Summer 2019 | Vol. 71, No. 2

CHEMICAL INFORMATION BULLETIN

A Publication of the Division of Chemical Information of the ACS

ISSN: 0364-1910

Spring 2019 National Meeting:
Chemistry for New Frontiers
Orlando, Florida
March 31-April 4

Table of Contents

Letter from the Editor

We have been experimenting lately with the format of the *Chemical Information Bulletin*. As a result, this issue may look different from the Spring 2019 issue or the Summer 2018 issue. This is in part because of the march of technological change. However, we aim to preserve the high quality of content that goes into the *Bulletin*.

You may notice that there is not much in the way of technical symposium reports in this issue. Every year, it seems, I have more and more difficulty finding participants to take notes and write summaries of the technical symposia. By the way, it is not necessary to be a symposium organizer to write a summary. It often has been the symposium organizer reporting on his or her own symposium, but sometimes the symposium organizer is too busy to do this. Also, it can be good to have the perspective of an "average attendee". So please consider volunteering for this activity later this year in San Diego or next year in Philadelphia.

While I am on the subject of volunteering, the CINF Division has a few positions open. For example, we still need a fundraising chair. (Remember: no fundraising means no funds for division activities! Thanks to Graham Douglas for filling this role in the interim.) Also, the division sometimes has difficulty recruiting more than one candidate for officer positions such as secretary. If you are interested in volunteering for any Division function, ask one of the current officers and I am sure they will be glad to help you get started.

Submitted by David Shobe

Notices

Wendy Warr has published six albums of photos from the ACS National Meeting in Orlando on the CINF Flickr stream at https://www.flickr.com/photos/cinf/albums. While you are visiting you might want to run through the whole photostream at https://www.flickr.com/photos/cinf/. Hover over each picture to see who is who. Double click a picture to see the "unshrunk" version. Enjoy!

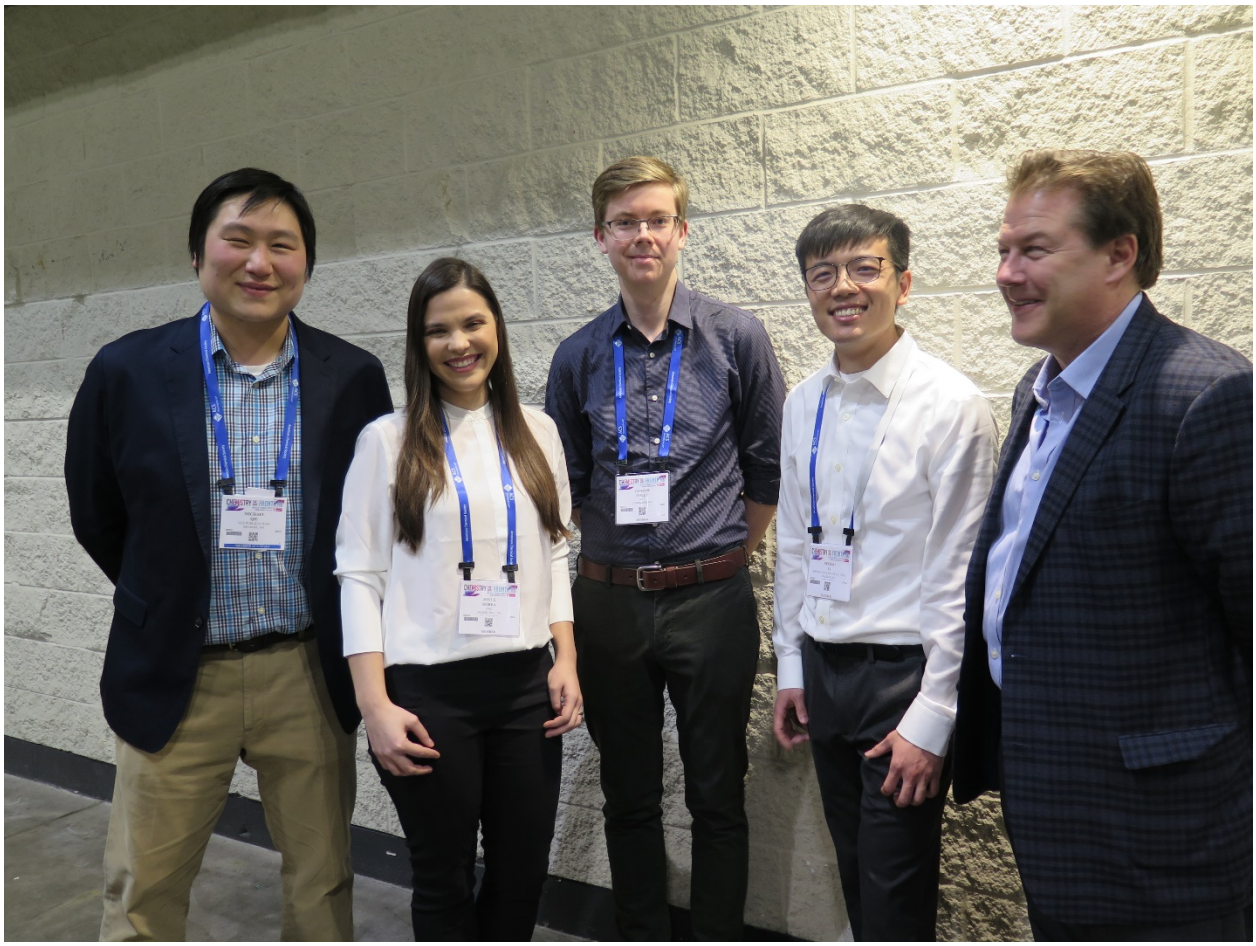
Submitted by Wendy Warr

Scholarships and Awards

Spring 2019 CINF Scholarships for Scientific Excellence Winners

The CINF Scholarship for Scientific Excellence program of the American Chemical Society Division of Chemical Information (CINF) is designed to reward outstanding graduate and postdoctoral students working in cheminformatics and chemical information addressing problems around knowledge representation, management, and modeling, and to foster their involvement with CINF. Since 2005 the program has awarded scholarships at each of the ACS national meetings. The awards at the spring 2019 national meeting in Orlando were sponsored by ACS Publications.

