

CHEMICAL Information BULLETIN

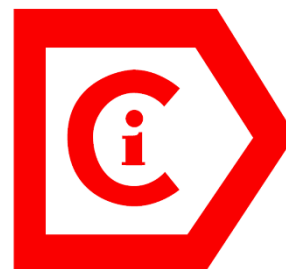


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Chemical Information Bulletin

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Teri M. Vogel, Editor
tmvogel@ucsd.edu

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Chemical Information Bulletin

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Program News for the Fall 256th ACS Meeting in Boston, August 19-23, 2018

We are all anticipating the fall CINF program in Boston. With over 170 submitted abstracts and triple program tracking on Sunday and Wednesday, we are certain to have presentations of interest to everyone! CINF has an excellent location for its technical sessions in the Westin Boston Waterfront, a hotel adjoining the convention center and very convenient to other divisions programming of interest.

Beginning on Sunday, we have three concurrent, full-day symposia. Jose Medina-Franco has organized a program dealing with cheminformatics and natural products. Martin Hicks, Bonnie Lawlor, Leah McEwen, and Vincent Scalfani, will preside over "Reporting and Reproducibility of Chemistry Research Data, cosponsored by ETHX and ORGN, with financial support from Chemical Structure Association Trust, and IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS). This will be followed with a symposium all day Monday on publishing chemical data. Elaine Chessman, Matt McBride, and Edlyn Simmons have organized a Sunday symposium dealing with patent and structure searching, in conjunction with CHAL and CPRM.

Sunday evening will feature the CINF poster session at our combined CINF Welcoming and Skolnik reception in the Galleria of the Westin Boston Waterfront, beginning at 6:30PM.

On Monday morning, we will have another program cosponsored by ETHX, this one on the ethics of data sharing organized by Judith Currano and Pam Mabrouk. Claire Bellamy, Evan Bolton, and David Deng will address another data standard Monday afternoon, with "Where are the Standards: Biologics Registration & HELM; Representation of Biologics: Informatics Standards & Challenges".

Don't forget the Monday night Sci-Mix poster session in the Convention Center Exhibit Hall B2/C, where CINF will have several poster presentations.

Tuesday features the Skolnik Symposium, honoring this year's awardee, Dr. Gisbert Schneider, Professor of Computer-Assisted Drug Design at the Institute of Pharmaceutical Sciences in the Department of Chemistry and Applied Biosciences, ETH Zurich. Among the invited speakers paying tribute to Dr. Schneider: Dr. Jürgen Bajorath, and Dr. David Winkler, both previous Skolnik awardees, and Dr. Bill Jorgensen. Also scheduled for Tuesday is "Chemistry Librarians of the Future," cosponsored by CHED and organized by Jeremy Garritano, Leah McEwen, and Vincent Scalfani.

Wednesday morning features a symposium on druggable targets organized by Rajarshi Guha and Tudor Oprea, a machine learning scoring function symposium organized by Suman Sirimulla, and "Semantics in Chemistry Vocabulary and Terminology," organized by Stuart Chalk and Leah McEwen.

Wednesday afternoon features programming on reaction analytics organized by Frederik van den Broek of Elsevier, along with a program on cheminformatics and drug discovery organized by Erin Davis. Thursday morning the CINF programming concludes with the second half of the reaction analytics and drug discovery symposia.

It will be very full four and half days of programming, and we hope you will join CINF for all of it from beginning to end. An outstanding program depends on the work and contributions of many people; I thank all those who suggested topical symposia and solicited speakers. If you have programming ideas and would like to suggest a topic for a future CINF symposium, or you would like to serve on the program committee, please reach out to me or our upcoming program chair, Sue Cardinal (scardinal@library.rochester.edu).

Rachelle Bienstock
CINF Program Chair
rachelleb1@gmail.com

From the CIB Editor

Welcome to another fall issue.

Inside you'll find a list of the CINF social events scheduled to take place at the upcoming fall National Meeting of the American Chemical Society. We also have Wendy Warr's report about the 1993 fall meeting in Chicago, Bob Buntrock's review of *What the Future Looks Like: Scientists Predict the Next Great Discoveries and Reveal How Today's Breakthroughs Are Already Shaping Our World*, Donna Wrublewski's interview with CINF member Kortney Rupp, and a new but slightly delayed installment of chemistry/science and popular culture. I did not attach the [CINF technical program](#) to this issue, but you can [access it from the CINF blog](#). The blog version was current at the time of printing, so please refer to the online program for the most current information.

I would like to thank our generous sponsors for supporting our meeting social events and providing updates on their products and services, as well as everyone who contributed a feature, or assisted with the copyediting. If you are interesting in writing something for an upcoming issue, please contact me or one of the other editors. The winter and summer issues that follow the national meetings are usually packed with symposium reports, so articles for the spring and fall issues are particularly welcome.

Have a great time in Boston!

Teri M. Vogel
CIB Editor, Fall Issue
UC San Diego
tmvogel@ucsd.edu

CINF Social Networking Events at the Fall 2018 ACS Meeting



Division of
Chemical
Information

Please Join Us At These Division of Chemical Information Events!

The ACS Division of Chemical Information is pleased to host the following social networking events at the Fall 2018 ACS National Meeting in Boston, MA.

Sunday Welcome Reception and Division of Chemical Information's 75th Anniversary Honoring Herman Skolnik Awardee Prof. Dr. Gisbert Schneider, ETH Zurich, Switzerland.

With Scholarships for Scientific Excellence Posters

6:30 - 8:30 pm, Sunday, August 19 – Galleria, Westin Boston Waterfront

Reception co-sponsored by: **Journal of Cheminformatics (Springer Nature)**,
Bio-Rad Laboratories, Collaborative Drug Discovery,
InfoChem, and PerkinElmer.

