive Substances, to be held in Vienna, Austria from August 23-23, 2017. He works on the development of novel methodologies for the in-the-field detection of novel psychoactive substances (NPS), where chemical structure and information play a crucial role.

Jessica Holien: St. Vincent's Institute of Medical Research, Fitzroy, Victoria, Australia, was awarded a grant to cover travel to present her work at the 2017 Computer-Aided Drug Design (CADD) Gordon Research Conference, scheduled to take place July 16-21, 2017 in Mount Snow, VT, USA. She is a postdoctoral researcher at St. Vincent's and is responsible for a range of computational molecular modeling, including compound database development, virtual screening, docking, homology modeling, dynamic simulations, and drug design

2016

Thomas Coudrat: Monash University, Australia, was awarded a Grant to cover travel to present his work at three meetings in the United States: the Open Eye Scientific CUP XVI, The American Chemical Society Spring Meeting, and the Molsoft ICM User Group Meeting. His work is in ligand directed modeling.

Clarisse Pean: Chimie Paris Tech, France, was awarded a Grant to cover travel to give an invited presentation at the 2016 Pacific Rim Meeting on Electrochemical and Solid State Science later this year.

Qian Peng: University of Oxford, England, was awarded a Grant to attend the 23rd IUPAC Conference on Physical Organic Chemistry. His research is in the development of new ligands for asymmetric catalysis.

Petteri Vainikka: University of Turku, Finland, was awarded a Grant to spend the summer developing and testing new methods for modeling organic solvents in organic solutions with Dr. David Palmer and his group at the University of Strathclyde, Glasgow, Scotland.

Qi Zhang: Fudan University, China, was awarded a Grant to attend a Gordon Conference on Enzymes, coenzymes and metabolic pathways. His research is in enzymatic reactions.

2015

Dr. Marta Encisco: Molecular Modeling Group, Department of Chemistry, La Trobe Institute for Molecular Science, La Trobe University, Australia was awarded a Grant to cover travel costs to visit collaborators at universities in Spain and Germany and to present her work at the European Biophysical Societies Association Conference in Dresden, Germany in July 2015.

Jack Evans: School of Physical Science, University of Adelaide, Australia was awarded a grant to spend two weeks collaborating with the research group of Dr. Francois-Xavier Coudert (CNRS, Chimie Paris Tech).

Dr. Oxelandr Isayev: Division of Chemical Biology and Medicinal Chemistry, UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, was awarded a Grant to attend summer classes at the Deep Learning Summer School 2015 (University of Montreal) to expand his knowledge of machine learning to include Deep Learning (DL). His goal is to apply DL to chemical systems to improve predictive models of chemical bioactivity.

Aleix Gimeno Vives: Cheminformatics and Nutrition Research Group, Biochemistry and Biotechnology Dept., Universitat Rovira i Virgili was awarded a Grant to attend the Cresset European User Group Meeting in June 2015 in order to improve his knowledge of the software that he is using to determine what makes an inhibitor selective for PTP1B.

2014

Dr. Adam Madarasz: Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences. He was awarded a Grant for travel to study at the University of Oxford with Dr. Robert S. Paton, a 2013 CSA Trust Grant winner, in order to increase his experience in the development of computational methodology which is able to accurately model realistic and flexible transition states in chemical and biochemical reactions.

Maria José Ojeda Montes: Department of Biochemistry and Biotechnology, University Rovira i Virgili, Spain. She was awarded a Grant for travel expenses to study for four months at the Freie University of Berlin to enhance her experience and knowledge regarding virtual screening workflows for predicting therapeutic uses of natural molecules in the field of functional food design.

Dr. David Palmer: Department of Chemistry, University of Strathclyde, Scotland. He was awarded a Grant to present a paper at the fall 2014 meeting of the American Chemical Society on a new approach to representing molecular structures in computers based upon on ideas from the integral equation theory of molecular liquids.

Sona B. Warriar: Departments of Pharmaceutical Chemistry, Pharmaceutical Biotechnology, and Pharmaceutical Analysis, NMIMS University, Mumbai. She was awarded a Grant to attend the International Conference on Pure and Applied Chemistry to present a poster on her research on inverse virtual screening in drug repositioning

2013

Dr. Johannes Hachmann: Department of Chemistry and Chemical Biology at Harvard University, Cambridge, MA. He was awarded the Grant for travel to speak on “Structure-property relationships of molecular precursors to organic electronics” at a workshop sponsored by the Centre Européen de Calcul Atomique et Moléculaire (CECAM) that took place October 22 – 25, 2013 in Lausanne, Switzerland.