Three scholarships valued at $1,000 each were awarded to Joyce Borba, Connor Coley, and Xinhao Li.



From left to right: Michael Qiu, Joyce Borba, Connor Coley, Xinhao Li, Brandon Nordin.

Joyce V.B. Borba, Laboratory for Molecular Modeling, University of North Carolina; and Laboratory for Molecular Modeling and Drug Design, Federal University of Goias, Brazil. *"In silico* platform as an alternative to animal testing for acute toxicity".

Joyce V. B. Borba is a Ph.D. candidate at the Federal University of Goias, Brazil, where she also received her M.S. in Tropical Medicine and Public Health and her B.S. in Pharmacy. Her research interests include

cheminformatics and bioinformatics with applications in toxicology and neglected tropical diseases. She attended the University of North Carolina in 2018-2019 as a visiting research scholar.

Connor W. Coley, Department of Chemical Engineering, Massachusetts Institute of Technology. “ASKCOS: Data-driven synthetic route design and validation for small organic molecules”.

Connor W. Coley received his B.S. in Chemical Engineering from Caltech and M.S. in Chemical Engineering Practice from MIT. He is a final-year Ph.D. Candidate in the Department of Chemical Engineering at MIT working with Professors Klavs F. Jensen and William H. Green on computer assistance in organic synthesis planning and execution. Much of his work has focused on the development of a data-driven synthesis planning program and other predictive chemistry tools.

Xinhao Li, Department of Chemistry, North Carolina State University. “Hierarchical H-QSAR Modeling Approach for Integrating Binary/Multi Classification and Regression Models of Acute Oral Systemic Toxicity”.

Xinhao Li is now a Ph.D. student in the Denis Fourches’ lab at the North Carolina State University. His research areas involve developing molecular informatics approaches and software for secure data storage and building QSAR models for molecular toxicity predictions.

Submitted by Elsa Alvaro and Michael Qiu

Lucille M. Wert Student Scholarship

The Lucille M. Wert Student Scholarship is awarded annually and is designed to help persons with an interest in the fields of chemistry and information to pursue graduate study in library, information, or computer science. The CINF Awards Committee reviewed the applications during the spring ACS meeting, and is very pleased to announce that the 2019 recipient is Steve Geier.

Steve holds a B.Sc. in Chemistry from Mount Allison University and a Ph.D. in Chemistry from the University of Toronto. Following a post-doctoral fellowship at the University of California Berkeley, he decided to pursue a master's in library and information studies from the University of Alberta. Steve continues to work part-time as a research associate in the Department of Chemistry and Biochemistry at Mount Allison University during his studies.

Steve is interested in a career helping students and researchers improve information literacy skills, disseminate their work, and access the work of others.

Congratulations to Steve!

Submitted by Rajarshi Guha

2018 Highlights of ACS Achievements

The following excerpt from the "2018 Highlights of ACS Achievements", an annual report by Thomas Connelly, Executive Director and CEO of the American Chemical Society, is relevant to the society's publications and abstracting services. This summary might be of interest to the chemical information community since an open meeting of the ACS Publications and CAS is no longer part of the CINF technical program. It is reprinted with permission from Thomas Connelly. The full report (21 pages) is at: https://www.acs.org/content/dam/acsorg/about/aboutacs/highlights-acs-achievements.pdf.

The year 2018 proved to be one of significant progress and great accomplishments for ACS on many fronts. The strength of the ACS publishing units, combined with excellent cost management across the society, produced the third consecutive record year for net from operations.

CAS generated its fastest revenue growth in more than a decade, through growth of enhanced products such as SciFinder^{n} and STNext. The new offering pipeline remains full, with new service offerings and a retrosynthesis tool (ChemPlanner).

- SciFinder^{n} finished the year at 400 sales. There were over 248 SciFinder^{n} converted customers and 86 new commercial customers. Penetration now amounts to 13.3% of the SciFinder market. New SciFinder^{n} capabilities include commercial customer self-registration, spectral property numeric searching, and full content corpus delivery twice per week.
- ChemPlanner development progressed on the retrosynthesis capability, positioning CAS for a release in 2019.
- CAS reported uptake on STNext continues with more than 40% of all STN usage through this platform.
- A new Interactive Insights Dashboard for the Science IP service was launched in November 2018.
- CAS completed development on minimum viable integration Application Programming Interface (API), which will enable customers to retrieve substance information by searching with a Registry Number, name, or Molfile.
- A new Data, Analytics, and Insights unit (DAI) was established at CAS in the fall of 2018. The first charter is to develop a solution to improve patent examiner efficiency by reducing the time needed to evaluate search results.
- There was added growth in content offered via CAS products in 2018. Most notable were again Chinese patent growth (double-digit percentage increases for more than three years now), PatentPak additions, and investment in formulations for the Formulus product offering.
- In its first full year, the Agile Marketing organization began to independently leverage emerging best practices in business-to-business marketing to generate sales leads and measurably influence revenue. The CAS blog was launched to promote thought leadership and engage C-level executives and has approximately 3,398 subscribers. Five whitepapers were published.

