CHEMICAL Information BULLETIN

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Division of Chemical Information
of the ACS

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David S. Shobe, Editor

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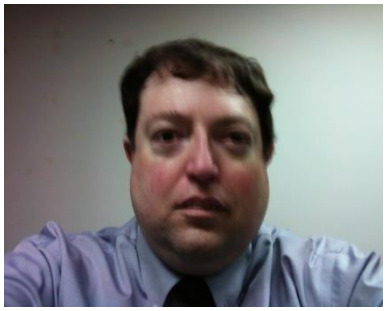
Chemical Information Bulletin

Letter from the Editor



The chosen theme of the recent spring ACS national meeting was “Nexus of Food, Energy, and Water”. All three of these are necessary for life and for standard of living, and the appetite for all three continues to grow as both population and wealth per capita increase. The link between these necessities and chemical information may seem tenuous. Note, however, that just as chemical technology will be needed to sustain the increase in availability of food, energy, and (clean) water, chemical information will be important in sustaining and enhancing this chemical technology.

The cover photo shows a Louisiana refinery at night. Not only is this an instance of an important, chemistry-related industry for the New Orleans region, but it illustrates two of the three elements of the “nexus”, water and energy. It is perhaps unfortunate that the third element, food, is absent from the photo, especially since New Orleans is known for its cuisine!

As usual, this issue of the *Chemical Information Bulletin* features summaries of the lectures at selected symposia from the spring 2018 ACS meeting. Teri Vogel starts the list with “Chemical Information Literacy: Innovation, Collaboration, and Assessment”. Note the word “collaboration”, as it appears to also be a theme of the next two selected symposia, “Enhance Discovery: Share Chemical Structures” summarized by Kortney Rupp, and “Community Sharing of Chemical Safety Data: Yes, No, Maybe?” summarized by Carmen Nitsche. The latter of these was designated a presidential event. A second presidential event, “CINF: Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web”, was the subject of a recent *Chemical & Engineering News* article by Stu Borman (1). Finally come two symposium summaries written by Rachelle Bienstock, “Workflows and Cheminformatics” and “Fragrances, Food, and Cheminformatics”.

Other features of this issue include a report of committee activity at the spring 2018 meeting, a book review of *Elements of Ethics for Physical Scientists* by Bob Buntrock, and a call for applications to the Chemical Structures Association (CSA) Trust Grant. There is also a preview of CINF events in the technical session of the fall 2018 ACS meeting.

CINF needs volunteers! Our division is in un urgent need for new committee chairs. The Fundraising Chair is the most crucial among all vacancies. Every CINF reception at a national meeting is in jeopardy. We like to continue sustaining this benefit for the division members and guests for social networking. Please consider volunteering or nominating someone to Erin Davis, erinsdavis@gmail.com.

References:

(1) Borman, Stu. “Impact factor creator and chemical information pioneer Eugene Garfield honored”, *Chemical & Engineering News*, 96(15), 30-31 (April 9, 2018).