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 21 – Grand Ballroom A, Westin Boston Waterfront

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

Speaker:

Dr. Alex M. Clark

Scientist at Collaborative Drug Discovery,
Founder of Molecular Materials Informatics



Presentation:

Leveling Up Chemical Information for the Era of Big Data.

Herman Skolnik Award Symposium: De Novo Design

Prof. Dr. Gisbert Schneider, ETH Zurich, Switzerland

Symposium: 9:00am - 5:00pm (estimate), Tuesday, August 21 - Harbor Ballroom II - Westin Boston Waterfront

CINF Business Meetings

Saturday, August 18: 12:30-2:30 PM

- Education Committee: Alcott – Westin Boston Waterfront
- Awards Committee: Adams – Westin Boston Waterfront

Saturday, August 18: 12:30-6:00 PM

- Program Committee: 12:30pm – 3:00pm, Douglass – Westin Boston Waterfront
- Executive Committee: 3:00pm – 6:00pm, Douglass – Westin Boston Waterfront



Chemical Structure Association Trust

Applications Invited for CSA Trust Grant for 2019

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 2019.

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 pounds sterling 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 2019 Grant is March 29, 2019. Successful applicants will be notified no later than May 8, 2019.

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

2018

Stephen Capuzzi, Division of Chemical Biology and Medicinal Chemistry at the University of North Carolina Eshelman School of Pharmacy, Chapel Hill (USA), was awarded a grant to attend the 31st ICAR in Porto, Portugal from 06/11/2018 to 06/15/2018, where he presented his research entitled “Computer-Aided Discovery and Characterization of Novel Ebola Virus Inhibitors.”

Christopher Cooper, Cavendish Laboratory, University of Cambridge, UK, was awarded a grant to present his current research on systematic, high-throughput screening of organic dyes for co-sensitized dye-sensitized solar cells. He presented his work at the Solar Energy Conversion Gordon Research Conference and Seminar held June 16-22, 2018 in Hong Kong.

Mark Driver, Chemistry Department, University of Cambridge, UK, was awarded a grant to offset costs to attend the 7th EUChEMS conference where he will present a poster on his research that focuses on the development and applications of a theoretical approach to model hydrogen bonding.

Genqing Wang, La Trobe Institute for Molecular Sciences, La Trobe University, Australia, was awarded a grant to present his work at the Fragment-Based Lead Discovery Conference (FBLD2018) in San Diego, USA in October 2018. The current focus of his work is the development of novel anti-virulence drugs which potentially overcome the problems of antibiotic resistance of Gram-negative bacteria.

Roshan Singh, University of Oxford, UK, was awarded a grant to conduct research within Dr. Marcus Lundberg’s Group at Uppsala University, Sweden, as part of a collaboration that he has set up between them and Professor Edward Solomon’s Group at Stanford University, California. He conducts research within Professor John McGrady’s group at the University of Oxford. The collaboration will look to consolidate the experiments on heme Fe (IV)=O complexes currently being studied by Solomon’s Group with future multi-reference calculations to be conducted within Lundberg’s Group.

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 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 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 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 was awarded a 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 was awarded a 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 was awarded a 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 was awarded a 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 was awarded a grant for travel to work with Professor Ernst Walter-Knapp at 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 was awarded a 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 was awarded a grant to do three months of research at the University of Innsbruck, Austria.

2008

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

2007

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

2006

Krisztina Boda: University of Erlangen, Erlangen, Germany was awarded a 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 were awarded a 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 was awarded a grant to purchase equipment needed for her research.

2003

Prashant S. Kharkar: Institute of Chemical Technology, University of Mumbai, Matunga, Mumbai was awarded a 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 was awarded a 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.

Committee Reports

Report on the Council Agenda for August 22, 2018

The Council of the American Chemical Society will meet in Boston, MA on Wednesday, August 22, 2018 from 8:00am until approximately 12:00pm in Ballroom A-C of the Hynes Convention Center. All ACS members are welcome to attend, although only Councilors are permitted to vote. A continental breakfast is usually available at 7:00am for all attendees. There are only six routine action items for Council Action and these are noted below. The petition for consideration may generate discussion, but there is not vote on it in Boston. There will also be a special discussion on what role(s) ACS should play in preventing sexual harassment.

Nominations and Elections

The Committee on Nominations and Elections has announced the list of candidates for membership on the Council Policy Committee (CPC). These are Lawrence J. Berliner, Michelle V. Buchanan, Alan B. Cooper, Ella L. Davis, Lissa A. Dulany, Lydia E. M. Hines, Lisa Houston, Will E. Lynch, Martin D. Rudd, and Barbara P. Sitzman. Council must elect five individuals. The four candidates receiving the highest numbers of votes will be declared elected for the 2018-2021 term, and the candidate receiving the fifth highest vote will be declared elected for a one-year term for 2019.

The slate of candidates for membership on the Committee on Nominations and Elections has also been announced. Candidates are Allison Aldridge, Christopher J. Bannochie, Mary K. Engelman, Kenneth P. Fivizzani, Anne M. Gaffney, David S. Gottfried, James M. Landis, R. Daniel Libby, Silvia Ronco, and Frankie K. Wood-Black. Council must elect five individuals. The five candidates receiving the highest numbers of votes will be declared elected for the 2019-2021 term.

And finally, the slate of candidates for membership on the Committee on Committees has been announced. Candidates are: Rodney M. Bennett, Richard S. Danchik, Jacqueline A. Erickson, Rick Ewing, Russell W. Johnson, Donivan R. Porterfield, Carolyn Ribes, Frank Romano, and Peter Zarras. Council must elect five individuals. The five candidates receiving the highest numbers of votes will be declared elected for the 2019-2021 term.