ACS Publications also experienced high revenue growth in its underlying sales. Manuscript submissions grew 12%, published articles grew 11%, and citations increased 8%. Six new titles were launched in 2018, and more than one third of the journals experienced record impact factors. ACS Publications increased its global programming and representation. New initiatives such as *ChemRxiv* and *ACS Omega* advanced significantly. *Chemical & Engineering News* (*C&EN*) launched a new online format, and its *C&EN Brand Lab* contributed to improved performance.

- In 2018, researchers worldwide provided nearly 178,000 author submissions for editorial consideration, from which more than 51,000 articles were published across the ACS journals portfolio. Achieving more than 133 million full text article downloads in 2018, ACS journals ensured that the research findings of authors are widely disseminated and read by the relevant global research communities. With over 3.1 million total citations reported, up 8% from the previous year, over one third of ACS journals achieved their highest Impact Factors (IF) ever.
- Six new journals were introduced with exceptional community support and one new journal, *ACS Materials Letters*, was approved by the Governing Board for Publishing for introduction in 2019. In 2018 five new titles under the *ACS Applied Materials & Interfaces* journal brand and *ACS Pharmacology & Translational Science* published their first issues.
- ACS Publications upgraded its Digital Publishing Platform and the user interface is being completely redesigned to deliver a modern, highly functioning interface for researchers to discover, peruse, and download integrated journal, book, and *C&EN* content.
- Authors of ACS journals can use the new innovative ACS Direct Correct system to both review and make direct edits to their manuscripts immediately prior to publication, all within a web browser. The authors' edits are electronically integrated into the work performed by ACS Publications production staff to prepare the article for publication.
- Information Technology launched an Artificial Intelligence (AI) powered tool to assist editors in matching the best journals to transfer manuscripts, and in locating relevant reviewers and potential new reviewers from an author pool for any given manuscript. They also implemented an AI-powered related articles engine for cen.acs.org.

Open Access Initiatives:

ACS Omega is firmly establishing itself and on track for future success:

- 3,600 submissions (up 75%)
- 2,044 published articles (more than double 2017 output)
- 1.5 million article downloads (up 210%)

ChemRxiv is developing successfully:

- Over 1,000 preprints posted
- Over 1 million article views and downloads

Strategic Open Access Developments, Plan S:

In September, a coalition of thirteen European-based funders announced far-reaching plans to require open access publication of research derived through their grants. Subsequently, implementation plans were released, and a consultation period started, designed to inform actions in time for the 2020 start date of the Plan S program. During December 2018, senior leaders from ACS Publications met with the key EU proponents of Plan S, and separately with the executive for the engagement of the United Kingdom with the Plan S coalition.

Market Outreach and Brand Awareness:

ACS on Campus had its biggest year to date. Supported as a joint program by ACS Publications, CAS and Membership & Society Services, Publications hosted 54 events at institutions and meetings in 14 countries, engaging with nearly 6,000 researchers in total, and featuring 69 editors drawn from across 37 journals as speakers.

ACS Publishing Center (https://pubs.acs.org/publish/), a new centralized portal that consolidated functionality previously in ACS *ChemWorx* and resources from the Author & Reviewer Resource Center, achieved an average of 1,249 sessions a day from 552 visitors within a month of launch. Other resource improvements for research authors were ACS Author University, a 15-video series showcasing editor advice on all aspects of the publication process, and translated versions of the online course *ACS Reviewer Lab*.

C&EN:

In 2018, *C&EN* accomplished the goal to publish all news content on the web ahead of it being released weekly in print. *C&EN's* new web design debuted on March 30. In addition, the redesign of *C&EN's* website was launched. Built for responsiveness, organized around newly designed taxonomy, and with expanded opportunities for advertising, the new cen.acs.org has a greatly enhanced user experience. The project transformed the members-only paywall on the site into a metered paywall that encourages visitors to cen.acs.org to register for more access to *C&EN* content or to become ACS members for unlimited access.

C&EN's Multimedia Team created a new monthly podcast, aptly named *Stereo Chemistry*, available on iTunes, Google Play, and Amazon's Alexa. Its goal is to provide a channel to discuss chemistry news and share *C&EN* reporters' expertise and analysis.

Submitted by Svetlana Korolev

Technical Program

Partnering Up in the New Frontier: Libraries & External Partners Working Together

Michael Qiu and I were curious about how librarians collaborate with external partners. What are some examples? What are the benefits and challenges of such partnerships? Our symposium was held on Sunday, March 31, 2019 at 8:30 – noon, at the Orange County Convention Center in Orlando, Florida. The audience learned that the local community and the library were enhanced by participating in partnerships with publishers, educational organizations, and both public and private database developers. Often these collaborations had a global impact.

The main benefits of partnerships are:

- Strengthening the network of the local community
- Enhancing expertise for both partners
- Sharing knowledge, skills, and data
- Building better tools for discovering and organizing information.

To begin with, **Grace Baysinger**, a librarian from Stanford University Libraries, and **Shannon O'Reilly**, from ACS Publications, described how universities can work with publishers to help students advance their research and get published. The abstract said "Stanford hosted an event with the theme 'GearUp for Scientific and Technical Publishing' and included a session on graphical abstracts, an important part of any publication since they help users understand the research and play a key role in helping users find and choose which articles to read." This event strengthened the local community by introducing people to each other in a learning environment and teaching them how to graphically summarize their work. The library was a strong partner, providing space and facilitation for the event. The American Chemical Society gained a new learning module that they could incorporate in future ACS on Campus events. ACS continues to partner with libraries and holds more events that draw on knowledge of the local community. See https://acsoncampus.acs.org/ for more information.