Dr. Robert S. Paton: University of Oxford, UK. He was awarded the Grant to speak at the Sixth Asian Pacific Conference of Theoretical and Computational Chemistry in Korea on July 11, 2013. Receiving the invitation for this meeting has provided Dr. Paton with an opportunity to further his career as a Principal Investigator

Dr. Aaron Thornton: Material Science and Engineering at CSIRO in Victoria, Australia. He was awarded the Grant to attend the 2014 International Conference on Molecular and Materials Informatics at Iowa State University with the objective of expanding his knowledge of Web semantics, chemical mark-up language, resource description frameworks and other online sharing tools. He will also visit Dr. Maciej Haranczyk, a prior CSA Trust Grant recipient, who is one of the world leaders in virtual screening.

2012

Tu C. Le: CSIRO Division of Materials Science & Engineering, Clayton, VIV, Australia. She was awarded the Grant for travel to attend a Cheminformatics course at Sheffield University and to visit the Membrane Biophysics group of the Department of Chemistry at imperial College London.

2011

J. B. Brown: Kyoto University, Kyoto, Japan. J.B. was awarded the Grant for travel to work with Professor Ernst Walter-Knappat the Freie University of Berlin and Professor Jean-Phillipe Vert of the Paris MinesTech to continue his work on the development of atomic partial charge kernels.

2010

Noel O'Boyle: University College Cork, Ireland. Noel was awarded the Grant to both network and present his work on open source software for pharmacophore discovery and searching at the 2010 German Conference on Cheminformatics.

2009

Laura Guasch Pamies: University Rovira & Virgili, Catalonia, Spain. Laura was awarded the Grant to do three months of research at the University of Innsbruck, Austria.

2008

Maciej Haranczyk: University of Gdansk, Poland. Maciej was awarded the Grant to travel to Sheffield University, Sheffield, UK, for a 6-week visit for research purposes.

2007

Rajarshi Guha: Indiana University, Bloomington, IN, USA. Rajarshi was awarded the Grant to attend the Gordon Research Conference on Computer-Aided Design in August 2007.

2006

Krisztina Boda: University of Erlangen, Erlangen, Germany. Krisztina was awarded the Grant to attend the 2006 spring National Meeting of the American Chemical Society in Atlanta, GA, USA.

2005

Dr. Val Gillet and Professor Peter Willett: University of Sheffield, Sheffield, UK. They were awarded the Grant for student travel costs to the 2005 Chemical Structures Conference held in Noordwijkerhout, the Netherlands.

2004

Dr. Sandra Saunders: University of Western Australia, Perth, Australia. Sandra was awarded the Grant to purchase equipment needed for her research.

2003

Prashant S. Kharkar: Institute of Chemical Technology, University of Mumbai, Matunga, Mumbai. Prashant was awarded the Grant to attend the conference, Bioactive Discovery in the New Millennium, in Lorne, Victoria, Australia (February 2003) to present a paper, "The Docking Analysis of 5-Deazapteridine Inhibitors of Mycobacterium avium complex (MAC) Dihydrofolate reductase (DHFR)."

2001

Georgios Gkoutos: Imperial College of Science, Technology and Medicine, Department of Chemistry, London, UK. Georgios was awarded the Grant to attend the conference, Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, (CMTPI-2001) in Bordeaux, France, to present part of his work on internet-based molecular resource discovery tools.

CINF Scholarship for Scientific Excellence: Call for Applications (Spring 2018)

The international scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) sponsored by ACS Publications (<http://pubs.acs.com>) is designed to reward students in chemical information and related sciences for scientific excellence and to foster their involvement in CINF.

Up to three scholarships valued at \$1,000 each will be awarded at the 255rd ACS National Meeting in New Orleans, LA, March 18-22, 2018. Student applicants must be enrolled at a certified college or university; postdoctoral fellows are also invited to apply. The applicants will present a poster during the welcoming reception of the Division on Sunday evening at the national meeting. Additionally, they will have an option to show their posters at the Sci-Mix session on Monday night. Abstracts for the poster must be submitted through MAPS, the abstract submission system of ACS.

To apply, first submit your abstract on <http://maps.acs.org> using your ACS ID (if you do not have an ACS ID, follow the registration instructions). Submit your abstract to the CINF program in the session "CINF Scholarship for Scientific Excellence Student Poster Competition". MAPS will be open shortly and submissions are due by October 16, 2017. Second, please send a 2,000-word abstract (including references) describing the work to be presented to Stuart Chalk (schalk@unf.edu) by January 31, 2018. Note: to be considered for the scholarship you must send the long abstract by the deadline. Any questions related to applying for one of the scholarships should be directed to the same e-mail address.

Winners will be chosen based on the content, presentation, and relevance of the poster, and their names will be announced during the Sunday reception. The content should reflect upon the student's work and describe research in the field of cheminformatics and related sciences.