Petitions for Vote

Petition of Affiliation with Other Technical Organizations

This petition proposes to add the Divisional Activities Committee (DAC) and the Local Section Activities Committee (LSAC) to Bylaw XI, Sec. 3, because each is charged under their respective duties in Bylaw III, Sec. 3, d, (1), (c), that DAC and LSAC act for Council, in collaboration with the Committee on Constitution and Bylaws (C&B), in approving the affiliation of divisions/local sections with other technical organizations:

DAC: (vii) acting for the Council, in collaboration with the Committee on Constitution and Bylaws, in approving the affiliation of divisions with other technical organizations. (6/1/73).

LSAC: (xi) acting for the Council, in collaboration with the Committee on Constitution and Bylaws, in approving the affiliation of local sections with other technical organizations. (11/7/07)

The Committee on Constitution and Bylaws has reviewed the petition and finds it to be legal and not inconsistent with the Bylaws of the Society. It will have no impact on the finances of the Society.

Petition to Remove Restrictions for International Chemical Sciences Chapters

This petition proposes to address concerns that were raised at the recent ACS Council Meeting in Washington, D.C. when a similar petition failed by fewer than eight votes; it did not receive the required two-thirds approval. Bylaw IX was written more than twenty-five years ago when International Chemical Sciences Chapters were created. In addressing concerns raised on the Council floor in D.C., this simplified petition creates a pathway for International Chapters to have a role in the Society to help to carry out Article II, Section 3 of the ACS Constitution: "The Society shall cooperate with scientists internationally and shall be concerned with the worldwide application of chemistry to the needs of humanity." The International Chapters are governed and operated by ACS member volunteers in the same way as divisions and local sections. International Chapter leaders are ACS members, including: U.S. citizens working and teaching abroad; chemists, chemical engineers and chemistry educators who have received their education in the U.S. or abroad; ACS award recipients, editors, authors, donors, and national and regional meeting presenters based outside the United States. In their countries, these volunteers donate their time to hold meetings and conduct activities to benefit chemistry and the Society. The leaders and members of these International Chapters provide ACS with valuable international networks within the worldwide chemistry enterprise. The Society cannot afford to be insular considering the value that members of International Chapters bring to the Society. The proposed, revised language removes the allotment restriction that International Chapters shall not receive funds but does not authorize any allotment of funds from ACS; this does not take away any dues funds from divisions or local sections. The Board of Directors may grant funds for a specific requested purpose. The petition also removes the restriction that International Chapters are not entitled to elected representation on the Council; it does not permit them to have Councilors, but it paves the way in case this is permitted in the future.

The Committee on Constitution and Bylaws has reviewed the petition and finds it to be legal and not inconsistent with the Bylaws of the Society. It will have no impact on the finances of the Society.

Petitions for Consideration

Petition to Streamline the ACS Governing Documents.

As a result of a Joint Board - Council Policy Committee (CPC) Task Force on Governance Design, a project was undertaken to reorganize the fundamental governing documents of the Society: the Constitution and Bylaws. The objective was to preserve the current governance structure and all current provisions, while creating a third document - Standing Rules. The manner in which the Standing Rules can be modified will have the additional benefit of

engaging more committees and members in the design and execution of ACS governance. Organizationally, these three documents should work as a hierarchy. The Constitution should define; the Bylaws should authorize, and the Standing Rules should operationalize. In general, moving from Constitution to Bylaws to Standing Rules on any topic should provide progressively more detail and become progressively easier to amend. The task force avoided making substantive changes, choosing to move blocks of text among the documents. A summary of document changes to the Constitution and Bylaws can be accessed at: <https://www.acs.org/content/dam/acsorg/about/governance/councilors/council-agenda-8-17.pdf> - see pages 93-148.

Committees are no longer named in the Constitution and Bylaws; rather, essential functions of the Council are named and Council is directed to create committees responsible for those functions. The names and duties of those committees are contained in the Standing Rules. A procedure has been created for amending the Standing Rules, which is in the Bylaws, and the committees responsible for the functions are generally tasked with being curators for those rules. A new term is created, units, meaning local sections, divisions, and International Chemical Sciences Chapters. The Society is permitted to create other units as necessary. The outcome of this process is to make the first two documents significantly smaller, while moving the bulk of the detail and thus the bulk of the language into Standing Rules.

The Committee on Constitution and Bylaws (C&B) has reviewed the petition and finds it to be legal and not inconsistent with the Charter, Constitution, and Bylaws of the Society. The proposed amendments meet the intent of the petitioners to reorganize the ACS Governing Documents while preserving the current governance structure and creating Standing Rules that include more details and are easier to amend than the Constitution and Bylaws. Members will be asked to vote on changes to the Constitution, as usual. The Council and Board will have to approve and confirm the approval of the petitions, as is now done. C&B suggests that the documents be edited for clarity and to remove duplication, but realizes that some of the more substantive edits falls outside the intent of the petitioners and should be left to future petitions. C&B has a number of suggested edits that will be sent to and discussed with the petitioners. For the most part, text that was moved from and to appropriate documents was verified; C&B will correct the references, as necessary, in the petition that will be up for action in the spring. Within thirty days after the Council meeting at which this petition is considered, comments and suggestions on the substance of the petition from opponents, committees, petitioners, and other interested members should be directed to the Chair of the Council Policy Committee, which has primary substantive responsibility for the petition. Comments and suggestions may be sent to bylaws@acs.org.

Petition for Action from the International Activities Committee (IAC)

A legal application has been received for the formation of a new international chemical sciences chapter to be known as the Colombia International Chemical Sciences Chapter. The Chapter will consist of the individual territory, and is not part of any other chapter or local section of the Society. The petition was initiated and signed by ACS members in good standing and residing in the territory. The application meets all of the requirements of Bylaw IX of the Society, and includes a statement that the applicants are familiar with and will abide by all governing documents of the Society including specifically Bylaw IX Section 2(c), which states that the Chapter and its officers as representatives of the Chapter shall not engage in political activity, shall avoid any activities that may adversely affect the interests and public

and professional image of the Society, and shall assure that all activities of the Chapter shall be open to all members of the Society. The application includes proposed budgets for Chapter operation. The petition has been reviewed by the ACS Joint-Board Committee on International Activities (IAC) which recommends Council approval. This action seeks the approval of the Council and is contingent on the approval from the ACS Board of Directors, after which, the Chapter will begin operation.

