



CSA Trust Newsletter

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2013 Herman Skolnik Award Winner



Left: Tony Williams, CINF Chair, presents Herman Skolnik Award to Richard (Dick) Cramer. Right: Bobby Glen, Brian Masek, Bernd Wendt, Dick Cramer, Tudor Oprea, Todd Wipke, Bob Clark, Yvonne Martin. Photo credits: Wendy Warr.

Dr. Richard ("Dick") Cramer was awarded the 2013 Herman Skolnik Award by the Division of Chemical Information (CINF) during the 246th American Chemical Society National Meeting held in Indianapolis, IN, September 8-12, 2013.

This award recognizes Cramer's outstanding contributions to and achievements in the theory and practice of chemical information science. Cramer's scientific breakthroughs include the invention of Comparative Molecular Field Analysis (CoMFA), the first and most widely-used 3D-QSAR technique for molecular discovery. Researchers use CoMFA to build statistical and graphical models that relate the chemical and biological properties of molecules to their 3D structures and the 3D steric and electrostatic properties. These models are then used to predict the activity of novel compounds. This information helps researchers to decide which molecules will likely make the best new drug candidates. This development earned Cramer one of the earliest cheminformatics patents. He continues to refine this technique through his work on topomeric descriptors and other QSAR innovations.

Dr. Cramer organized a one-day symposium for the occasion, which included the following presentations:

Adventures in CoMFAland / Robert D Clark, bob@simulations-plus.com, Department of Life Sciences, Simulations Plus, Inc., Lancaster, CA 93534, United States

My introduction to Comparative Molecular Field Analysis (CoMFA) and Dick Cramer came in the early 1990's while I was still working at Monsanto Agricultural Co. I continued working with the technology and the man for most of the next 20 years, many of them spent at Tripos Inc. This presentation will describe the history of both from the perspective of someone directly involved in the many and varied developments along the way.

2013 Herman Skolnik Award Winner continued

Adventures in drug discovery: For now we see through a glass, darkly / Robert C Glen, *rcg28@cam.ac.uk, Department of Chemistry, University of Cambridge, Cambridge, Cambridgeshire CB21EW, United Kingdom*

The fascinating thing about discovering drugs is that we learn more from our many mistakes than from our few successes – it is an incomplete puzzle with no clear answer. There are a few hundred successful drugs, and probably a few million attempts at drugs. The problem is that drug discovery is unfortunately multi-dimensional, with a response surface that is non-linear and disjoint, with polypharmacology and biological variability – and this is just for starters. Finding a new medicine is a really challenging problem. But there is hope – this is just the kind of problem we ought to make progress with using computational methods - embedding the transferable nuggets of knowledge or technique in computer software not only helps what we do today, but encapsulates this knowledge for future generations of drug hunters. There are a multitude of methods available, but a few like CoMFA or Topomers stand out as innovative attempts at solving parts of the puzzle. I would like to describe some problems, solutions and recent developments in computer-aided drug discovery applied to current projects at different stages of development.

Three paradigm shifts in computer-assisted drug design: The inventors and by-standers / Yvonne C Martin, *yvonnecmartin@comcast.net, Martin Consulting, Waukegan, Illinois 60087, United States*

In 1963 Hansch and Fujita invented 2D QSAR, which signaled the conversion of drug design from chemists' intuition and ease of synthesis to property-based considerations aided by computer analysis. Left as by-standers were researchers who ignored the use of statistical analysis with computers or who ignored the importance of hydrophobicity to drug potency. Some twenty-five years later Richard Cramer III and colleagues united molecular modelling and QSAR with the CoMFA method that showed that it is possible to correlate the potency of existing and forecast the potency of untested compounds with their 3D properties. Left as by-standers were researchers who focussed on complex descriptions of 3D properties or who ignored the use of multivariate statistical methods. Five years after that, Martin and colleagues showed that it is possible to use a computer to identify the 3D pharmacophores present in a set of diverse molecules, thus providing a starting hypothesis for CoMFA analysis. Left as by-standers were those who developed methods that required the user to specify the corresponding atoms in the molecules or who focussed on the 3D structures of the molecules, not their properties in 3D space. In each of these examples, the paradigm shift was catalyzed by the focus of the investigators to solve a problem.

Look back at 3D-QSAR and Dick Cramer / Anton J. Hopfinger, *hopfingr@gmail.com, Department of Pharmaceutical Sciences, The University of New Mexico, Albuquerque, NM 87131-0001, United States*