Stuart Chalk
Coordinator
CINF Scholarship for Scientific Excellence

Committee Reports

Report on the Council Agenda for August 23, 2017

The Council of the American Chemical Society will meet in Washington, DC on Wednesday, August 23, 2017 from 8:00 am until approximately 12:00 pm in the Marriott Ballrooms 1-6 of the Marriott Marquis Washington, DC hotel. All ACS members are welcome to attend, although only Councilors are permitted to vote. A continental breakfast will be available at 7:00 am for all attendees.

There are four items for Council Action and they are summarized below.

Nominations and Elections

Elections will be held to fill 2018-2020 terms on the following three committees:

Committee on Committees: Council will vote to fill five slots on the Committee on Committees. There are ten nominees as follows: Mitchell R. M. Bruce, Jetty Duffy-Matzner, Rick Ewing, Barbara R. Hillery, Martha G. Hollomon, Judith M. Iriarte-Gross, Russell W. Johnson, Diane Krone, Robert A. Pribush, and Susan M. Schelble. The five candidates receiving the highest numbers of votes will be declared elected for the 2018-2020.

Council Policy Committee: Council will vote to fill five slots on the Council Policy Committee. There are ten nominees as follows: Karl S. Booksh, James C. Carver, Dwight W. Chasar, Ella L. Davis, Mark D. Frishberg, Lydia E. M. Hines, Will E. Lynch, Zaida C. Morales-Martinez, Barbara P. Sitzman, and Linette M. Watkins. The four candidates receiving the highest numbers of votes will be declared elected for the 2018-2020 term and the candidate receiving the fifth highest vote will be declared elected for a one year term for 2018.

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: Anthony W. Addison, Joe D. Allison, Michael Appell, Mark A. Benvenuto, Arindam Bose, Neil D. Jespersen, Mamie W. Moy, Eleanor D. Siebert, Julianne M.D. Smist, and Keith R. Vitense. The five candidates receiving the highest numbers of votes will be declared elected for the 2018-2020 term.

Petitions

The Committee on Membership Affairs (MAC) will seek approval for a petition on *International Chemical Sciences Chapters*. The petitioners propose changes to the ACS's Bylaws to allow an International Chemical Sciences Chapter to receive financial support from the Society. The Society Committee on Budget and Finance has examined this petition and concludes that it will have no impact on the finances of the Society. The Committee on Constitution and Bylaws suggested revisions and finds the revised petition to be legal and consistent with other provisions of the Society's documents. A two-thirds (2/3) vote of Council is required for approval of amendments to the Bylaws. If approved by Council, the amendments will become effective upon confirmation by the Board of Directors.

This petition appears on pages 82-84 of the Council Agenda at:

<https://www.acs.org/content/dam/acsorg/about/governance/councilors/COUNCIL%20Agenda%208.17.pdf>.

The Committee on Divisional Activities (DAC) will ask Council to act on the request to establish the Division of Space Chemistry. DAC received a request to establish the Division of Space Chemistry and then shared key information of the proposed division with the leadership of all 32 existing divisions. After discussing the matter on several occasions, DAC voted to oppose the creation of this new division (8 opposed – 6 support). The primary concern was a belief that the leadership of the proposed division was not sufficiently representative of the larger space chemistry community it hopes to serve. Other concerns included the absence of a compelling argument regarding the need for a new division, the vitality of a division operating in this area of chemistry, and counter-productive competition of division memberships at a time when membership in several divisions is in decline. These appear on pages 89-92 of the Council Agenda at:

<https://www.acs.org/content/dam/acsorg/about/governance/councilors/COUNCIL%20Agenda%208.17.pdf>.

The Committee on Local Section Activities (LSAC) will seek approval requested by the South Jersey Local Section for annexation of the unassigned territory of Ocean County, New Jersey. LSAC voted in favor of the petition at its meeting in San Francisco in April 2017. This petition appears on page 94 of the Council Agenda at:

<https://www.acs.org/content/dam/acsorg/about/governance/councilors/COUNCIL%20Agenda%208.17.pdf>.

Petitions for Consideration

There will be two petitions for consideration by Council: 1-Petition on the Composition of Society Committees, and 2-Petition for Election of Committee Chairs.

The first petition changes the Councilor requirement of Society Committee members from a least two-thirds (2/3) to a majority in order to provide for greater flexibility in member appointments and continuity of committee membership. This petition also removes the Councilor requirement for the Chair and Vice-Chair of a Society Committee. Committee members with expertise and strong leadership abilities should not be disqualified to serve as Chair or Vice-Chair because of status as a non-Councilor.