Note: The Council Agenda Book can be accessed at:

<https://www.acs.org/content/dam/acsorg/about/governance/councilors/council-agenda-8-17.pdf>.

Respectfully submitted July 30, 2018

CINF Councilors

Bonnie Lawlor
Svetlana N. Korolev
Andrea Twiss-Brooks

CINF Member Profile

Who are you?

Kortney K. Rupp

What do you do? (Institution, position, job description/duties)

University of California Berkeley (UCB) Chemical Information Librarian and Liaison to Lawrence Berkeley National Laboratory (LBNL)

My main job duties include all aspects of collection development, outreach, and reference and instruction for the College of Chemistry, which includes chemistry, and chemical and biomolecular engineering. Providing instruction to a range of learners is one of the best parts of my job. Those interactions often occur through individual appointments, course-integrated instruction, or library-wide events. I also serve as a campus-wide consultant for data management strategies in the sciences and have recently become more involved in creating programming for addressing unconscious bias in STEM fields. One interesting aspect of my position is my role as the liaison to LBNL, which involves collection development for a multidisciplinary government-funded research laboratory managed by UCB. I also work closely with the librarians at LBNL to provide outreach and reference services when needed.



Why are you in the chemical information field? (Your background, what led you to chemical information, etc.)

My original career intentions were not unlike many other chemistry undergraduates: go to graduate school for a Ph.D. and become a faculty member at a research institution. Through my research experiences at a small liberal arts college, a large pharmaceutical company, and a large research institution during graduate school, I started seeing the complexity of information management issues facing all scientists. I began having conversations with science librarians and quickly realized I could combine my background in chemistry and develop my skills as a librarian to help solve these issues. I could also still be involved in scientific research; now my research questions look at information transfer and organization within the research lifecycle. My hope is to help scientists become more efficient and effective in their work so we can make bigger and better scientific discoveries, faster.

What makes CINF valuable to you? (Include anything relevant, but especially any committees or projects in which you are involved.)

The American Chemical Society has been a part of my life for seven years. I have served as the president and secretary of my undergraduate chapter. I have attended the ACS leadership symposium and received the Women Chemist Committee Overcoming Challenges Award. It

is ingrained in my professional identity. When I was making the transition to the field of librarianship, I became concerned that I would no longer be able to maintain that strong connection to ACS, as I was no longer a “practicing chemist.” Enter the Chemical Information Division, and suddenly I found that I still had a community to belong to within ACS. I have been able to meet many of my amazing colleagues and continue to build relationships as I slowly take on more leadership roles, first as the *Chemical Information Bulletin* Editor for spring 2019 and soon as a member of the publications committee.

Donna Wrublewski
Chair, Membership Committee
July 2018

Twenty-five Years Ago in Chicago

The fall 1993 ACS meeting (in Chicago) marked the fiftieth anniversary of the Chemical Information Division. The anniversary was recognized, amongst other things, by a reception sponsored by CAS, InfoPro Technologies, MDL Information Systems, Questel, ISI, Dialog, Springer-Verlag, and Hampden Data Services. *C&EN* ran a small feature on the anniversary, with photographs, on September 13, 1993.

Symposia were presided over by Judith Leondar, Bruce Slutsky, Tom Wolff, Bill Milne, Peter Willett, Richard Love, Karen Landsberg, Stephen Schmidt, Bob Buntrock, and me. My own symposium was on new technologies for the delivery of chemical information: genetic algorithms, flexible 3D searching, fuzzy mathematical methods, neural networks, structure retrieval from large in-house databases, automatic chemical structure recognition (concerning PSI International's Kekulé "OCR for chemists"), and visualization and modeling. The structure retrieval talk was the revelation of Beilstein CROSSFIRE (later XFIRE or CrossFire). COMP division ran a full symposium on the Beilstein database, causing some CINF members to complain that COMP was straying onto CINF's patch. *C&EN* ran a full article about the COMP symposium.

The Herman Skolnik Award was presented to Professor Peter Willett of the University of Sheffield. An evening reception in his honor was sponsored by TRIPOS Associates, the Upjohn Company, Abbott Laboratories, and the Chemical Structure Association.

The Open Meeting of the Committee on Chemical Abstracts Service was a low-key meeting; Stu Kaback was not present to ask the first question. The open meeting of the Copyright Committee was entitled "Copyright law and electronic media" but in my own report it has the arcane title "Legal aspects of electrocopying". Much of the question and answer session arose from the protests of academic librarians who do not like having to return CD-ROMs and tapes to publishers; books never used to be returned.

CD-ROMs were much in evidence at the meeting. CASurveyor was demonstrated. It was described as a "personal science library". InfoChem announced a new product CD-React: a database on CD-ROM containing 1.8 million reactions from the 1975-1988 literature, derived from the VINITI/ZIC structural database of 2.2 million compounds. CD-React could be used in conjunction with the reaction database, ChemSelect, which was searched on a PC using PC Select, written by InfoChem. ISIS/Base was unsuitable for searching ChemSelect because it did not have reaction site searching.

At about this time, ISIS version 1.1 was "withdrawn" for further beta testing, to the chagrin of many MDL users. I have on file a copy of Phil McHale's carefully worded letter to customers on the subject. Also in 1993, MDL Information Systems, Inc. was born. An extract from my meeting report states: "MDL Information Systems, Inc. of Catalina Drive, San Leandro, is a publicly quoted company which bought Molecular Design Limited of Farallon Drive, San Leandro. Actually, the company occupies the same premises it has occupied for a long while. There are two buildings across the road from each other and by closing up a door to one building on Farallon Drive and leaving entrances opposite each other on Catalina, a new address could be created to make it seem in the public offering that a new company was buying old MDL. The value of the company was \$90 million: 8.2 million shares at \$11."