Ye Li, a librarian previously from Colorado School of Mines and now at MIT, described two partnerships she had with non-profit stakeholders: Wiki Education and Carpentries. She partnered with Wiki Education in order to facilitate Wikipedia editing assignments. "Don't cite Wikipedia, Write Wikipedia." Students needed help navigating the Wikipedia world and avoiding editing wars. Even though each student does a small amount of writing and editing, together there are many classes making many changes that together have a global impact. Ye's faculty colleagues created assignments that required students to actively improve the world's most-read source of information making it more accurate and complete than before. In my opinion, this is better than creating writing assignments that are destined to be forgotten and thrown out. For more, see https://wikiedu.org/.

In addition, Ye described how she became a certified trainer with the Carpentries movement and offered workshops on FAIR (findable, accessible, interoperable and reusable) data. Trainers can also develop new curricula for libraries and for use in software. For more see https://carpentries.org/.

Leah McEwen, a librarian at Cornell University, collaborated with **Evan Bolton**, National Institutes of Health (NIH), to create Laboratory Chemical Safety Summaries in PubChem. These summaries assemble and unite quality safety data. Evan and Leah brought complementary skills to this project. Evan had the

data-harvesting skills, the tools, and the raw data. Leah had the knowledge of how to organize this information to meet people's needs based on use cases. They had a shared vision of keeping people safer in the laboratory. While machines could do a reasonable first attempt to put the data together, humans were required in order to make the presentation of the data usable to other people. The quality of multiple sources of similar data could be evaluated based on provenance cited in the PubChem database. For more about PubChem, see https://pubchem.ncbi.nlm.nih.gov/.

Leah is also involved in creating FAIR data workshops. She brought interested parties together, enabling them to form new collaborations around the topic of standardizing and improving data. At the workshop, "FAIR chemical data for health and safety connects the dots between cheminformatics and librarianship", everyone developed a richer understanding of the nuances of common challenges, and new projects emerged. For more about FAIR, see https://www.go-fair.org/fair-principles/.

Jürgen Swienty-Busch, from the publisher Elsevier, discussed the evolution and current state of the database currently known as Reaxys. Reaxys has its roots in old print handbooks called Beilstein and Gmelin. It was difficult to use these and find information. The information in these handbooks was digitized in 1989 and made available through STN, first as Crossfire and now as Reaxys. This new Interface is more intuitive. Searches can be performed in natural language. Combinations of structure and properties can be searched. This database helps people find useful information across disciplines and across publications.

Judith Currano, a librarian at University of Pennsylvania, described her collaboration with Jürgen. Training on Reaxys was embedded in her courses. She required the students to show their work on homework assignments. This work was sometimes shared with Reaxys developers so that they could learn how students approach and use the product. Librarians can introduce students and researchers to developers so that the product can be improved. Librarians are expert searchers and can beta-test products and give advice.

Jozica Dolenc and **Oliver Renn** from ETH Zürich joined us virtually and asynchronously. They described how they interview people and understand their needs. At ETH, they have "coffee lectures" to teach students how to use Reaxys. They show students how to find properties and the best synthetic routes. Additionally, researchers provide feedback that leads to specific product development and improvements.

Sunghwan Kim, from NIH, delved deeper into the potential usefulness of the PubChem database as a freely available public database. Many younger researchers are using it for their research. It is stable and government-funded. It is especially useful for educational organizations such as community colleges where resources are limited. Data provenance is preserved to help a person evaluate the quality of the data. The context is key to understanding the values. If data appear to disagree, one should identify the source, how they were measured, and for what purpose they were measured. There is easy and quick access to Laboratory Chemical Safety Summaries using a mobile device. The data can be downloaded and manipulated by computers, which is nice for teaching cheminformatics. Potential course materials are on LibreTexts for free, and cover PubChem data, tools, and services. PubChem has great potential as a cheminformatics training tool. However, the interface keeps changing, so training materials will need updating. For more about LibreTexts see https://chem.libretexts.org/.

Submitted by Susan K. Cardinal

Preview of Fall 2018 Meeting

I encourage you to register for the San Diego conference, August 25-28, 2019. With over 175 submitted abstracts and triple program tracking on Sunday and Wednesday, we are certain to have presentations of interest to everyone!

To start with, we are celebrating the most recent Herman Skolnik Award winner, Kimito Funatsu. He is well known for his contributions to structure elucidation, *de novo* structure generation, and applications of cheminformatics methods to materials design and chemical process control.

While on the subject of materials, we have a session on materials informatics and a related session on materials in the machine learning and artificial intelligence symposium. There are many more sessions for our computational colleagues, including sessions on text mining and natural language processing, machine learning and artificial intelligence, drug discovery via innovative data visualization, biologic informatics, and drug discovery informatics.

With great joy and many talks, we will celebrate one million crystal structures in the Cambridge Structural Database (https://www.ccdc.cam.ac.uk/Community/blog/an-acs-symposium-one-million-crystal-structures/). For librarians and information providers, we will explore chemical nomenclature and representation. Additionally, there will be sessions on patent novelty searching, extended reality, and the importance of collaboration to create student success, sponsored by CAS.