Dick Cramer and I began to discuss the future of QSAR analysis in the mid- to late- 1970s. There was little we did agree upon, but we were in concurrence that 3D information about molecules somehow needed to be included in the then 2D-QSAR paradigm. Much of our discussion and focus was directed at issues that remain familiar even today - a) how to represent the 3D information as descriptors, b) how to select 'active' conformations, c) what is the best way to select alignments, and, d) is there a good approach to develop a scheme to simultaneously do data reduction and model/function optimization. Obviously Dick was enormously successful with CoMFA by cleverly bringing together diverse computational and statistical methods to first generate and then parse through and neatly package large amounts of 3D molecular field data to generate a significant 3D-QSAR. At the same time, I struggled with first developing a methodology called molecular shape analysis, MSA, and making it operational. Subsequently, MSA morphed into what is now called 4D-QSAR analysis which can be considered a hybrid of CoMFA and MSA. Along the way, namely the last 35 years or so, the interesting discussions between Dick and I hopefully, on occasion, have served as substrates leading to advances, ideas and concepts, as well as more interesting discussions among our colleagues. I don't want this interplay between Dick and I to end so I'm going to mention in this presentation some recent advances, or perhaps better stated, hidden features, of 4D-QSAR analysis relating to alignment, pharmacophore delineation, 'active conformation' and mixing of different types and classes of descriptors within a 3D-QSAR formalism. Hopefully, this will once again garner interest from Dick for more discussion.

Evolution of QSAR from regression analysis to physical modeling / Ajay N Jain, *ajain@jainlab.org, Department of Bioengineering and Therapeutic Sciences, UCSF, San Francisco, CA 94158, United States*

This symposium honors a scientist whose work began a shift from predictive modeling of chemical and biological properties of molecules based on correlative analyses to modeling of biological activity in a manner related to underlying physical principles. Our work has been greatly influenced by the trail that was initially broken by CoMFA. Over the past twenty years, we have followed a course of increasingly more physically realistic model induction, beginning with abstract machine-learning models that addressed ligand pose variation and continuing now with methods that combine protein structural information with ligand activity information to produce truly physical models of binding sites. Such models are capable of accurate binding affinity predictions and accurate predictions of bioactive molecular poses.

2013 Herman Skolnik Award Winner continued

Scientific analysis of baseball performance / David W. Smith, dwsmith@retrosheet.org, Department of Biological Sciences, University of Delaware, Newark, DE 19716, United States

Science may be understood as a method of organized analysis which follows principles of objectivity, reproducibility and testability of clearly defined hypotheses. There is no limitation to specific topics such as Chemistry, Physics, or Biology. One non-traditional area in which the scientific approach has had great success is the analysis of baseball performance. Terms such as "baseball analytics" and "sabermetrics" have become increasingly common as science has moved into the sports world. There are three especially interesting aspects of scientific baseball analysis: 1) The innovations and sophisticated thought originated outside of the professional teams, many of which have been slow to accept what they see as intrusions; 2) Empirical observations have been important, but there has been a substantial component of modeling as well; 3) The collection of high quality, reliable data has been an essential underpinning to the entire effort. Retrosheet is a volunteer organization which has an extensive database of detailed baseball data that has been used in many studies. It is therefore not at all surprising that professional scientists and mathematicians have combined a passion for baseball with this rigorous analysis of a game. As a result, most teams now use a scientific approach to some degree, with the book (and later movie) "Money Ball" as a clear example along with the aggressive and successful use of these techniques by the Boston Red Sox. But the value of science in baseball is much greater, as a deeper and expanded understanding of the game's complexities has enhanced appreciation and enjoyment for fans and professionals as well as analysts.

Synthesis planning: Something about reactions, representation, relationships, and reasoning / W. Todd Wipke, wipke@ucsc.edu, Department of Chemistry and Biochemistry, University of California Santa Cruz, Santa Cruz, CA 95064, United States

This paper explores the technology of computer-assisted synthesis planning, its beginning, evolution, and impact. Once chemists could communicate in their natural language (structural diagrams) and the computer could carry out the symbolic algebra of chemical reactions we entered a new era for organic chemists and chemical information processing. Chemists had a new co-worker, one that would work faster, smarter, and cheaper each year. Fast forward 44 years, has the new partnership achieved all it was capable of? What can we expect for the future?

Think local, act global: Some challenges in cheminformatics and drug research / Tudor I Oprea, toprea@salud.unm.edu, Department of Internal Medicine, Translational Informatics Division, University of New Mexico School of Medicine, Albuquerque, NM 87131, United States

This retrospective will highlight some nonlinearities related to models and their usage in cheminformatics. From Cramer's BC(DEF) [1] to ChemGPS [2], and from ligand-based virtual screening [3] to Benet's BDDCS [4], this cheminformatics journey will highlight some of the evolving facets of cheminformatics, as it moves from understanding of chemical properties towards translational research. [1] Cramer RD. *J. Am. Chem. Soc.* 1980, 102:1837-1849 [2] Oprea TI, Gottfries J. *J. Comb. Chem.* 2001,3:157-166 [3] Bologa CG, et al. *Nature Chem. Biol.* 2006, 2:207-212 [4] Wu CY, Benet LZ. *Pharm. Res.* 2005, 22:11-23

From library design to off-target prediction: A wide array of topomer applications / Bernd Wendt, bernd.wendt@certara.com, Certara, Munich, Deutschland 81829, Germany

The topomer is a molecular descriptor that provides one solution to the molecular alignment problem. It produces a highly consistent set of 3D representations of fragments and allows for 3D alignment-based comparisons of molecules. The topomer has been widely used in various discovery research applications such as library design, virtual screening, 3D-QSAR and off-target prediction. Examples from several applications will be illustrated and discussed^{1,2}.