The second petition proposes changes to the ACS's Bylaws to allow the voting members of all ACS Committees to select their own Chairs. The members of the Committees have the career and ACS experience as well as judgment to select their own Chairs. This will free up the President, the Chair of the ACS Board, and the Committee on Committees to focus on priorities only they can deliberate and act upon. The proposed Bylaws changes will also make the Society, in a small way, more representative and democratic, and less bureaucratic.

The two petitions for consideration appear on pages 96-101 of the Council Agenda at:

<https://www.acs.org/content/dam/acsorg/about/governance/councilors/COUNCIL%20Agenda%208.17.pdf>.

Town Hall Meeting

A Town Hall meeting organized by the Committee on Nominations and Elections is scheduled for Sunday, August 20, 2017 in the Marquis Ballroom Salons 1-3 of the Marriott Marquis Washington, DC hotel from 4:30pm - 5:30pm. It will feature a Q&A session with the candidates for Director-at-Large: Kenneth P. Fivizzani, Wayne E. Jones, Jr., **Bonnie A. Lawlor**, and Barbara A. Sawrey. It is a great way to gather first-hand information and decide for whom you might want to vote in the fall election. All ACS members are encouraged to attend.

The Council Agenda book can be accessed at:

<https://www.acs.org/content/dam/acsorg/about/governance/councilors/COUNCIL%20Agenda%208.17.pdf>

Respectfully submitted July 25, 2017

CINF Councilors

Bonnie Lawlor
Andrea Twiss-Brooks
Svetlana N. Korolev

Book Review: Science and the Law: Analytical Data in Support of Regulation in Health, Food, and the Environment

Science and the Law: Analytical Data in Support of Regulation in Health, Food, and the Environment; Town W. G., Currano, J. N., Eds; ACS Symposium Series 1167; American Chemical Society: Washington, 2014. 178 p. +ix, ISBN 978-0-8412-2947-1. Hardcover \$150.

This book is the first in the series of the result of two related symposia presented at the fall 2012 ACS meeting in Philadelphia, the second previously reviewed by Bob Buntrock (1). Both remain timely, especially given continuing political developments on these topics. This book is especially prescient given current developments in regulation in the last half year. Most of the symposium presentations are included and often expanded to what are effectively mini-reviews with updated material. Each chapter terminates with a conclusion and a list of references with an index. In most cases, the title acts as a mini-abstract.

Chapter 1, "Looking Forward: Science-Based Policy Making" is by co-editor Bill Town and is not only an introduction to the subject area but also acts as an outline and abstract for the 10 remaining more specialized chapters. Communication between scientists and policy makers is difficult given differences in perception and interpretation on the influence of science on policy making. The typical lack of scientific knowledge of politicians and civil servants has a large and often negative effect on resulting policy. Therefore, "education" of politicians is paramount. All too often legislation is enacted without input from scientists and if input is requested it is often along the lines of "Here's the policy we want, find the science to support it". Concepts to aid in the evaluation of research are outlined and include error and bias, control and repeatability, and interpretation of data.

Chapter 2, "Hunting and Gathering: Locating and Evaluating Information on the Cusp between Science and Legislation", is by co-editor and master searcher Judith Currano. All sides on the debates (scientists, legislators, general public) often exhibit emotional responses and cite "hard facts" to add credibility to their stands (Plus ça change, plus c'est la même chose). In possibly the meatiest chapter, the author not only describes data and information location techniques but methods for evaluation of the information to attempt to determine the reliability. Two case studies are illustrated (fracking in the Marcellus Shale, and health effects of low-level RF energy) with line drawings as reliability guides. These methods were developed for an engineering ethics class at UPenn. Involved are four steps: 1) determining the breadth of the information required, 2) use of appropriate resources for searching, 3) evaluating the retrieval for credibility, and 4) use of ethical analysis to yield informed decisions. In the evaluation, criteria are discussed including accuracy, data integrity, authority, source quality, bias, timeliness, references, impact, and relevance. The line drawings and graphs range from positive to negative attributes with degrees of evaluation in between. In the course of searching and evaluation, sources include scientific information, news sources, sources for legislation, legal, and case law, along with hidden agendas and interests. Query building is also illustrated.

Chapter 3, “Environmental Databases: A Trip Down memory Lane and New Journeys into the 21st Century”, an equally meaty and thorough chapter, is by Fred Stoss (SUNY Buffalo). In the introduction and beginning sections, an extensive history of searching and resources in the age of online information is presented (for more background, see chapters in another Symposium Series book (2)) including the development of STEM databases, computerization, and further developments such as retrieval methods and analysis methods, and the trend toward end-user searching. Table I lists major abstracting and indexing services by beginning year including name changes and notes that all are currently available online. Table II lists environmental science and pollution management databases by year of onset. Newer data analysis programs as well as databases and sources close out the chapter.