We are having another round of the student poster competition, sponsored by ACS Publications. Two more symposia are on web-based chemistry databases and on successful projects fueled primarily by open-source tools or data. This is just the CINF program. We are cosponsoring with CHAS, HIST, CHAL, PROF, PRES and other divisions on other programs.

The organizers have done a fabulous job recruiting talented speakers. Please come and listen, discuss, and be enriched by this wealth of knowledge, skill, and experience. We hope you will join CINF for all of it from beginning to end. More details about programs, including organizers and program descriptions, can be found at https://callforpapers.acs.org/sandiego2019/CINF.

As you know, an outstanding program depends on the work and contributions of many people. This starts with simple suggestions of symposia topics and extends to speakers, organizers, reporters, committee members, attendees, and especially sponsors. 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 contact me, Sue Cardinal, your 2019 Program Chair, at scardinal@library.rochester.edu. Make sure to include "ACS CINF" in your subject line. If you like what you are reading, please tweet at #ACSCINF.

Submitted by Susan K. Cardinal

Report on the Council Meeting

The Council of the American Chemical Society met in Orlando, FL on Wednesday, April 3, 2019 from 8:00 am until approximately 12:00 pm in the Orlando I/II ballroom of the Hilton Orlando hotel. The council took action for the following six motions summarized below.

Nominations and Elections

President-Elect: The Committee on Nominations and Elections (N&E) presented the following nominees for selection as candidates for President-Elect 2020: Magid Abou-Gharbia, H.N. Cheng, Carol A. Duane, and Christopher J. Welch. By electronic ballot the Council selected H.N. Cheng and Carol A. Duane. These two candidates, along with any candidates selected via petitions, will stand for the fall national election.

CINF note: Carol A. Duane served as CINF Program Chair 1985-88 and Division Chair 1997 (Chair-Elect 1996, Nominating Chair 1998).

Directors from Districts II and IV: N&E announced the results of the election held prior to the Orlando meeting for Directors from District II and District IV on the Board of Directors for the term 2020-2022. By internet ballot, the councilors from these districts selected Christina C. Bodurow and Dawn Mason as District II candidates; and Rigoberto Hernandez and Lisa Houston as District IV candidates. Ballots will be distributed before October 1 to all ACS members in District II and District IV for election of a director from each District.

Candidates for Directors-at-Large: N&E announced the selection of the following candidates for Directors-at-Large for 2020-2022 terms: Harmon B. Abrahamson, G. Bryan Balazs, D. Richard Cobb, and Dorothy J. Phillips. The election of two Directors-at-Large from among these four candidates and any selected via petition will be conducted in the fall. Ballots will be distributed to the Councilors before October 1, 2019.

Member Dues for 2019

The council voted on the recommendation of the Committee on Budget and Finance to set the member dues for 2020 at the 2019 rate of $175.

Membership

The ACS ended 2018 with 151,012 members, a net membership growth of one-tenth-of-one-percent. This is the first membership growth ACS has recorded in the better part of a decade. Of the 25,000 new members who joined in 2018, about 20% were incentivized by market testing initiatives. Without these new members, ACS would have seen a continued decline.

The council voted to extend the provision of the international dues discount test based on World Bank country income levels for an additional three years (August 2019-August 2022).

Petition to Streamline the ACS Governing Documents

The council approved the *Petition to Streamline the ACS Governing Documents* (Constitution Articles I-XIX, Bylaws I-XIV, and Standing Rules I-IX), which will reorganize the fundamental governing documents of the society, i.e. the constitution and bylaws, and create a third document, standing rules. These three documents will function as a hierarchy. The constitution should define; the bylaws should authorize; and the standing rules should operationalize. Additionally, an amendment was voted upon, and passed by recorded vote:

That the language proposed as Standing Rule II, Sections 2 a, 2 b, and 2 g be moved to the bylaws as new Sections 2 a, 2 b, and 2 c of proposed Bylaw III with appropriate renumbering of the other sections of Bylaw III and Standing Rule II.

The petition will become effective if and when the proposed changes to the constitution are approved by the membership of the society, and if and when the Board of Directors approves the petition. Because the changes to the ACS Governing Documents are substantial, the council authorized the ACS Secretary and General Counsel and the Committee on Constitution & Bylaws to correct minor technical mistakes in the petition.

International Chemical Sciences Chapter

On the recommendation of the Committee on International Activities, the council approved the establishment of the ACS Pakistan International Chemical Sciences Chapter, subject to confirmation by the Board of Directors.

Recommendation to Continue Committees

On the recommendation of the Committee on Committees, the council approved the continuation of the Committee on Nomenclature, Terminology, and Symbols and the Committee on Senior Chemists, contingent on approval by the Board of Directors.

REPORTS OF COMMITTEES

Budget and Finance (B&F)

In 2018, ACS generated a net from operations of $41.1 million, which was $13.3 million higher than 2017. Total revenues were $571.6 million, increasing $34.2 million (6.4%) over 2017. Expenses ended the year at $530.5 million, which was $20.8 million (4.1%) higher than the prior year. These results were attributable to strong performance from the society's Information Service units (CAS and ACS Publications) and a continued emphasis on expense management across the ACS.

Additional information of the society's audited financial statements and IRS 990 filings can be found at http://www.acs.org/. At the bottom of the page click About ACS, then ACS Financial Information.

CINF note: Bonnie Lawlor is a member on B&F.

Council Policy

As required by the society's bylaws, the Council Policy Committee (CPC) has set the divisors for allocation of councilor seats among local sections and divisions for the 2020-2023 term. Official notification of the number of councilors permitted for each local section and division will be sent to the respective local sections and divisions prior to May 1, 2019.