Dialog was another company that figured large in meetings of that era. The company appears on many pages of Volume 45(3) of the *Chemical Information Bulletin*. The Dialog customer appreciation breakfast at ACS meetings was always well attended: there is such a thing as a free breakfast.

I wonder if in 25 years' time someone will be writing about the upcoming meeting in Boston in August 2018. I can guarantee that it will not be me, but, Deo volente, I will offer another trip down memory lane for the *CIB* in February 2019.

Wendy Warr
July 2018

Science and Popular Culture, Part IV

Not surprisingly, one of the hot science topics this spring was vibranium, the metal that drives the economic and technological power of Black Panther's Wakanda, but for the first time in this occasional series, I get to include a source from an ACS journal. In a letter published in *Journal of Chemical Education* and briefly reported on in [Chemical & Engineering News](#), two Lawrence Technological University instructors included exam questions on vibranium for their general chemistry students. Where would they place [vibranium on the periodic table](#), what would the shorthand electron configuration be, and what symbol they would assign to it? Collins and Appleby further noted that the film provides an opportunity for class discussions about women and people of color in STEM disciplines. Kyle Hill weighed in on The Nerdist's Because Science channel on how T'Challa's Black Panther suit could [absorb, store, and release kinetic energy](#), while Bownamey Thirukkumar and Faeza Lorgat from the University of Leicester went into greater detail on the [suit and kinetic energy](#). Their conclusion: "For an ordinary human this would be impossible; as Black Panther is fictitious these values seem reasonable." USC physicist and TV and film science advisor Clifford Johnson also wrote about the film's potential impact on science education and engagement through its [representation of scientists](#).

Moving to cinematic universe in another galaxy, Sarah Jeong takes us on a journey through the bizarre array of [data storage formats](#) in the Star Wars films, from the lone disk with the Death Star plans in the original film, and coming full circle to the theft of those plans in *Rogue One*, a film whose climatic battle relied on our scrappy band of heroes essentially trying to get a good internet connection. Cloud City, and the physics behind suspending this [city above a giant gas planet](#), is covered in Patrick Johnson's recent book, *The Physics of Star Wars* (and excerpted here in *Popular Science*). Ryan Smith reached out to Johnson to discuss the accuracy of that powerful [ten seconds of silence](#) in the film, as well as a few other science "plot holes", some of which were also touched on in another [Because Science](#) video. For another unusual intersection between science and Star Wars, Jennifer Tsang wrote about mitochondria and the [much criticized midi-chloridians](#), which inspired one microbiologist to name a bacterium they discovered *Candidatus Midichloria mitochondrii*.

Rachel Becker looked into chemistry behind the [weapons used in Wonder Woman](#), speaking with St. Edwards University chemist, Raychelle Burks. While the science behind the gas (a hydrogen-based mustard gas that would be worse than the sulfur-based) does not make much sense, what the film does get right is the devastating role that chemical weapons played in the war as the "villain." The article also cited a [longer Chemical & Engineering News](#) piece by science journalist Sarah Everts, on the first chlorine gas attack in 1915 at the Battle of Ypres, part of a larger series, "[100 Years of Chemical Weapons](#)". There's [another article](#) in that series focusing specifically on Fritz Haber, plus this one written more recently by Matt Brady for "The Science Of..." website on Haber, a likely inspiration for the [Dr. Poison](#) character in *Wonder Woman*. David Hambling at *Popular Mechanics* also wrote about [Wonder Woman and WWI chemical weapons](#).

Moving from film to television, there's *The Expanse*, which is moving to Amazon for its fourth season next year. Hill wrote about why the show uses [science to depict a future](#) that feels more plausible, while Rhett Allain at *The Wired* [took a deeper dive](#) into the physics behind an important season two event: crashing a spacecraft into an asteroid to crash it into the sun. *Science Friday* interviewed *The Expanse*'s executive producer and one of the series authors

to talk about how they use science to keep the show grounded. More recently, Alan Boyle interviewed the cast and crew about the [science behind the show](#), and we also have Chris Mahon's list of the [top five science moments](#). (That number two moment, was a 'wow' moment.) Speaking of shows that will return in 2019, we have Stranger Things. Corey Mueller at *Popular Science* interviewed Columbia's Brian Greene about [parallel universes](#) and calculated how much salt would be needed to recreate [the isolation tank](#), while Clifford Johnson [broke down the science](#) for Screen Junkies.

Finally, this year marked the 200th anniversary of [Mary Shelley's Frankenstein](#); Nobel Prize winner, Roald Hoffmann, reflected on this seminal work, for *Chemical & Engineering News*: "The science in Mary Shelley's classic is just a stand-in, a prompt for our struggles with what is natural and what is not, with what being human means."

Teri M. Vogel
UC San Diego
July 2018

Book Review: *What the Future Looks Like: Scientists Predict the Next Great Discoveries and Reveal How Today's Breakthroughs Are Already Shaping Our World*

What the Future Looks Like: Scientists Predict the Next Great Discoveries and Reveal How Today's Breakthroughs Are Already Shaping Our World, Al-Khalili, J., Ed.; The Experiment, New York, 2018.

You might ask what relevance a book like this has for the audience of the *CIB*? Even though the information covered is broader than chemical information, the topics covered do have direct or indirect relevance to us both in our professions and in our daily lives. Topics including The Cloud, Cybersecurity, AI, Quantum Computing, and Robotics have direct relevance to most or all of us. Hopefully I've set the hook, and you are encouraged to continue reading.