(Not to quibble, but the evolution of searching STEM information in academia differed from that in industry. As described, in academia, librarians and information specialists were trained in computer-based searching methods and performed searches at the request of scientist customers which led to end-user training. In industry, chemists and engineers, many already familiar with printed information resources, became self-taught in computerized retrieval methods and provided searches for customers on a cost recovery basis for both searcher billable hours and computer expenses. This latter aspect led to many in industry doing online searches earlier than our colleagues in academia because of cost recovery without pirating library acquisition budgets. Several programs also led to end-user training.)

Chapter 4, “Regulatory Toxicology: Progress in Law”, describes and compares product regulation and animal welfare legislation in both Europe and the United States. Current dependence on animal testing is discussed and the alternatives to it are described in detail, especially the efforts of CAAT, The Center to Alternatives to Animal Testing, at Johns Hopkins. The chapter concludes with 47 references, most authored by T. Hartung, one of the chapter authors.

Chapter 5, “Analytical Procedures and Regulation of New Drug Development”, activities in the Center for Drug Evaluation and Research within the FDA are described. Requirements of submission to the FDA, are set by statute and the Code of Federal Regulations, and other guidance documents. The amount of information required at each stage increases at each stage of the approval process. The example of analytical procedures is described in detail.

Chapter 6, “Steps Towards the Analytical Standards Required for Science-Based Tobacco Product Regulation”, somewhat surprisingly from the British American Tobacco Co. R&D, describes FDA analytical results and their impact on regulation. More than 90 harmful components of tobacco have been identified. Margins of exposure and modes of action for these and other components are determined, and standardization, especially of smoking machines, is developed. Evaluation of smokeless tobacco products and e-cigarettes is becoming important.

Chapter 7, “Regulatory Toxicology: Progress in Science”, covers the topic of non-animal based testing in greater depth. Worldwide, \$3 billion is spent on testing of pesticides and drugs (but not food additives), most of it on animals. However, many countries ban animal testing for cosmetics. Beginning with the motto, “Humans are not 70 kg rats”, progress at CAAT and elsewhere is discussed. Previous testing has contributed extensively to public safety, but many false positives and other inaccuracies exist (e.g., aspirin would fail most

tests). Testing in the 21st Century should be evaluated on economics, efficacy, and accuracy. Pitfalls in preclinical testing (only 5% of such submissions are eventually marketed) are shown. Predictability of cell culture testing needs improvement and integrated testing and mapping the human genome (a very current hot topic) are discussed as well developments such as ToxCast, which uses high-throughput screening, evaluation of endocrine disruptors, and advances in developmental neurotoxicity. The chapter concludes with 78 references.

Further developments in non-animal testing are discussed in Chapter 8, "Cooperation Between the United States EPA and Industry to Develop an *in vitro* Ocular Hazard Strategy". Three alternative tests to the Draize test on rabbits are being evaluated. No one test will suffice and a flow chart for effective evaluation is shown. Chapter 9, "Ensuring that Nutrition and Health Claims in the European Union on Foods and Food (Dietary) Supplements are Justified and Scientifically Substantiated", discusses achieving consumer protection along with fair trade and promotion of research. Scientific evidence of health claims is paramount and the process in the EU is described, especially for antioxidants and cardiovascular health claims. Communication understandable to the public is very important, and future challenges are discussed.

Chapter 10, "Comprehensive Nuclear Magnetic Resonance Analysis of Honey", is important to the analysis of mixtures and possible adulterants in general. NMR active isotopes of H, C, and P are analyzed. Chapter 11, "Rapid Screening Methods for Pharmaceutical Surveillance", discusses the problems of monitoring all ingredients (including inactives) in pharmaceuticals for purity and other factors including adulterants and even counterfeit drugs. Developments in portable or handheld spectroscopy in the field (Raman, IR, XRF, fluorescence) are discussed. I am familiar with such research at the University of Maine.

I also attended the ACS meeting in Philadelphia, presenting at another CINF symposium, and I was able to attend most of the presentations covered here. It's great to be able to acquire documentation of these valuable and timely presentations. A must read for anyone, chemist or not, concerned with scientific data and information used in the regulatory process.

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(1) *Science and the Law: How the Communication of Science Affects Policy Development in the Environment, Food, Health, and Transport Sectors*; Town W. G., Currano, J. N., Eds; ACS Symposium Series 1207; American Chemical Society: Washington, 2015. (Reviewed in *CIB*, 2017, 69 (2), p. 34-35)

(2) *The Future of the History of Chemical Information*; McEwen, L. R., Buntrock, R. E., Eds; ACS Symposium Series 1164; American Chemical Society; Washington, 2014.