[ol][li]Wendt B, Mülbaier M, Wawro S, Schultes C, Alonso J, Janssen B, Lewis J (2011) *J Med Chem* 54:3982-3986[/li][li]Wendt B, Uhrig U, Bös, F (2011) *J Chem Inf Model* 51:843-851[/li][ol]

Whole template CoMFA: The QSAR grail? / Richard D Cramer, cramer@tripos.com, Tripos, Certara, Santa Fe, NM 87507, United States

3D-QSAR's fundamental challenge is generating appropriate 3D superpositions, or "alignments", of training and test set candidate structures. Whole Template CoMFA alignment is based on one or more template structures, whose conformations may be experimentally determined and/or pharmacophorically hypothesized. Alignment of a candidate structure first identifies and overlays the candidate bond having maximal "similarity" to any bond in any template structure, then copies the coordinates from all the "matching" atoms within that template to the corresponding candidate atoms, and finally positions the remaining candidate atoms by topomer canonicalization. Virtues of this new protocol include its full utilization of both structural and SAR information, ready interpretability and applicability, objectivity, and (foreseeably complete) automatibility. In addition to this method and some sample applications, its potential relevance to such fundamental QSAR challenges as the scope and reliability of a particular QSAR's predictions will be discussed.

For more information, please see: **Herman Skolnik Symposium Report** by Wendy Warr. *Chemical Information Bulletin*, 2013, 65 (4): 23-42.

People and Places

Engelbert Zass Selected to Receive 2014 Herman Skolnik Award



Dr. Engelbert Zass has been selected as the recipient of the American Chemical Society Division of Chemical Information's 2014 Herman Skolnik Award.

The award recognizes outstanding contributions to and achievements in the theory and practice of chemical information science and related disciplines. The prize consists of a \$3,000 honorarium and a plaque. Dr. Zass will also be invited to present an award symposium at the Fall 2014 ACS National Meeting to be held in San Francisco.

Dr. Zass, head of the Chemistry Biology Information Center at ETH Zürich (retired) is being recognized for outstanding contributions and achievements in the practice of chemical information science, notably for his lifelong work in education, research and development activities. Throughout his career he has been a true bridge-builder and mediator between database producers, vendors, publishers, librarians and end-users in chemistry, contributing to advancing chemical information as a whole.

Specializing in chemical information after receiving his Ph.D. in organic chemistry, Dr. Zass has more than 30 years of experience in searching, operating and designing chemistry databases, as well as in support, training and education of users of chemical information. He has given numerous lectures and courses in Europe and the U.S., is author of more than 60 papers on chemical information, and served on several publisher advisory boards. From 1999 till 2004, he was a partner in the BMBF Project "Vernetztes Studium – Chemie", where he was engaged in the design of multimedia educational material for chemical information. Through his leadership, vision, and collaborative efforts with his staff, he developed a model 21st century library that serves chemists and biologists at ETH.

To his many friends and admirers, "Bert" has been a true leader in the profession, generous in sharing his expertise with colleagues. His dedicated, sustained efforts and the transformative impact he has had on chemical information systems, database producers, chemists, and librarians make him a worthy recipient for the Herman Skolnik Award.

Dr. Zass did his undergraduate studies in chemistry at Universität zu Köln, followed by a Master's degree (Diplom) in Chemistry with Prof. E. Vogel. He went on to complete graduate studies with Prof. A. Eschenmoser at the Laboratorium für organische Chemie der ETH Zürich, culminating with a Ph.D. in Organic Chemistry (Dr. sc. nat.). Upon completing his education, Dr. Zass was a lecturer and senior scientist at the ETH, Laboratorium für organische Chemie ETH / Chemistry Information Center, later serving as Head of the expanded ETH Chemistry Biology Pharmacy Information Center until his retirement in 2012.

Andrea Twiss-Brooks, Chair, CINF Awards Committee
(Source: CHMINF-L, 25 September 2013)

Dave Winkler Receives 2013 Adrien Albert award for Medicinal Chemistry



Congratulations to [Dave Winkler](#) for receiving the 2013 Adrien Albert award for Medicinal Chemistry! His research "focuses on using computational methods to understand and predict the behaviour, hence design, of complex materials."

Given by the Division of Biomolecular Chemistry of The Royal Australian Chemical Institute, the [Adrian Albert Award](#) is the premier award of the Division and is given for sustained, outstanding research in the field of medicinal or agricultural chemistry, related to biomolecular chemistry.

[Adrien Albert](#) established medicinal chemistry in Australia and was the author of many important books including *Selective Toxicity*.

People and Places—continued



Guenter Grethe receiving congratulations from Antony Williams, CINF Chair

2013 CINF Lifetime Award Presented

Guenter Grethe was presented the CINF Lifetime Award during the Division Luncheon in Indianapolis on Tuesday, September 10, 2013.

The award was established by the Executive Committee of the Division of Chemical Information in 2006. It recognizes long-term membership, and outstanding service and active contributions to the Division over the years. The recipient must have been a member of the Division for at least 20 years.