The book (the subtitle makes a good abstract) is multi-authored and most of the authors, experts in their fields, are British. In the Introduction, the book editor describes the approach as "...neither celebratory nor alarmist ... instead ... objective as possible." The 18 chapters are organized into five sections. Most chapters conclude with a summary or final thoughts. The book concludes with a list of further reading, author bios, and an index.

The section on the Future of our Planet includes a chapter on demographics which covers a host of issues including population trends, sustainability, aging, urbanization, migration, populism, and topics that overlap with other chapters, including cell phones, the Internet, climate change, and robotics. The Biosphere chapter covers extinctions, threatened populations, and the anthropocene, with a possibly too-restrictive concentration on sea turtles. The currently topical subject of climate change is next, covering sources, pace, human enterprise, statistics, the climate in 2050, ice-free Arctic, monsoon disruption, seacoast flooding, choices, the Paris agreement, and energy usage.

The section, The Future of Us, contains four chapters. The first, the Future of Medicine, covers resistance to antibiotics, pandemics, personalized medicine, communication, spread of diseases by travel, and remote medical consultation (but no mention of AI). Genomics and Genetic Engineering covers complete gene data, decreasing costs, CRISPR developments, optogenetic DNA information storage (relevant!), cell programming, smart drugs, personalized medicine, and privacy issues. Synthetic Biology covers spider silk from yeast, standardized parts of DNA, reinvention of DNA, combatting malaria (all-time top killer), artemisinin from engineered yeasts, and facilitation of long-term space travel. The Transhumanism chapter covers "post-humans", enhancement of happiness, enhancement of virtue and morality, extension of life (cf Lazarus Long, a character in Robert Heinlein novels), brain injury repair, immortality by upload to computers, and brain enlargement. A host of ethical and desirability issues is also discussed, should versus will or would developments, transhumanism versus

religion and politics, and other cultural considerations.

The Future Online section contains four chapters. The Cloud and the Internet of Things covers reliable access to data and information, smart cities, share cars, and collaboration, plus a plethora of issues including privacy, security, coverage, costs and fees, plus societal benefits versus costs including what jobs are left, education, and even kitchens versus more eating out. (The chapter even provides the source of my favorite descriptor, DIKW: data, information, knowledge, wisdom). The Cybersecurity chapter expands on the downsides of enhanced computing including security improvements over the likes of DARPA, overload of ToT (the Internet of Things), the Dark Web, Bitcoin, cyber law enforcement, cybercrime, hacking, and copyright. The chapter on Artificial Intelligence (AI) continues the developments and debates in this exploding and explosive area. Coverage includes machine learning via Big Data, multilayer neural networks, artificial general intelligence (cf Alan Turing), uses of Watson (but no mention of Watson's "cheating" on Jeopardy), military drones, and the multitude of issues of the possible singularity of AI surpassing human intelligence including robotic takeover, human work versus machines, caregiving, and inevitable changes in living versus (un)intended consequences. Quantum Computing is changing so rapidly that any chapter rapidly becomes out of date. However, this chapter sets the stage by describing how quantum computers (QCs) would operate. QCs are not just fast computers, they operate entirely differently from conventional computers, and will be used for jobs other than those done by conventional systems. Such tasks include molecular calculations, weather prediction, and enhanced database searching.

The section on Making the Future also contains four chapters. The first deals with smart materials including devices that could sense, adapt, morph, and repair themselves, all without robotics or electronics. Opportunities could be as mundane as bicycles and weather adaptable clothing. Development for real items from demonstrated lab bench examples is difficult, and yet to come, but downsides of applications are minimal. The chapter on energy has obvious involvement with climate change, and greenhouse gases and sources. Smart energy systems and the need for globality and other political issues are discussed. The chapter concludes with an interesting question: "What if energy were free?" These topics lead directly to the chapter on Transportation. Topics covered are costs, time, capacity, and convenience, environmental impacts, public transport, and autonomous vehicles (a very hot topic). The last chapter in this session covers robotics. Topics include self-driving cars, domesticating robots, multi-purpose robots, and robots that care, as well as robotic soldiers and police, stealing jobs, repair of climate change damage, and the future.

The section on The Far Future literally gets "far out". The chapter on Interstellar Travel and Colonization covers time and thrust requirements, possibility of "wormholes", human frailty, and outposts such as the Moon, Mars, Venus, and icy moons. Possibilities are compared with probabilities. The Apocalypse is covered in the penultimate chapter. What if the future does not go as planned? Civilization collapse, risk of global catastrophe, climate change, extraterrestrial impacts, super volcanoes, solar coronal mass ejection, and global pandemics are discussed. Do we need a backed-up "save" file for civilization? The final chapter discusses Teleportation and Time Travel. The former would require quantum mechanics and entanglement, and the latter would involve time loops and worm holes. Both have been and are active topics in science fiction.

If this review seems verbose and formulaic, it is actually terse compared to the amount of information contained in this book. It is recommended for all who like to speculate on their profession and their future lives. After all, we've already done that for chemical information, both in a symposium (1) and the derived ACS Symposium Series book (2) (shameful plugs).

References

(1) The Future of the History of Chemical Information, CINF, 244th Meeting of the American Chemical Society, Philadelphia, PA, Aug. 20, 2012.

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

R. E. Buntrock
Buntrock Associates
Orono, ME



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In 2017, the Royal Society of Chemistry and Portland Press, the wholly owned publishing arm of the Biochemical Society, agreed to a partnership enabling the Royal Society of Chemistry to sell Portland Press journals content.

Speaking from the Frankfurt Book Fair, our commercial director, Dan Dyer said: "I am excited by the opportunities this announcement presents to both the Royal Society of Chemistry and the Biochemical Society. With the strategic alliance of the two societies, our customers will benefit by having a single sales contact to discuss all their chemistry and biochemistry content requirements. Working collaboratively in this way will benefit the whole community, by extending our content offering into each other's respective markets."