CINF note: Andrea Twiss-Brooks is a member on CPC.

Education

The Committee on Education (SOCED) held a strategic planning retreat in September framing their vision, mission, and goals, and establishing the teams to carry out the strategies. SOCED and the Division of Chemical Education coordinate efforts in support of the American Association of Chemistry Teachers (AACT). AACT ended 2018 with 5,690 members. In 2018, 100 new teaching resources were created for AACT members, and the option of dual membership with ACS was made available.

Together with many ACS units, SOCED participated in the second ACS Safety Summit in March, 2019.

The ACS comment "Improving graduate education: career paths and competencies" in the October 29, 2018 issue of *C&EN* highlighted activities that build on graduate STEM education for the 21st century. Progress on those activities included forming a taskforce to define competencies for graduate students in the chemical sciences in both Master's and Ph.D. programs, and establishing the Bridge Project to help diversify the graduate student population in the chemical sciences.

CINF note: Jeremy Garritano is a member on SOCED.

Science

The Committee on Science (ComSci) remains active on the science policy front. In Orlando, ComSci considered revisions to the ACS policy statement on forensic science. ComSci is collaborating with the Committee on Divisional Activities for thematic programming. For Orlando, they organized a symposium on *Exploring the Frontiers of Chemistry through NASA Research.* For San Diego, ComSci is planning a symposium on *Water for Two Worlds*.

Meetings and Expositions

The theme of the Spring 2019 ACS National Meeting & Exposition was *Chemistry for New Frontiers*. As of Tuesday, April 2, the attendance was:

Attendees	7,887
Students	6,019
Exhibitors	869
Expo only	404
Guests	426
Total	15,605

Attendance at the spring national meetings since 2004 is as follows:

2004 Anaheim, CA:	14,141
2005 San Diego, CA:	15,385
2006 Atlanta, GA:	12,546
2007 Chicago. IL:	14,520
2008 New Orleans, LA:	13,454
2009 Salt Lake City, UT:	10,668
2010 San Francisco, CA:	18,067
2011 Anaheim, CA:	14,047
2012 San Diego, CA:	16,758
2013 New Orleans, LA:	15,473
2014 Dallas, TX:	13,498
2015 Denver, CO:	13,958
2016 San Diego, CA:	16,310
2017 San Francisco, CA:	18,917
2018 New Orleans, LA:	16,585
2019 Orlando, FL:	15,605

Divisional Activities

The Committee on Divisional Activities (DAC) is developing novel approaches to persuade a higher percentage of new ACS members to join divisions. Since March 2018, new members have been given the option to join up to three divisions at no cost for the first year. Preliminary data indicate that many are taking advantage of this new offer. There were 13,331 free divisional memberships activated in 2018 compared to 6,787 in 2017.

CINF note: Marge Matthews is a member on DAC.

Local Section Activities

The Committee on Local Section Activities (LSAC) approved 31 Innovative Project Grant proposals for a total of $86,230 in 2018. LSAC hosted the Local Section Pre-Leadership Institute webinar on January 8, 2019 with 66 local section officers in attendance. A link to the recorded webinar is available at www.acs.org/getinvolved: click on “Local Sections” and then “Training and Support”.

Economic and Professional Affairs

The Committee on Economic and Professional Affairs (CEPA) updated the Chemical Professional’s Code of Conduct which expects ACS members to adhere to the highest ethical and safety standards. The current version can be found at: https://www.acs.org/content/acs/en/careers/career-services/ethics/the-chemical-professionals-code-of-conduct.html.

CEPA is continuing to reimagine the National Meeting Career Fair by adding one-on-one career consulting options with ACS Career Consultants, centralizing society-wide career resources at the fair and promoting networking amongst industry members. CEPA will organize a career day in several cities.

Constitution and Bylaws

There were no petitions for consideration in Orlando. The deadline for new petitions to amend the constitution or bylaws must be received by the Executive Director (bylaws@acs.org) by May 8 to be included in the council agenda for the fall 2019 meeting in San Diego, CA.

CINF note: Svetlana Korolev is a member on C&B.

Chemical Safety

The Committee on Chemical Safety (CCS) led the organization of the 2018 and 2019 ACS Safety Education Summits. The 2019 Summit identified six strategies for ACS and its partners to enhance chemical safety education and safety cultures. A complete report on the second summit will be available this summer. A new ACS safety website (www.acs.org/safety) was launched this winter. The website aligns to the ACS strategic directions identified at the 2018 Safety Summit (https://www.acs.org/content/acs/en/about/governance/committees/chemicalsafety/advisory-panel/2018-summit-findings.html) focusing on safety information, education, partnerships and communication.

CINF note: Leah McEwen is a member and Grace Baysinger is an associate member on CCS.

Women Chemists

On March 21, 2019, the Women Chemists Committee (WCC) launched the first webinar, *Advocating for Yourself: Stop Looking for Yoda in Your Career*. Among the panelists included were Kathleen Schulz and Dorothy Phillips from the ACS Board of Directors.

Special Discussion

ACS President Bonnie Charpentier led a special discussion on *ACS Relevance to Current and Future Members: Challenges and Opportunities.* Councilors provided recommendations, including increased support for local sections and industry members, helping student transitions into their professional careers, and implementing a monthly payment tool for ACS dues. These, and all the other ideas and input submitted, will be shared with the Committee on Membership Affairs and the ACS Membership Division for further research or implementation.