Guenter has served CINF in various offices, and has been especially active in promoting the development of international partnerships and activities for CINF, including the XCITR project and the International Conference on Chemical Structures.

Guenter was the recipient of the 2001 Herman Skolnik Award and the 2004 Val Metanomski Meritorious Service Award from the Division. Congratulations, Guenter!

Andrea Twiss-Brooks, Chair, CINF Awards Committee

Reprinted from the Chemical Information Bulletin. 2013, 65 (4): 5.

In Memory of Monty Hyams

On 9, October 2013, Monty Hyams, the founder of Derwent, passed away peacefully in his own home at the age of 95 years and 7 months.

Monty was a visionary who pioneered the patent information industry in the 1950's with the realisation that Belgian patent information at that time offered the fastest source of important inventions. This led to the foundation of Derwent which he continued to run until 1984, when he retired to become Life President.

His influence on IP and Derwent in particular were profound. His achievements were recognised for his immense contributions to the patent information industry, including the creation of the unique Derwent World Patents Index database, by receipt of the Hermann Skolnik award in 1984 and at the turn of the millennium, becoming the inaugural recipient of the IPI Award in 2000. He was always quick to acknowledge the contributions of his colleagues at Derwent as he remarked in his acceptance speech for that award: "I am naturally very honored to be the first recipient of the award, which is a tribute not only to me personally, but also to all those at Derwent who helped to develop the company into the world leader in patent documentation service provision." In an interview with Richard Poynder in 2000, Monty was modest about his achievements: "All I really did most of the time was simply see chances, and then organise the people to do the work".

He will be fondly remembered by his many friends and colleagues as a unique individual who was still actively involved in information services until recently.

Monty was sometimes referred to as the father of the patent family, but he was also a father to two sons, Peter and Stephen.

Source: [Sad news - Monty Hyams, father of Derwent, passed away yesterday](#), *PIUG Discussion Forum*, 10 Oct., 2013.

For more information about Monty's career, please see: [The Proud Father—The History of Derwent](#)



CSA Trustees at the ACS 2013 Fall Meeting in Indianapolis



Top Left: Peter Loew, Guenter Grethe, Wendy Warr, Valentina Eigner- Pitto

Middle Left: Corinne Wipke, Steve Heller

Bottom Left: Andrea Twiss-Brooks, Martin Braendle, Edlyn Simmons

Top Right: Wendy Warr, Jignesh Bhate

Middle Right: David Wild, Jan Kuras, Tony Williams

Bottom Right: Tony Williams, Wendy Warr

Pictures taken by Wendy Warr. Used with permission from the ACS Chemical Information Division (<http://www.flickr.com/photos/cinf/>).

Photo Album from the ACS Fall National Meeting 2013 in Indianapolis



- 1st row left: Andy Berks, Andrea Twiss-Brooks
 1st row right: Johannes Hachmann and Abhik Seal (scholarship winners), Guenter Grethe
 2nd row left: Pamela Scott, Sally Peters, Howard Peters
 2nd row right: David Martinsen, Judith Currano
 3rd row left: Sarah Tegen, Brian Crawford
 3rd row right: Curt Breneman, Dusanka Janezic, Terry Stouch, Woody Sherman
 4th row left: Sarah Rouhi

Pictures taken by Wendy Warr. Used with permission from the ACS Chemical Infor-

CSA Trust Grant Call for Applications for 2014

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 currently inviting the submission of grant applications for 2014.

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. Grants will be awarded annually up to a maximum of a total combined value of ten thousand U.S. dollars (\$10,000). 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; 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.
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 13, 2014. Successful applicants will be notified no later than May 2, 2014.

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.

Chemical Structure Association Trust Award

The Chemical Structure Association Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In particular, the Trust strives to create a heightened and sustained awareness of the *essential* role that is played in scientific research by the systems and methodologies used for the storage, processing and retrieval of information related to chemical structures, reactions and compounds. In support of its charter, the Trust has created the Chemical Structure Association Trust Award as well as a unique Grant Program. These programs are financed by investments managed by the Trust and through funds donated by industrial, academic, and government organizations that recognize the value of and benefit from research, development, and education in the fields supported by the Trust.

The Trust is now seeking submission of nominations for its Award for its next round of deliberations.

AWARD PROGRAM

Purpose: To recognize and encourage *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 compounds.

Nature: The award, given on a tri-annual basis beginning in 2002, consists of five thousand U.S. dollars (\$5,000) and an appropriate memento. The award will be presented at a prestigious, relevant conference to be identified prior to each presentation. The awardee will be asked to give a presentation at the conference.

Eligibility: The Trust Award shall be granted to an individual without regard to age or nationality for outstanding achievement in education, research or development in the area of systems and methods used for the storage, processing and retrieval of information about chemical structures, reactions and compounds. Nominations of persons known to be deceased will not be considered. Posthumous awards will be made only when knowledge of the recipient's death is received after the Award Committee has announced their decision.