Twenty-five Years Ago in Washington

As we prepare for yet another ACS national meeting in Washington, DC, I thought it might be amusing to look back at the fall 1992 meeting, also in Washington, DC. The very first of my ACS meeting reports was based on that meeting. (The 49th report in the series is now being advertised at <http://www.warr.com>.) Back in those days the report was distributed to only a small number of trusted readers and I was able to employ a much more gossipy style than the more objective one I currently use. Since so many years have passed, I feel able to repeat some of the gossip verbatim, but first some fact and figures:

Attendance was about 11,000, plus 1,500 exhibitor registrants. There were about 400 booths at the exhibition, representing about 220 companies. CINF presented a program of 35 talks (compared with 147 planned for the fall 2017 meeting); COMP had 59 (compared with over 400 in 2017). The Herman Skolnik Award was presented to Jacques-Emile Dubois, and the reception was held “in France” at La Maison Française de Washington (part of the French embassy). Apart from the Award symposium (on topological information in molecular modeling), there were sessions on genome information, the use of hypermedia, biotechnology patent information, and information for the bottom line.

In the exhibition, Fein-Marquart’s Kekulé software was demonstrated. My report says: “Kekulé takes a scanned chemical structure as input and makes a connection table from it. A structure is displayed from the connection table, and superimposed on the scanned version, so that it is easy to make any minor corrections using the molecule editor.”

The InfoChem reaction databases, ChemReact, ChemSynth, and ChemSelect were being shown in the Springer-Verlag booth. ChemReact and ChemSynth were REACCS-compatible; ChemSelect could be searched on a PC using MDL’s ChemBase software. MDL was still “Molecular Design Limited” and still had the lovely “M” logo. Who remembers the advert: “To ordinary draw programs it could be a caterpillar. Only ISIS/Draw knows it’s Friedelin”? I think I still have the T-shirt. In fall 1992 MDL was also demonstrating polymer solutions in MACCS-II. The company had a year of uncertainty after the death of Robert Maxwell in November 1991. In my report on the fall 1992 ACS meeting I noted that something like 60% of Maxwell Online staff had now left or been “let go”.

CAS had a large advert in the *Chemical Information Bulletin* proclaiming “Move into the 21st century: use CASREACT on STN”. In fall 2017 no doubt SciFinderⁿ will be the 21st century wonder. Databases on CD ROM were all the rage in 1992. There were even requests for CA on CD-ROM, as the 12th Collective Index on CD-ROM was about to be released. Beilstein’s Current Facts in Chemistry on CD-ROM was being touted. Do you remember the Lawson Number? Springer New Media was advertising “Draw a structure, AutoNom names it, within seconds”. Molecular Solutions Inc. were selling a rather useful book called the *Computational Chemistry Yellow Pages*.

More product news verbatim from my report: “At the last ACS meeting, AUTODESK could not do ‘lectures’ in their booth because they were told that microphones are banned. Piped music is, however, not banned, so this time they blasted ‘Also Sprach Zarathustra’ to all and sundry”. AUTODESK were promoting HyperChem in a big way.

Last but not least, I must mention the open meeting of the Society Committee on CAS (SOCAS). This always used to form the last item of the CINF technical program on the Monday afternoon, and it was always very well attended. For the fall 1992 event I reported:

“This time it was characterized by a great deal of smugness and back-slapping on the part of those on the platform: Joe Dixon, Larry Thompson (Chairman of the Committee), Clayton Callis (until recently, Acting Director of CAS) and Bob Massie (the new Director of CAS). Joe Dixon started by introducing Bob Massie, mentioning that the search process for the new Director had been long and thorough and denying the rumors (in *Monitor*) that three people had turned the job down. Massie’s background was outlined (linguist, lawyer, marketing manager, and ex-CEO of Gale Research). Bob Massie replied to the accolade but said that Clayton Callis would do a more substantive report on this occasion since he (Massie) had only been in office for five weeks [...] Larry Thompson said that he (Larry) was now about to retire from the committee after a three-year term. He reckons that communications between CAS and CINF have improved during his term of office and a ‘kinder and gentler’, less adversarial regime has begun [...]

And at last Stu Kaback (Exxon) rose to his feet. He had not intended to speak, he claimed. Larry Thompson congratulated him on waiting all of 26 minutes. It was, said Stu, eight years since the fall 1984 meeting where the attendees erupted in front of Dale Baker, and Seals and Dunn promised that as soon as STN was strong enough the data would be licensed to other hosts. ACS members are now paying over the odds to strengthen STN. It saddens him that no one has found a way around the lawsuit from which only the attorneys benefit. [Cries of ‘hear, hear’ and much applause.] Arleen Somerville then cooled things down by waffling about her useful communications with CAS, and Larry Thompson announced that the hour was up.”

And with that, my article also concludes. I hope to continue my history theme when the spring 2018 national meeting approaches. I expect I can find some gems in my report on the spring 1993 meeting in Denver.