The Board Open Session

The Board held a regular session on March 31, which featured a presentation by Susan Butts, Chair of the Working Group on Immigration and Work Visas, entitled *Workforce Immigration and its Relationship to the U.S. Economy, Innovation, and Global Competitiveness*.

Supplemental Information

- Council Agenda, April 3, 2019
  https://www.acs.org/content/dam/acsorg/about/governance/councilors/council-agenda-4-19.pdf
- 2018 Highlights of ACS Achievements, an annual report from Thomas Connelly
  http://www.acs.org/acshighlights
- Governing Documents http://www.acs.org/bulletin5
- Membership Special Discussion engage@acs.org
- Office of Secretary & General Counsel secretary@acs.org
- President Bonnie A. Charpentier b.charpentier@acs.org
- President-Elect Luis Echegoyen l.echegoyen@acs.org
- Immediate Past President Peter K. Dorhout p.dorhout@acs.org
- Safety Resources http://www.acs.org/safety

Submitted by Svetlana Korolev, Bonnie Lawlor, and Andrea Twiss-Brooks

Book Review

Chemoinformatics: Basic Concepts and Methods, Engel, T., Gasteiger, J., Eds.; Wiley-VCH, Weinheim, Germany, 2018, 575 pp + xxvii, ISBN 978-3-527-69378-8 (paperback), $120.

So, is this tome a textbook (as described) or a reference book? I would say it is both. It weighs 2.5 pounds, putting it in the same class as my psychology textbook which is 4.5 pounds (although hardcover, larger format, and 645 ++ pages). ALA CHOICE considers it a textbook and they don't review textbooks. It is formatted like a textbook with references at the end of each chapter as well as exercises (answers and index at the end of the book). It's also a reference book due to the incredible amount of information. The first edition of the book (*Chemoinformatics: A Textbook*) was published in 2003 and this second edition is updated and has additional subjects. It has 22 authors including the two editors (one of which is Engelbert Zass).

Their definition of chemoinformatics is broader than that used for the development of pharmaceuticals and drugs and is here defined as the application of informatics methods to solve chemical problems. The authors correctly state that the knowledge and use of chemoinformatics is essential to the conduction of chemical research. (Is CINF due to evolve into the ACS Division of Chemoinformatics? Although that would require merger with COMP, stay tuned).

There are 14 chapters which are briefly described below. However, the table of contents (TOC) is multi-faceted, and the complete TOC is listed on 12 print pages on the Wiley catalog record. Current practices and resources as well as the history are covered in each chapter. The objectives of chemoinformatics are discussed in the introduction, as well as the learning processes necessary, such as the data (measurements, calculations)-information (context)-knowledge (abstraction) pyramid; to which I've been known to add numbers at the bottom and wisdom at the top. The inductive learning processes range from empiricism (special examples) to theory (models) at the top.

After an introduction, chapter 2 describes the principles of chemical structure information and chapter 3 covers the processing of that information. Chapter 4 covers the representation of chemical reactions. Chapter 5 discusses the types of chemical data and chapter 6 covers databases and data sources in chemistry. Chapter 7 covers finding chemical information in the chemical databases. Chapters 8 through 12 discuss computational chemistry. Chapter 8 covers the basics of computational chemistry and chapters 9 and 12 discuss modeling and prediction of physicochemical properties including QSPR and QSAR. Chapter 10 covers the calculation of chemical structures and chapter 11 covers inductive methods for correlation of chemical compounds and chemical properties. Chapter 13 is a brief overview of bioinformatics, including sequence databases of proteins and nucleic acids and searching those databases.

Chapter 14 discusses future directions of chemoinformatics. More information on several topics can be found in resources listed for free energy relations, chemometrics, neural nets, fuzzy logic, genetic algorithms, and expert systems. A chapter in the original textbook also spawned an entirely new book (*Applied Chemoinformatics: Achievements and Future Opportunities*) which will be reviewed in a future *Chemical Information Bulletin*.

Needless to say, I did not attempt to cover all topics, but instead concentrated on topics of interest and importance to me, past and present. Primary interests include chemistry databases, and chapter 6, Databases and Data Sources in Chemistry (by Engelbert Zass and Thomas Engel), is a trove of information.

Section 6.3, Major Chemical Databases, is of special interest particularly the descriptions of SciFinder and Reaxys, their missions and their database contents. Section 6.3.3 describes SciFinder vs. Reaxys and a table is given for database performance for two searches, MEDLINE/CAplus vs. Reaxys for paracetamol and Registry/CAplus vs. Reaxys for substituted naphthalenes. SciFinder outperforms Reaxys, except in finding references before 1950, or before 1900. I did a similar brief comparison study in 2013 (*Online Searcher*, **37** (5), 44-48), which is cited, and similar results were found. Other searching parameters including author searches are discussed. STN and its large stable of databases is mentioned only briefly and, curiously, is not indexed. STN is described as for information specialists, and is more difficult to search but more powerful and precise. I heartily agree except that I think it's easier to search.

Comparing coverage of chemical reactions is discussed, but the situation is more complicated. In general, once again Reaxys is more comprehensive than SciFinder/CASREACT.

Citation searching, from the Science Citation Index (originally print, now available on STN) through availability on Web of Science is described and evaluated. My paper on the subject (2016, *J. Chem. Educ.*, **93** (3), 560-566) is cited. Reaxys/Scopus is also described, as is Google Scholar. Additional uses of citation metrics as applied to journals and individuals are briefly described in one paragraph. Patent databases, availability and searching, are discussed.