Nominations: Any individual may submit one nomination or one seconding letter for the Award in any given year. In nomination by petition, the person whose signature is first will be considered to be the nominator. The required nominating documentation is as follows: 1) A letter that evaluates the nominee's accomplishments and the specific relevant work that is to be recognized; 2) A biographical Sketch, including a statement of academic qualifications, as well as contact information; 3) At least two seconding letters that support the nomination and provide additional factual information with regard to the scientific achievements of the nominee. If appropriate, a list of the nominee's publications and/or patents may also be submitted. The Award will not be given in any year in which the nominees do not meet the award criteria.

The information should be submitted via email to Rene DePlanque, Chair of the Awards Committee (deplanque@gmx.de) and to Bonnie Lawlor, CSA Trust Secretary (Blawlor@nfais.org) by January 15, 2014.

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Report from the American Chemical Society Council Meeting Held on Sept. 11, 2013

The following report is adapted from the ACS Office of the Secretary's Councilor Talking Points. Items of particular interest to members of the Division of Chemical Information have been selected for inclusion in this report.

ACTIONS OF THE COUNCIL

Election Results

- Elected to the **Committee on Committees** beginning in 2014: Janet L. Bryant, Dee Ann Casteel, Amber S. Hinkle, Wayne E. Jones, Jr., and V. Michael Mautino for the 2014-2016 term.
- Elected to the **Council Policy Committee** beginning in 2014: Harmon B. Abrahamson, Judith H. Cohen, Alan M. Ehrlich, and Angela K. Wilson for the 2014-2016 term.
- Elected to the **Committee on Nominations and Elections** beginning in 2014: Lisa M. Balbes, Jeannette E. Brown, Martha L. Casey, D. Richard Cobb, and Lissa Dulany for the 2014-2016 term.

Candidates for President-Elect and Board of Directors

- The candidates for the fall 2013 ACS national election were announced as follows:

Candidates for President-Elect, 2014

Dr. G. Bryan Balazs, Associate Program Leader, Lawrence Livermore National Lab, Livermore, CA

Dr. Charles E. Kolb, Jr., President and CEO, Aerodyne Research Inc., Billerica, MA

Dr. Diane Grob Schmidt, Section Head R&D, The Procter & Gamble Company, Cincinnati, OH

Candidates for Directors-at-Large, 2014-2016 (two will be elected)

Dr. Susan B. Butts, Independent Consultant, Susan Butts Consulting, Midland, MI

Dr. Thom H. Dunning, Jr., Director, National Center for Supercomputing Applications and Professor, Distinguished Chair for Research, University of Illinois at Urbana-Champaign, Urbana, IL

Dr. Dorothy J. Phillips, Retired, Waters Corporation, Milford, MA

Dr. Kathleen M. Schulz, President, Business Results, Inc., Albuquerque, NM

Candidates for District II Director, 2014-2016

Dr. George M. Bodner, Arthur Kelly Distinguished Professor of Chemistry Education and Engineering, Purdue University, West Lafayette, IN

Dr. Alan A. Hazari, Director of Chemistry Labs and Lecturer, University of Tennessee, Knoxville, TN

Candidates for District IV Director, 2014-2016

Dr. Rigoberto Hernandez, Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA

Dr. Larry K. Krannich, Professor Emeritus of Chemistry, University of Alabama, Birmingham, AL

Committee Reviews and Committee Charters

- Council voted to continue the joint Board-Council Committee on International Activities and the Council Other Committee on Nomenclature, Terminology and Symbols. Continuation of the Committee on International Activities also requires Board of Directors concurrence.
- The Council voted to approve amendments to the charters of the committees on International Activities and on Nomenclature, Terminology and Symbols.

Selected Committee Reports (Highlights)

Society Committee on Education

SOCED recognized the achievement that is present in the Next Generation Science Standards, including their basis in research on teaching and learning, their formulation as performance standards, and their basis in the NRC framework and its dimensions of Science and Engineering Practices, Disciplinary Core Ideas, and Cross Cutting Concepts. SOCED supported the Standards as a document that is broadly applicable as a basis for K-12 science instruction and called upon the Society to develop innovative programming to support the implementation of the Standards.

Standing Committee on Economic and Professional Affairs (CEPA)

Committee on Economic and Professional Affairs reported that employment is up and unemployment is down for ACS chemists. The complete review of the Comprehensive Salary Survey will appear in the September 23 issue of *C&EN*.

Report from the ACS Council Meeting Held on Sept. 11, 2013 continued

Realignment of Electoral Districts

- ACS Bylaws require that the six electoral districts – from which six directors are elected to the ACS Board of Directors – be balanced in their total member populations. The Council voted to approve a proposal by the Committee on Nominations and Elections to realign these districts. The realignment meets the specified criteria for redistricting as required by Bylaw V, Section 4a and brings all six districts within permissible population range. This change takes place in 2014 and does not affect the 2013 national ACS elections. Councilors and others may visit the N&E website to look at the actual proposal and its impact.