Wendy Warr
July 2017



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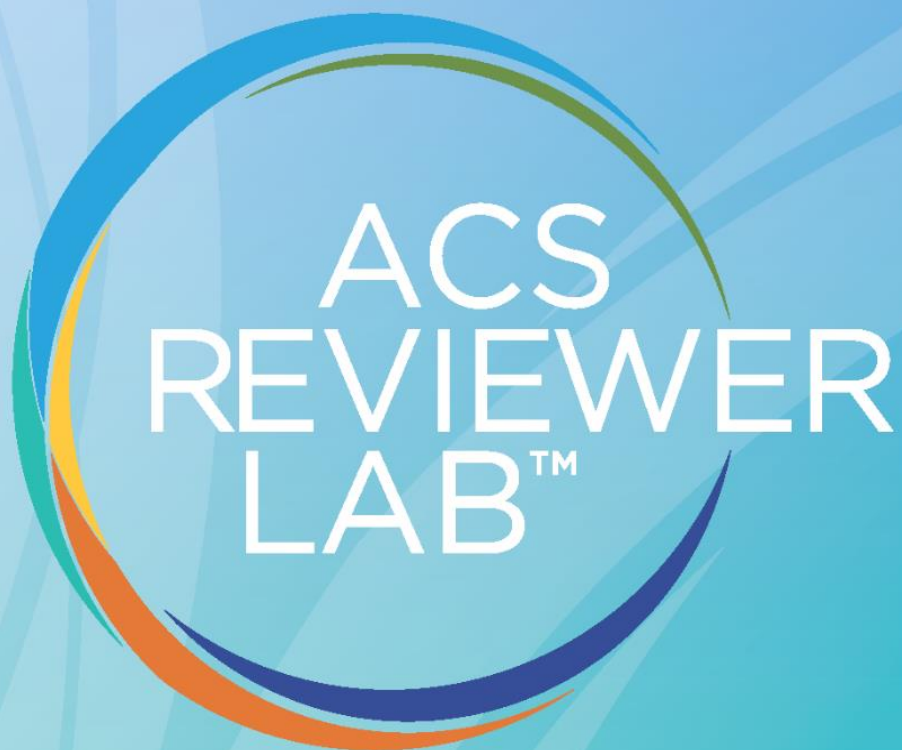
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- Earlier this year we published the first ever issue of our new journal, *Sustainable Energy & Fuels*. The journal contains research that contributes to the development of new and next-generation sustainable energy technologies, complementing our other energy journals including [Energy & Environmental Science](#) and [Journal of Materials Chemistry A](#).
- We also published the first issue of [Materials Chemistry Frontiers](#) as the third journal in the Frontiers portfolio, which we deliver in partnership with the Chinese Chemical Society.
- In our books portfolio we have launched two new professional reference series, [Chemical Biology](#) and [Food Chemistry, Function and Analysis](#). All books published in these new series will be included in our [2017 eBook collection](#).

RSC Advances – the story so far

Last year, we announced that from January 2017 our largest chemistry journal, *RSC Advances*, would be converted from a subscription journal to a gold open access (OA) journal.

Context for the change

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RSC Advances was launched in 2011 to provide a high quality publishing option for all sections of our community, including emerging scientific areas and markets. It supports early-career researchers and researchers from nations which are developing their research base.

Since its launch, the journal has become a home for high quality research that advances the development of the field. With a broad scope and focus on interdisciplinary research, it is now the largest chemical science journal in the world in terms of number of articles published. Since 2011 we have published over 26,000 articles covering 133 subjects.

The way scientists communicate their research has naturally evolved in the last five years, with the demand for OA publishing on the increase. Many funding bodies and institutions also now require authors to publish their research open access.

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*Data based on 2016 Journal Citation Reports, (Clarivate Analytics, June 2017).

Journal of Chemical Information & Modeling (ACS Publications)

Journal of Chemical Information and Modeling is excited to be sponsoring the Division of Chemical Information and our team looks forward to working with many of its members in the coming months. In the past I mentioned changes at the Journal in which involved creating two new manuscript types: Reviews and Application Notes. We have published several Application Notes describing software appropriate to chemical information and other areas and are in the process of publishing several Reviews. If you have an idea for a Review please contact me at eic@j cim.acs.org and we can discuss your idea further. We also are expanding our support in the area of molecular simulation and materials informatics, so please consider sending your manuscripts in these areas to the journal. All the best in 2017!

JOURNAL OF
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– Editor-in-Chief Kennie Merz

IC_{SYNTH} Version 3.0 Launched

InfoChem is pleased to announce the release of IC_{SYNTH} version 3.0 in Q2 2017.