Notices

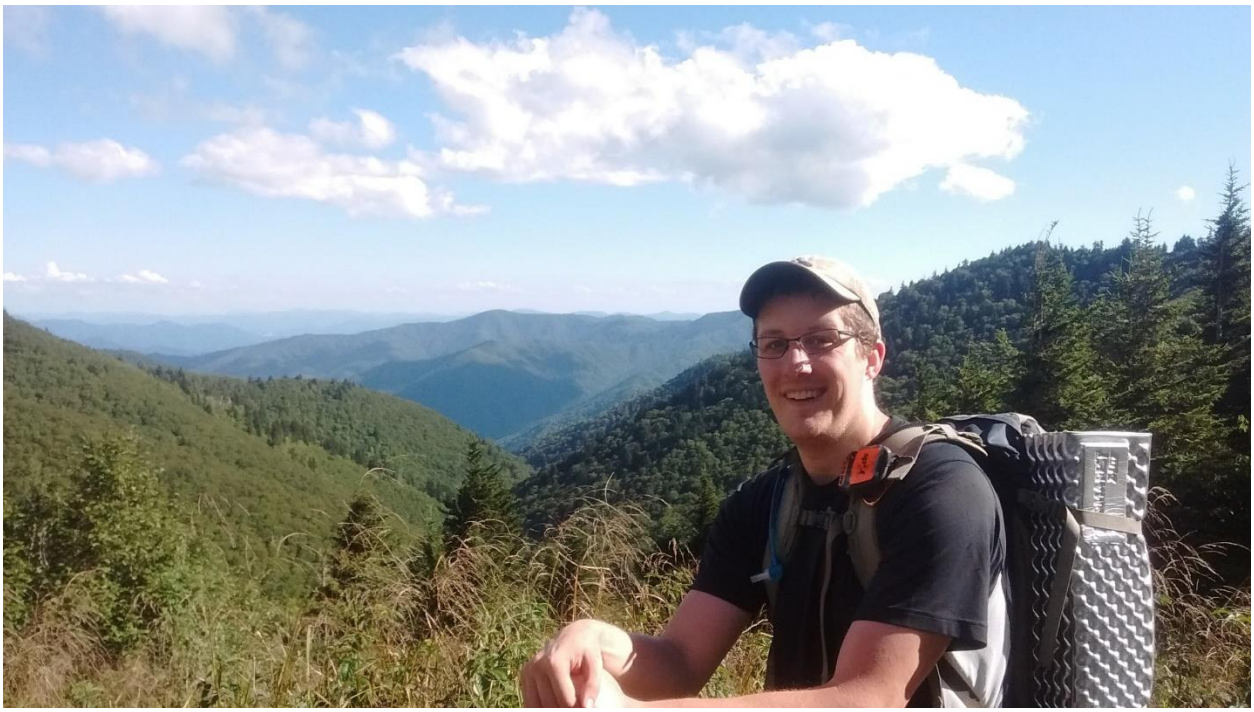
Wendy Warr has published her photos from the ACS National Meeting in Washington, DC on her Flickr stream. Visit https://www.flickr.com/photos/cinf/collections/72157693888982061/ to access the photos. They appear in four albums:

- ACS New Orleans 2018 CINF technical sessions
- ACS New Orleans 2018 CINF welcome reception
- ACS New Orleans 2018 COMP division social
- ACS New Orleans 2018 CINF executive committee

While you are there, check out the photos from other past national meetings and special CINF events at https://www.flickr.com/photos/cinf/albums!

Awards and Scholarships

Lucille M. Wert Student Scholarship



Joshua Borycz has been selected as the 2018 recipient of the Lucille M. Wert Student Scholarship. The award is for $1500 to “help persons with an interest in the fields of chemistry and information to pursue graduate study in library, information, or computer science.”

Joshua holds a B.S. in Chemistry and Mathematics from Hope College, and a Ph.D. in Chemistry from the University of Minnesota. He is currently pursuing a M.S. in Information Science at the University of Tennessee-Knoxville.

Joshua is currently working with a team on the NSF DataONE project, looking at how scientists share, reuse, and manage research data. Upon obtaining his M.S. degree, Joshua intends to focus on applying his knowledge of research data management and the research process to informing the community of chemical researchers of new ways of sharing data.

2018 Scholarship for Scientific Excellence

https://www.flickr.com/photos/cinf/41431526902/in/album-72157694954041364/

On the photo from left to right: Michael Qiu (ACS Publications, sponsor), Yannick Djoumbou Feunang, Bethany Cook, Jana Gurinova, Stuart Chalk (Scholarship for Scientific Excellence, coordinator)

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) is designed to reward students and postdoctoral fellows in chemical information and related sciences for scientific excellence, and to foster their involvement in CINF. Since 2005, the program has awarded scholarships at each of the ACS National Meetings, 74 scholarships in total. The awards at the 255th National Meeting in New Orleans were sponsored by the American Chemical Society (ACS) Publications. Three full scholarships valued at $1,000 each were awarded to Yannick Djoumbou Feunang, Bethany Cook, and Jana Gurinova.