Professor Richard Reece, Chair of Portland Press Board commented: “Portland Press is dedicated to promoting and sharing scientific research. As such I am delighted that our journals will be exposed to a wider market. We can continue to further our aim to offer the best service to the librarian community, whilst increasing the dissemination of our published content to researchers.”

Dr Niamh O’Connor, Director of Publishing, Portland Press added: “This aids achievement of the Biochemical Society’s strategic objective to further develop international links and networks, supporting scientists to share their work on a global scale.”

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Ralf Schimmer

Head of Information at the Max Planck Digital Library

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To find out more about any of the above, please [get in touch](#).

New deputy chief executive

Paul Lewis joined the Royal Society of Chemistry as the new Deputy Chief Executive (Head of House) in March 2018.

An experienced senior leader in the private and not-for-profit sectors, Paul was previously at City & Guilds where he was Executive Director, International and Strategy. He has substantial leadership experience in the education, skills and knowledge sectors with specialist government-to-government and international operating expertise.

Paul has a B.Sc. (Hons) Geographical Sciences, PGCE (qualified teacher status) and MBA (Distinction). He is a graduate of the Royal Military Academy, Sandhurst. Paul is a Freeman of the City of London, a Fellow of the Institute of Leadership and Management, and a Fellow of the Royal Society for the Arts.

Dr. Robert Parker, Chief Executive of the Royal Society of Chemistry, said: "I am delighted to welcome Paul to the Royal Society of Chemistry. He brings with him valuable knowledge, skills and experience that, in partnership with Helen Pain, our DCEO (Head of Profession) and our wider leadership team, will contribute towards our strategic delivery, and achieving our mission to advance excellence in the chemical sciences."

Paul said: "I am delighted to be joining the highly-respected Royal Society of Chemistry and honored to be appointed Deputy Chief Executive. I very much look forward to meeting and working with colleagues, members and stakeholders around the world and feel privileged to be part of the chemical sciences community."

Paul will be responsible for leading the organization's publishing, commercial and technology delivery with a strong focus on developing and maintaining our position as a leading, high-quality publisher and knowledge provider, which is core to our Royal Charter and strategic ambitions.

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InfoChem News



[PubChem](#) is, arguably, the largest corpus of publicly-available chemical information. It collects chemical information from hundreds of data sources, and disseminates it to the public free of charge. Yet, although it contains 94.6 million unique chemical structures, very few of them (around 470,000) had direct links back into the primary literature. Enter [Springer Nature](#), delivering on its commitment to Linked Open Data. In October 2017 PubChem added more than 26 million links to scientific articles, thanks to contributions from the publisher. Of these, 1.6 million links point to open access or free-to-read documents.

The new data are created using InfoChem's Chemical Named Entity Recognition engine [ICANNOTATOR](#). It is a [smart ranking algorithm](#), ensuring that only relevant citations and molecules are deposited (who needs articles where, for example, an uninteresting solvent was mentioned just once?). Now Springer Nature and InfoChem have gone one step further by implementing a fully-automated workflow for the deposition of chemical compounds to PubChem, including links to scientific documents from Springer Nature.

While in the first phase of the [project](#) many parts of the processing had to be done manually, the great advance now is having a workflow in place that no longer requires human interaction. All the postpublication processing steps are fully-automated, from chemical annotation and relevancy calculation, to finally uploading and ingesting the literature data into the [PubChem Compound](#) database, which makes the process smart, rapid, and cost effective.

InfoChem has also added new Nature.com titles like *Nature Chemical Biology*, *Nature Chemistry* and *Nature Catalysis* to the workflow, so that links into these journals from compounds extracted from full-text are also visible on PubChem. All extracted compounds are linked to at least one Springer Nature document; from February 2018 until now more than 900,000 links back into the primary literature have been added (Fig. 1). Over 1,000 new compounds per month on average were delivered in the period from February to May 2018.

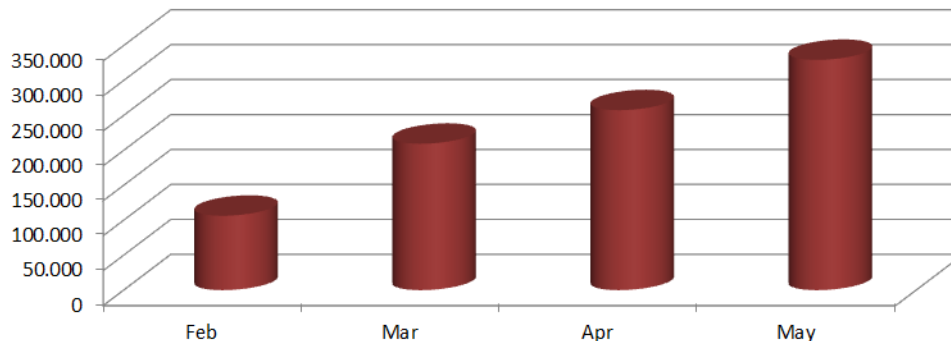


Fig. 1: New Citation Links from PubChem Compounds to Springer Nature Documents

Chemical compounds and their source documents in Springer Nature can be searched by substructure through PubChem, improving the accessibility and discoverability of information about chemical compounds. Each chemical record in PubChem with a "Springer Nature References" literature section includes a table with links to

SpringerNature documents (Figs. 2-3).