Meeting Registration Report

As of the morning of September 11, 2013, the ACS fall national meeting had attracted 10,840 registrants, including 6,630 regular attendees and 2,584 students. The history of attendance at ACS fall national meetings since 2004 is as follows:

2004: Philadelphia, PA	14,025
2005: Washington, DC:	13,148
2006: San Francisco, CA	15,714
2007: Boston, MA:	15,554
2008: Philadelphia, PA:	13,805
2009: Washington, DC:	14,129
2010: Boston, MA:	14,151
2011: Denver, CO:	10,076*
2012: Philadelphia, PA:	13,251
2013: Indianapolis, IN:	10,840

Note for 2011: decline assumed to be due to timing (the week before Labor Day) [but there was also a major storm warning shortly before this ACS Meeting]

Local Sections

- The Council voted, on the recommendation of the Committee on Local Section Activities (LSAC), to approve a request from the Syracuse Local Section to change its name to the Central New York Local Section. Council also approved a recommendation from LSAC that the Monmouth County Local Section (in New Jersey) be dissolved, effective January 1, 2014, due to a decline in activity over the last several years. The North Jersey Local Section has contacted LSAC and will submit a petition in 2014 to annex the Monmouth County territory.

Divisions

- After much debate, a proposed name change for the Division of Colloid and Surface Chemistry to the Division of Colloids, Surfaces, and Nanomaterials was defeated by the Council in a close vote.

Special Discussion Item

- ACS President Marinda Wu presented and moderated a discussion on "What can we – as the Society and as individual citizens – do to help create jobs or demand for chemists?" She shared five recommendations from the presidential task force "Vision 2025: Helping ACS Members to Thrive in the Global Chemistry Enterprise" and what they might imply for our efforts to help create jobs: discover and share information about the skills and competencies that a wide range of employers will need; continue to expand resources which help our members to position themselves for successful careers in the global chemistry enterprise; enable entrepreneurs to create and strengthen their startups that hire chemistry professionals; advocate for policies that improve the business climate and promote the creation of chemistry jobs; and work with other stakeholders to understand and influence the supply and demand of chemists and jobs. Following the presentation, numerous Councilors engaged in a discussion of this focused topic on possibilities to encourage jobs creation and offered several suggestions.

ACTIONS OF THE BOARD OF DIRECTORS

At this meeting, the ACS Board of Directors considered a number of key strategic issues and responded with several actions.

The members of the Division of Chemical Information may be particularly interested in the specific bullets below regarding the formation of a National Association of Chemistry Teachers and the appointment of Manny Guzman as the President of Chemical Abstracts Service (CAS).

The Board's Committees and Working Groups

- The Board held a discussion on the topic "Connecting Chemists with Each Other." It considered what the role of ACS should be in helping chemists develop relationships with other chemists and the strategies that enable those relationships; how these strategies encourage and support younger and international members; and how these strategies develop relationships to leverage the world renowned chemists/innovators that comprise our membership.

Report from the ACS Council Meeting Held on Sept. 11, 2013 continued

The Board's Committees and Working Groups continued

- On the recommendation of the Committee on Grants and Awards, the Board voted to approve Society nominations for the National Science Board's Public Service Award and the National Science Foundation's (NSF) Alan T. Waterman Award. The National Science Board's Public Service Award honors individuals and groups that have made substantial contributions toward increasing public understanding of science and engineering in the US. The Alan T. Waterman Award recognizes an outstanding young researcher in any field of science or engineering supported by the NSF.
- The working group on Society Program Portfolio Management briefed the Board on its activities. The working group is charged with delivering a process for portfolio management of Society programs in the divisions of Membership and Scientific Advancement, Education, and the Office of the Secretary and General Counsel (Office of Public Affairs) and pilot programs.
- The Board received a briefing and approved a recommendation from its Committee on Executive Compensation. The compensation of the Society's executive staff receives regular review from the Board.
- On the recommendation of the Committee on Budget and Finance (B&F), the Board voted to approve an advance member registration fee of \$380 for national meetings held in 2014. The Board also voted to reauthorize funding in next year's proposed budget for the ACS International Center, and the ACS Entrepreneurial Initiative, and to authorize funding for a new initiative, the National Association of Chemistry Teachers (NACT). This association will be an ACS program to provide teachers a professional home. Through NACT they will have access to specialized resources and the broader ACS community.
- The Board confirmed the recommendation of the ACS Executive Director/CEO of the new President of Chemical Abstracts Service (CAS). He is Manuel (Manny) Guzman, most recently Executive Vice President of Learning and Research Solutions of Cengage Learning. Mr. Guzman succeeds Robert J. Massie, who is retiring in March 2014 after leading CAS for 21 years. Mr. Guzman will begin September 30. Mr. Massie will assist in the transition when he returns from medical leave.

The Executive Director/CEO Report

- The Executive Director/CEO and her direct reports updated the Board on the following: highlights and high-level recommendations on the ACS global presence; and the activities of CAS (Chemical Abstracts Service) and the ACS Publications Division. As a follow-up to the Publications report, the Board voted to approve one journal editor appointment and several editor re-appointments.

Other Society Business

- The Board also voted to hold the December 2015 Board of Directors meeting in Honolulu, Hawaii, in conjunction with the 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem). The ACS is the host society for the 2015 Pacifichem meeting, and co-location will allow Board members to participate in this very successful Pacifichem meeting.