The names of the recipients and the titles of their posters are (listed from left to right on the photo):

Yannick Djoumbou Feunang
Biological Sciences, University of Alberta, Edmonton, Alberta, Canada
BioTransformer: A tool for metabolism prediction of small molecules
Abstract:
https://plan.core-apps.com/acsnola2018/abstract/6f02edf9fa1f10ca80fb6786b065a8a5

Bethany Cook
Chemistry, North Carolina State University, Raleigh, North Carolina, United States
Designing CDK2 inhibitors using the molecular chimera approach
Abstract:
https://plan.core-apps.com/acsnola2018/abstract/6f02edf9fa1f10ca80fb6786b063dba1

Jana Gurinova
Pharmaceutical Chemistry, University of Vienna, Vienna, Austria
Triangulation of repurposing candidates for orphan diseases
Abstract:
https://plan.core-apps.com/acsnola2018/abstract/6f02edf9fa1f10ca80fb6786b0a03273

Submitted by Svetlana Korolev

Chemical Structure Association Trust

Applications Invited for CSA Trust Grants 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 research relating to chemical information 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. Proposals from those who have not received a grant in the past will be given preference. 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. Grants will not be given for activities completed prior to the grant award date.

***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 and a recent photograph;
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**:*

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.

A list of previous awardees and their corresponding award-funded activities may be found at http://bulletin.acscinf.org/node/955.

Submitted by Bonnie Lawlor

ACS Salute to Excellence Award

On April 19, 2018, the Philadelphia Section of the American Chemical Society presented **Marge Matthews** with a “Salute to Excellence” award in recognition of her outstanding service to the Local Section, especially with her work on the Section's Communication Committee. In 2005 Marge received the Meritorious Service Award from the ACS Division of Chemical Information where she has served as Editor of the *Chemical Information Bulletin*, Treasurer, and a member of several committees, currently serving on the Awards Committee. Congratulations, Marge. ACS has been well-served by your hard work!

Submitted by Bonnie Lawlor

Technical Program

Chemical Information Literacy: Innovation, Collaboration, and Assessment

Ye Li provided introductory remarks for this all-day symposium by highlighting some of the works that inspired us to organize the session: Information Competencies for Chemistry Undergraduates (2011), the 2016 *Journal of Chemical Education* special issue on chemical information, *Integrating Information Literacy into the Chemistry Curriculum* (ACS Symposium Series, volume 1232) and the Association of College & Research Libraries (ACRL) *Framework for Information Literacy for Higher Education* (2016).

Kortney Rupp at UC Berkeley opened the symposium with a talk about her initial, targeted outreach activities in the Departments of Chemistry and Chemical Engineering and the Lawrence Berkeley National Laboratory. As an early career librarian in a position that had not been permanently staffed in more than two years, Kortney has used her own experiences as a graduate student to know where best to engage with graduate students and their faculty, including attending seminars and social events, and when she has been able to get in, research group meetings. Highlighting several recent successes, she noted that needs will vary among research groups, but all have a common interest in time-saving activities. Topics that have come up include citation management, Reaxys training, Overleaf for dissertations, research data management, and ChemRxiv. Her "big picture" goal is to continue her strategic engagement efforts to reach more of the roughly 100 research groups, which will provide ample opportunities to provide chemical information education to the community she supports. (Presentation)