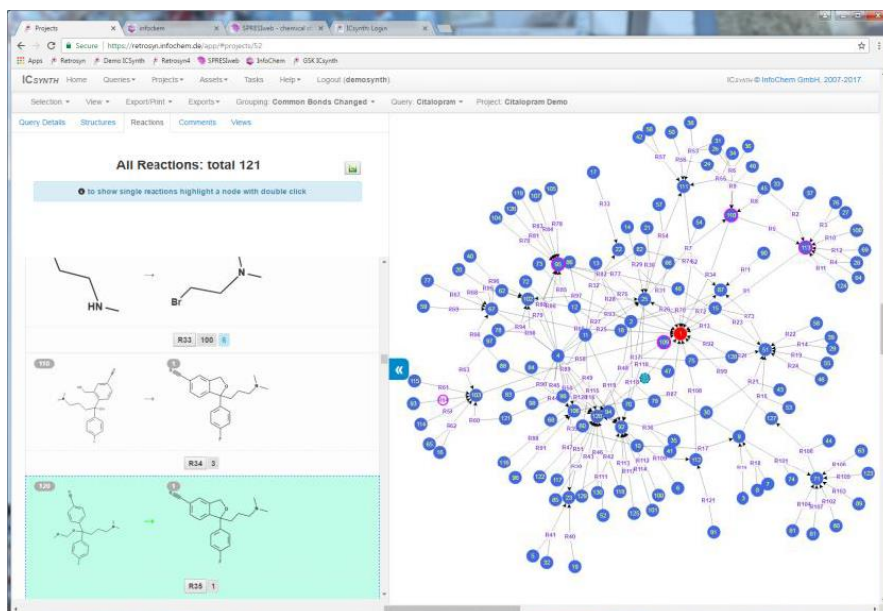
IC_{SYNTH} is a powerful synthesis-planning tool able to define synthesis routes based only on fully algorithmic chemical knowledge, and not on literature based synthesis path analysis. The system builds multistep, interactive synthesis trees taking advantage of automatically created transform libraries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



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Two major enhancements characterize version 3.0 of IC_{SYNTH}. First, the reaction layout view introduced with V.2.2 has been enhanced to become a genuine reaction graph: precursors can be visualized as molecules or just kept as nodes. The side panel enables magnification of the information in the graph, giving users an immediate scan of the highlighted reaction, empowering easy browsing of the retrosynthetic analysis results. The second major improvement provides the possibility to work in a team. IC_{SYNTH} V.3.0 enables project managers to define user groups able to work on the same target molecule, adding comments and exchanging information directly in the web application. Furthermore the algorithm responsible for the precursor search has been improved, resulting in better pathway suggestions.

For more information about IC_{SYNTH}, please visit our homepage (<http://www.nature.com/content/infochem/icsynth/index.html>) or contact us (info@infochem.de).



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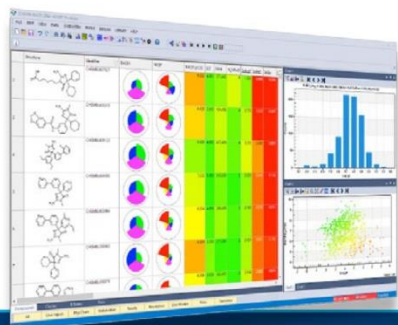
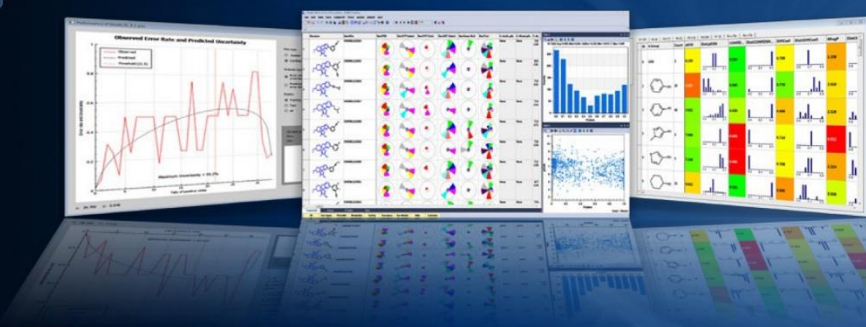
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Schedule of Future ACS National Meetings

255 th	Mar. 18–22	2018	New Orleans, LA
256 th	Aug. 19–23	2018	Boston, MA
257 th	Mar. 31–Apr. 4	2019	Orlando, FL
258 th	Aug. 25–29	2019	San Diego, CA
259 th	Mar. 22–26	2020	Philadelphia, PA
260 th	Aug. 23–27	2020	San Francisco, CA
261 th	Mar. 21–25	2021	San Antonio, TX
262 th	Aug. 22–26	2021	Atlanta, GA