ADDITIONAL INFORMATION FOR COUNCILORS

The following is a selected list of URLs and email addresses presented on slides at the Council meeting.

- www.my.acs.org

Showcases stories and photos submitted by members describing what best defines their ACS membership experience. If your story is selected, you receive a T-shirt.

- www.acs.org/getinvolved

ACS offers many ways to get involved at the local, regional, and national levels. There are opportunities for everyone, whether you are a student, just starting your career, or a seasoned professional.

- www.ACS.org/ChemistryAmbassadors

Visit the Chemistry Ambassadors website for ideas and resources to engage your community with positive messages about chemistry.

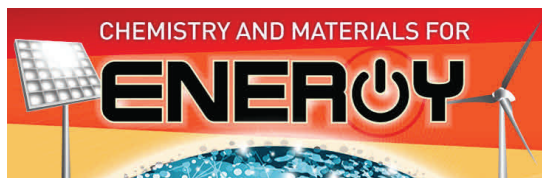
Submitted by:

Andrea Twiss-Brooks and Bonnie Lawlor, Councilors, CINF

Themes for Future ACS National Meetings

Themes for Future ACS National Meetings

The future of thematic programming at ACS meetings looks bright. More and more technical divisions organize symposia related to the theme of a meeting, often co-sponsored by other divisions indicating the interdisciplinary nature of chemistry. We definitely have seen a strong upwards trend in the last few meetings. Below are the themes for future ACS national meetings (F=Fall, S=Spring):



- S2014 *Chemistry and Materials for Energy* (Dallas)
- F2014 *Chemistry and Global Stewardship* (San Francisco)
- S2015 *Chemical Resources: Extraction, Refining and Conservation* (Denver)
- F2015 *A History of Innovations: From Discovery to Application* (Boston)
- S2016 *Computers in Chemistry* (tentative) (San Diego)
- F2016 *Chemistry and Education* (tentative) (Philadelphia)
- S2017 *Water and Chemistry* (proposed) (San Francisco)
- F2017 *Chemistry and Globalization* (proposed) (Washington)

From Guenter Grethe, CINF Representative to Multidisciplinary Program Planning Group

Joint CINF-CSA Trust Symposium at the ACS Spring National Meeting 2014 in Dallas

Energy Information Resources to Help Catalyze Your Research

Financially supported by Chemical Structure Association Trust

G. Baysinger, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 Trends in bio-based chemicals: Business intelligence from published literature. **S. M. Watson**

9:05 Chemistry databases and alerting services for finding the best energy research content. **S. Dabb**, R. Kidd

9:35 Sustainable chemistry in the CAS databases. **C. Dumitrescu**, R. Schenck

10:05 Intermission.

10:20 Fading shades of gray? ACS Meeting preprints past, present and future. **D. Flaxbart**

10:50 On the fly collection development to support emergent energy research initiatives. **D. T. Wrublewski**, G. Porter, D. Roth

11:20 X marks the spot: Using xSearch for discovering energy information. **G. Baysinger**

11:50 Concluding Remarks.

Abstracts

Trends in bio-based chemicals: Business intelligence from published literature / Steve M Watson. Radarweg 29, Amsterdam, North Holland, The Netherlands, s.watson@elsevier.com

A new information solution, Elsevier Biofuel, has been used to review the literature landscape, revealing trends in R&D towards the production of valuable chemicals from biomass. Elsevier Biofuel comprises advanced search and analysis tools, using a domain specific taxonomy to automatically classify over 21 million documents, many in full text, covering relevant journal publications, patents, technical reports, conference proceedings and trade publications. The analysis highlights emerging technology areas, commercial opportunities, and the leading companies staking a claim to this space.

Joint CINF-CSA Trust Symposium at the ACS Spring National Meeting in Dallas: Energy Information Resources to Help Catalyze Your Research—Abstracts continued

Chemistry databases and alerting services for finding the best energy research content / *Serin Dabb*, Richard Kidd. Royal Society of Chemistry, Thomas Graham House, Science Park, Cambridge, CB4 0WF, UK, dabbs@rsc.org

Chemistry research underpins the pursuit of sustainable and renewable materials for energy generation and storage. Due to the interdisciplinary nature of energy research, tools are needed to provide relevant chemical-related content to a researcher in this field, whether they have a chemistry background or not. As with all fields of research, services which condense, validate, or filter information are even more valuable due to the sheer quantity of information available on-line. Current literature updating services (such as Catalysts and Catalysed Reactions), highly curated information (such as The Merck Index Online), or information aggregators (such as ChemSpider), are all useful portals for energy researchers to find chemical information. This talk will outline the different types of content and subject coverage of these databases and tools, and how they relate to researchers in the field of energy generation and storage.

Sustainable chemistry in the CAS databases / *Cristian Dumitrescu*, Roger Schenck. CAS, 2540 Olentangy River Road, Columbus, OH 43202 cdumitrescu@cas.org

Covering chemistry in its broadest sense, the CAS databases are a reflection of the research efforts in the area of chemistry for environmental sustainability. From greener syntheses of pharmaceutical candidates, to more efficient conversion of the biomass, to new energy storage materials, this presentation will cover discovering insights into these technologies. In the area of planning greener synthetic procedures, a focus will be on finding more environmentally friendly catalysts and solvents in CAS's collection of chemical reactions.