The Georgia Gwinnett College library and chemistry department have been working collaboratively for years. **Adrienne Harner**, the library's instruction coordinator, with chemistry instructor **Derek Behmke** in attendance to share his perspective, spoke about their collaboration for information literacy in general chemistry. Whether she and her fellow instruction librarians are developing one-shot sessions or credit-bearing courses, they incorporate backward design, designing for significant learning, and ADDIE design into all of their information literacy activities. (ADDIE stands for Analysis, Design, Development, Implementation, and Evaluation). The focus for this talk was on Chem 1211, the first of the two-quarter general chemistry sequence taken by all of their science students. For this course, students are required to use a variety of information resources for a poster project (followed by a research paper in the second course). Adrienne walked us through how she used ADDIE design in this course. She matched information literacy learning objectives to department and campus goals, using ACRL Framework and ACRL Standards as guides. Then she considered motivational design to develop ways to engage the students and increase their level of confidence with the scientific literature. Chem 1211 uses a flipped instruction model that includes a Guide on the Side tutorial and a Google Forms pre-test to gather information about the students' prior online searching experiences. This allows for more active learning in the actual library sessions. For one group exercise, students are assigned a particular resource and asked to identify what kind of source it is and how they made that determination. The evaluation piece includes a post-test and reviewing the sources they used in their posters. Did they use a variety of sources, is there evidence they integrated those sources into their work, and were the sources cited correctly? The scope of the librarians' engagement with this course was impressive, with three librarians meeting with 850 students just this spring. Adrienne's next goal is to create a rubric to replace the existing information literacy checklist used to evaluate the posters. They are also working with some biology and allied health courses, and she also hopes to get the library embedded in upper-division chemistry courses, including the senior capstone. However, scalability will continue to be a challenge for their instruction program.

Mary Ellen Sloane spoke about how the librarians at Middle Tennessee State University are connecting with the chemistry faculty for information literacy. They used the ACRL Framework as the foundation, focusing on "students creating new knowledge" and "faculty fostering engagement". The librarians saw this as an opportunity to match the library's learning outcomes with the departments' curricular goals, and to support faculty who were modifying their courses for MT Engage, a program to incorporate high impact

pedagogies into the curriculum that enhance student engagement. The librarians started with the Association of American College and Universities (AACP) integrated learning rubric, which they further refined after interviews with faculty. From there they created 16 information literacy assignments that faculty can download and customize for their classes, along with suggested ways to scaffold the assignments, which range from single-source evaluations to research papers.

Chemistry professor **Judith Iriarte-Gross** shared her perspective next. She teaches an introductory chemistry class for MT Engage, and she connected with SENCER (Science Education for New Civic Engagements and Responsibilities) and used one of their videos as a starting point for her students to think about real-world science issues. Her students' information literacy project includes six tasks, with four coming from the library assignments, such as completing a literature review and explaining how science connects to their chosen topic. Their final task is to submit an e-Portfolio document where they reflect on their learning experiences. In a final note, Mary Ellen and Judith also reminded the audience not to be afraid to extend beyond the Framework.

Longwood University assistant professor **Andrew Yeagley** shared with us his department's efforts to scaffold information literacy into their chemistry curriculum. The department, consisting of just four faculty, has some flexibility to make the changes that other departments might not have. Being a new instructor and aware of how much the libraries had changed in just a few years, he referred to the guidelines in sources like the ACRL Standards and *Information Competencies for Chemistry Undergraduates* (Special Libraries Association Chemistry Division and CINF) to map how information literacy outcomes could be incorporated throughout the curriculum. Even with a small group of instructions, they faced challenges one would expect, like assuming "someone else" was already covering this information in their own courses. Andrew and his colleagues used a stepping stone approach, starting with the first organic chemistry lab course. Students looked up safety data sheets and answered "soft" questions about articles to help them better understand the conducted studies. There was not much writing in the course, but it engaged the students and made them more comfortable to work independently. Sophomore and junior courses served as a bridge to the senior-level courses, with guided tasks such as literature reviews and the practice writing of abstracts. These scaffolded activities prepared students for their final, two-quarter capstone series, where they write up an abstract, literature review, project proposal, and final research report for their project. Then the university added new writing requirements for the general education courses, including the first year, general chemistry course. Andrew and his colleagues were able to shift the information literacy plan to make the general chemistry lab that first stepping-stone course, and with that a new approach to writing lab reports that mirrored journal article organization with abstracts, introductions, and experimental sections. The second organic lab course was modified into a bridge course with a new, discovery-based project. Along with getting the library more involved, faculty also swapped out lectures to focus more on information literacy skills, reading and interpreting journal articles, and student peer reviewing of lab reports. The last bridge course, Introduction to Chemical Lab Problem Solving, was also modified to place greater emphasis on lab report writing, better preparing students for the capstone project. The instructors do not have much data yet due to the small class sizes, but the student feedback so far has been positive. Andrew and the other instructors will learn more from the next cohort of students, who will be using the updated scaffolding. (Slides available upon request from yeagleyaa at longwood dot edu.)