A few of us information specialists, especially Edlyn Simmons, the late Stu Kaback, and myself, advocated repeatedly for database services like STN. Stu and I often referred to "one stop shopping" because of the large number of databases on STN, especially for patents and other topics like toxicology data and information. Since a large number of databases were available in one place, not only was simultaneous searching of several databases possible, but also the ability to "dedup" (eliminate duplicate original references). To information professionals, these efficiencies are not only convenient but cost-effective. Apparently, STN is only rarely available in academia. If you know of any remaining academic use of STN, please contact me.

I briefly glanced at some of the exercises and they appeared to be relevant. Bottom line: this is an excellent textbook AND reference book, a must-buy for many.

Submitted by Robert E. Buntrock

Sponsor Announcements

Bio-Rad Laboratories, Inc.

Bio-Rad is a leader in spectral databases and software with their award-winning KnowItAll solutions. Here are some excellent resources to consider for your college campus this school year.

KnowItAll U - Campus-Wide Access to the World's Largest Spectral Database –

Get a Trial for Your School

Bio-Rad's KnowItAll U offers every student and faculty member unlimited access to over 2 million spectra, including Infrared (IR), Raman, NMR (CNMR, HNMR, XNMR), UV-Vis, and Mass Spectra (MS). A KnowItAll U Spectral Library subscription provides the most affordable option for campus-wide access the largest and highest quality collection of spectra available today.

Learn more:
http://www.knowitall.com

Set up a trial for your school:
http://www.knowitall.com/contactus

Choose access to the complete KnowItAll U collection or spectra from a specific technique!

Product Code	Library Name	Spectra
877010	KnowItAll U (all techniques)	2,043,000
891050	KnowItAll U - IR	264,000
892050	KnowItAll U - MS	829,000
895050	KnowItAll U - NMR	895,000
894050	KnowItAll U - Raman	25,000
896050	KnowItAll U - UV-Vis	30,000

Free Software for Chemistry Students & Professors

Bio-Rad offers the KnowItAll Academic Edition, a FREE chemistry software package for the academic community. Tools include ChemWindow chemical structure drawing software and reporting and publishing tools, along with spectral analysis tools.

Download here: www.knowitall.com/academic

CINF Officers and Functionaries

Chair
Elsa Alvaro
Northwestern University
elsa.alvaro@nortwestern.edu

Chair-Elect
Jeremy Ross Garritano
University of Virginia
jg9jh@virginia.edu

Past-Chair
Erin Davis
Schrödinger, Inc.
erindavis@gmail.com

Secretary
Tina Qin
Harvard University
qinnamsu@gmail.com

Treasurer
Stuart Chalk
University of North Florida
schalk@unf.edu

CINF Councilors
Bonnie Lawlor
chescot@aol.com

Andrea Twiss-Brooks
University of Chicago
atbrooks@uchicago.edu

Svetlana N. Korolev
University of Wisconsin, Milwaukee
skorolev@uwm.edu

CINF Alternate Councilors
Rachelle Bienstock
RJB Computational Modeling LLC
rachelleb1@gmail.com

Charles Huber
University of California, Santa Barbara
huber@library.ucsb.edu

Jeremy Ross Garritano
University of Virginia
jg9jh@virginia.edu

Archivist/Historian
Bonnie Lawlor
chescot@aol.com

Awards Committee Chair
Rajarshi Guha
Vertex Pharmaceuticals
rajarshi.guha@gmail.com

Careers Committee Chair
Neelam Bharti
Carnegie Mellon University
nbharti@andrew.cmu.edu

Communications and Publications Committee Chair
Graham Douglas
communications@acscinf.org

Education Committee Chair
Grace Baysinger
Stanford University
graceb@stanford.edu

Finance Committee Chair
Stuart Chalk
University of North Florida
schalk@unf.edu

Fundraising Interim Committee Chair
Graham Douglas
communications@acscinf.org

Membership Committee Chair
Donna Wrublewski
Caltech Library
dtwrub@caltech.edu

Nomination Committee Chair
Erin Davis
Schrödinger, Inc.
erindavis@gmail.com

Procedures Chair
Bonnie Lawlor
chescot@aol.com

Program Committee Chair
Susan Cardinal
University of Rochester
scardinal@library.rochester.edu

***Chemical Information Bulletin* Editor Spring**
Kortney Rupp
University of California, Berkeley
kortneyrupp@berkeley.edu

***Chemical Information Bulletin* Editor Summer**
David Shobe
Patent Information Agent
avidshobe@yahoo.com

***Chemical Information Bulletin* Editor Fall**
Teri Vogel
UC San Diego Library
tmvogel@ucsd.edu

***Chemical Information Bulletin* Editor Winter**
Judith Currano
University of Pennsylvania
currano@pobox.upenn.edu

Webmasters
Rachelle Bienstock
RJB Computational Modeling LLC
rachelleb1@gmail.com

Stuart Chalk
University of North Florida
schalk@unf.edu

Contributors to This Issue

Articles and Features

Elsa Alvaro
Robert Buntrock
Susan K. Cardinal
Rajarshi Guha
Svetlana Korolev
Michael Qiu
David Shobe
Wendy Warr

Committee Report

Svetlana Korolev
Bonnie Lawlor
Andrea Twiss-Brooks

Sponsor Information

Graham Douglas

Cover photo

Antoine Gady, under Creative Commons License

Production

Rachelle Bienstock
Svetlana Korolev
Bonnie Lawlor
Kortney Rupp
David Shobe
Wendy Warr