Fading shades of gray? ACS Meeting preprints past, present and future / *David Flaxbart*. Mallet Chemistry Library, University of Texas at Austin, Welch Hall 2.132, Austin TX 78713 flaxbart@austin.utexas.edu

Meeting preprints from the energy-related divisions of ACS have been a part of the disciplinary literature since the 1930s. But the march of time seems to be leaving them behind, and even access to the legacy content is under threat from several quarters. This presentation will offer a quick history of this unique format of gray literature, the present state of affairs, and some advice for the future.

On the fly collection development to support emergent energy research initiatives. *Donna T. Wrublewski*, George Porter, Dana Roth. California Institute of Technology, 1200 E. California Blvd. MC 1-43, Pasadena, CA 91125, dtwrublewski@library.caltech.edu

Within the last few years, two major energy research initiatives have been undertaken on the Caltech campus: the Resnick Sustainability Institute (RSI) and the Joint Center for Artificial Photosynthesis (JCAP). RSI's research includes the production of electricity and fuels from renewable sources, the distribution and storage of energy, and other sustainability projects. JCAP's area of research is focused on achieving a system of artificial photosynthesis for utilizing solar energy. Both of these projects require resources from a broad range of fields, including chemistry, physics, biology, environmental & systems engineering, and more. This talk will give a brief description of some of the research being done in these projects, along with an overview of where energy research has traditionally been categorized in terms of collection development. A publication analysis will be presented to elucidate where information is being referenced from and where affiliated researchers are publishing, and how this correlates with the current collection holdings. Other considerations, such as identifying resources, outreach to groups about availability, and re-use of the collections, will also be discussed.

X marks the spot: Using xSearch for discovering energy information / *Grace Baysinger*. Stanford University, Swain Chemistry & Chemical Engineering Library, 364 Lomita Drive, Stanford, CA, 94305-5081, graceb@stanford.edu

Online collections in academic research libraries are growing at a rapid pace. To help users discover relevant information in the "digital stacks", robust yet intuitive discovery tools are needed. Multidisciplinary researchers in areas such as energy and the environment need to a broad array of resources to meet their information needs. xSearch is a locally customized federated search service that lets users search 250+ sources (databases, data & statistics, full-text books, full-text journals, grant & funding sources, government documents, images, streaming media, news, patents, reference materials, reports, and theses & dissertations). This presentation will cover energy-related resources selected for xSearch and will summarize search features available for finding relevant information.

News and Announcements



ICCS
International Conference
on Chemical Structures

GCC
German Conference
on Chemoinformatics



10th International Conference on Chemical Structures 10th German Conference on Chemoinformatics

June 1-5 2014, Noordwijkerhout
The Netherlands

<http://www.int-conf-chem-structures.org/>

The 10th International Conference on Chemical Structures (ICCS) and the 10th German Conference on Chemoinformatics (GCC) are teaming up for their 2014 conferences. Building on past successes of both conference series the 2014 event will offer a strong scientific program covering all aspects of cheminformatics and molecular modeling. Both conferences bring together an international audience interested in handling chemical structures and related topics. Participants discuss research and development in the processing, storage, retrieval and use of chemical structures. The conference fosters cooperation among organizations and researchers involved in the increasingly interwoven fields of cheminformatics and bioinformatics and combines in-depth technical presentations with ample opportunities for one-on-one discussions with the presenters.

The joint conference is the tenth in the series of the triennial ICCS conferences and in the series of the annual GCC conferences and will be held from 1-5 June, 2014 at the beautiful Conference Center in Noordwijkerhout, The Netherlands. The conference is jointly organized by:

- Division of Chemical Information of the American Chemical Society (ACS)
- Chemical Structure Association Trust (CSA Trust)
- Division of Chemical Information and Computer Science of the Chemical Society of Japan (CSJ)
- Chemistry-Information-Computer Division of the German Chemical Society (GDCh)
- Royal Netherlands Chemical Society (KNCV)
- Chemical Information and Computer Applications Group of the Royal Society of Chemistry (RSC)
- Swiss Chemical Society (SCS)





CSA Trust website:
<http://www.csa-trust.org>

CSA Trust Brochure:
<http://www.csa-trust.org/files/CSATBrochure.pdf>

Newsletter Calendar for 2013

Spring Issue:

Submission Deadline: May 10
Review Copy: May 27
Publication Date: June 3

Fall Issue:

Call for Content: Aug. 2
Reminder: Sept. 4
Submission Deadline: Sept. 27
Review Copy: Oct. 4
Publication Date: Oct. 7

About the CSA Trust

The Chemical Structure Association Trust (CSA Trust) is an internationally recognized, registered charity which promotes education, research and development in the field of storage, processing and retrieval of information about chemical structures, reactions and compounds. Since 2003, it has incorporated the activities of the former Chemical Structure Association.

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