PubChem OPEN CHEMISTRY DATABASE

Search Compounds

Compound Summary for CID 5394

Download Share Help

Temozolomide

Cite this Record

STRUCTURE VENDORS DRUG INFO PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

Fig. 2. How to Link from Compound to Literature

Download

1 to 5 of 7,080 1 2 3 ... 1,416 Relevance

Title	Journal or Book	Year	PMID
Temozolomide/PLGA microparticles: a new protocol for treatment of glioma in rats	Medical Oncology	2010	20396980
Role of temozolomide in the treatment of newly diagnosed diffuse brainstem glioma in children: experience at a single institution	Child's Nervous System	2010	20217098
Population pharmacokinetics of temozolomide and metabolites in infants and children with primary central nervous system tumors	Cancer Chemotherapy and Pharmacology	2003	13680158
ATM inhibitor KU-55933 increases the TMZ responsiveness of only inherently TMZ sensitive GBM cells	Journal of Neuro-Oncology	2012	23054561
JCOG0911 INTEGRA study: a randomized screening phase II trial of interferonβ plus temozolomide in comparison with temozolomide alone for newly diagnosed glioblastoma	Journal of Neuro-Oncology	2018	29557060

from Springer Nature

Fig. 3: Links from the Compound "Temozolomide" to the Primary Literature

Springer Nature's initial contribution of links had the effect of doubling, from roughly 470,000 to more than one million, the number of chemical structures in PubChem having links to scientific documents. Moreover some 40% of the compounds added were novel to PubChem. Now in 2018, yet more links have been added, increasing yet more the value of PubChem for researchers worldwide. And as the deposition is continuous, the number of links and structures will continue to increase. Enthusiastic feedback from users has made it clear that there is a demand for more literature information in PubChem: hopefully other scientific publishers will follow the example of Springer Nature.

Dr. Josef Eiblmaier
je@infochem.de

PerkinElmer Inc.

Elsevier teams up with PerkinElmer to enable faster, more intuitive chemistry research

First phase of a long-term collaboration set to improve the research experience by integrating flagship solutions ChemDraw and Reaxys.



[Elsevier](#), the information analytics business specializing in science and health, has today announced a strategic collaboration with [PerkinElmer](#). The first phase of this collaboration will see the integration of Elsevier's flagship chemistry database, [Reaxys](#), with PerkinElmer's [ChemDraw®](#) software. The ChemDraw® JS software will be available directly through Reaxys, allowing academic and industry users to access the structure editor from within Reaxys to create publication-ready drawings, and simplifying access to a range of commonly used features.

Following this initial phase, Elsevier and PerkinElmer intend to integrate Reaxys into ChemDraw Desktop, enabling Reaxys subscribers to draw structures in ChemDraw and immediately search for them in the Reaxys database. Elsevier and PerkinElmer anticipate that the integration with ChemDraw JS will be available Q2 2018, with the ChemDraw Desktop integration expected to be launched in Q4 2018.

The integration of Reaxys and ChemDraw demonstrates a recognition from both Elsevier and PerkinElmer of how important world-class digital tools are to modern chemists and researchers, whether in academia or industry. This demand has been underlined by [recent research](#) from Elsevier showing that 84 percent of chemists believe having the facility to use digital tools was either "critical" or "very important" to their progression in the field. This integration is the beginning of a strategic collaboration to help provide the best possible research tools to scientists around the world.

"By integrating ChemDraw with Reaxys we are enhancing the user experience, allowing chemists and researchers to work in whatever way is most natural and familiar to them," said Neal Katz, Director of Life Science Solutions Marketing at Elsevier. *"At Elsevier, we are consistently working to understand how the ways chemists work on a day-to-day basis are transforming, and to develop solutions that help them achieve their goals faster. We're so excited about collaborating with PerkinElmer. This is the first step in a collaboration that will benefit chemists and researchers around the world."*

The integration will provide users with greater flexibility and seamless workflow transitions by allowing them to use their preferred structure editor directly within Reaxys whenever they wish to create graphics for publication or queries for chemistry search solutions, rather than having to adapt or be trained on a new tool. It also gives users multiple ways to initiate a structure search depending on their particular needs for each task. With the introduction of ChemDraw into Reaxys, organizations can spend less time training chemists to master different tools, resulting in lower costs and increased productivity per user.

“We are delighted that ChemDraw will be integrated with Reaxys as we are dedicated to enhancing scientific discovery. This integration means our users will enjoy a fluid and seamless research process, accelerating discoveries and opening up new areas of scientific inquiry,” said Michael Swartz, Business Segment Leader, Research, at PerkinElmer. *“Bringing together these two top-tier solutions gives users the best of both worlds by combining our informatics capabilities with Elsevier’s vast searchable content library. We look forward to finding more ways to collaborate with Elsevier in the future.”*

[Reaxys](#) contains more than 240 years of unparalleled chemistry content, including 105 million organic, inorganic and organometallic compounds, 42 million chemical reactions, 500 million published experimental facts, 16,000 chemistry related periodicals and six indexing sources for a cross-disciplinary view of chemistry.

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erinsdavis@gmail.com

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elsa.alvaro@northwestern.edu

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carmen@cinformaconsulting.com

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jg9jh@virginia.edu

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Procedures Chair

Bonnie Lawlor
chescot@aol.com

Program Committee Chair

Rachelle Bienstock
RJB Computational Modeling LLC
rachelleb1@gmail.com

Teller

Susan Cardinal
University of Rochester
scardinal@library.rochester.edu

Webmaster

Erin Davis
Schrödinger, Inc.
erindavis@gmail.com

Chemical Information Bulletin Editor – Spring Issue

Kortney Rupp
University of California Berkeley
kortneyrupp@berkeley.edu

Chemical Information Bulletin Editor – Summer Issue

David Shobe
Patent Information Agent
avidshobe@yahoo.com

Chemical Information Bulletin Editor – Fall Issue

Teri M. Vogel
University of California San Diego
tmvogel@ucsd.edu

Chemical Information Bulletin Editor – Winter Issue

Judith Currano
University of Pennsylvania
currano@obox.upenn.edu

Fall 2018 CINF Bulletin Contributors

Articles and Features

Robert E. Buntrock
Bonnie Lawlor
Teri Vogel
Wendy Warr
Donna Wrublewski

Sponsor Information

Graham Douglas

Production

Rachelle Bienstock
Erin Davis
Bonnie Lawlor
Kortney Rupp
Teri Vogel
Wendy Warr