Chapel Cowden, University of Tennessee at Chattanooga, spoke about the information literacy scaffolding work her library has done with their chemistry department. Her instruction focuses more on evaluating and effectively using information resources, while the faculty cover topics like SciFinder searching. Chapel and her fellow instruction librarians developed what they call the Information Skills Pathway, a branded and systematic way to communicate with faculty about scaffolding and embedding information literacy in their courses and programs. While Chapel already had a relationship with the department, her dean wanted these relationships to be more formalized. The librarians started with a profile of each department, including a historical sketch of any previous library or faculty involvement. Once the profile was completed, the librarian met with the faculty to discuss mapping information literacy outcomes to selected courses. The faculty gave feedback on the proposed course map, which is periodically reviewed for possible improvements. Information literacy learning outcomes have been mapped to two general composition courses, as well as three courses in the chemistry department: the

one-credit chemical literature course, the biochemistry senior capstone, and a new scientific communication course focusing on digital literacy and presentation skills. While the library did not officially adopt the ACRL Framework, the instruction librarians used it as a springboard. Chapel and her colleagues identified learning outcomes for the five courses and how those outcomes would be assessed (e.g., pre- and post-test surveys, in-class search challenges, and literature reviews). They also designed a schedule for how and when outcomes would be introduced, reinforced, and mastered. The librarians then presented a two-page document to the department that would serve as their agreement with the library. This document included the expected learning outcomes, and where and how the librarians will be incorporated into specified courses. The document is not fixed in stone; in fact, Chapel's next step is to "redo the whole thing". She concluded her talk with some tips for librarians and instructors who are planning a project like this. Not all engagement needs to be instruction-based, digital literacy is information literacy and should be factored in, relationships are critical, change is constant, compromise is acceptable, and you should allow for opportunities to be creative. (Presentation and scaffolding documents)

Ashley Neybert from University of Northern Colorado gave an interesting talk about synthetic speech markup language (SSML) and its importance for chemistry students who are visually impaired or have print reading disabilities like dyslexia. She demonstrated some of the limitations that text to speech (TTS) readers have with chemical expressions. For example, KOH and NaCl were sounded out like actual words. A student unfamiliar with NaCl may trust that the TTS reader is correct in pronouncing it "nackle." When Ashley comes across longer molecular formulas, she must decipher them character by character to figure out if what is being read aloud is a two-element compound or two one-letter elements. TTS readers can sometimes handle chemical expressions if there are spaces, albeit with "dash" sounds between every element. Some molecular formulas can be read properly, such as HCl, HF, and CCl_4, though the last sounded like "tetachloride." However, when the TTS reader encounters a vowel, it treats it like a word. SSML can contribute to student learning because of some of its advantages, including regional customization, fixing pronunciation errors, and setting pronunciation preferences like "amĭd" vs. "amīd".

Grace Baysinger (Stanford University) shared how librarians can help students use the chemical safety literature. Though librarians may have a lesser comfort level with this aspect of chemical information, she pointed out these searches are similar in concept to other property data searches. The campus Environmental Health & Safety unit (EH&S) is the primary authority on safety issues, but they can also be your potential partner for outreach and training. She highlighted a number of reference works, databases, and websites for safety data, including the ChemSafety federated search that Stanford helped to develop. Provenance is important, and researchers should follow up with the values they find in these handbooks and databases to the original sources, going to the full-text articles if possible. (Slides available upon request from graceb @ stanford dot edu.)

National Library of Medicine's **Sunghwan Kim** focused on property data for his talk on chemical information literacy. It is thought that about 50% of PubChem use is coming from 18-to-24-year-olds who are accessing PubChem through Google results. With so much data available, mostly in the public domain, there are new educational opportunities for data processing, integration, assurance, and analysis, as well as teaching metadata and highlighting the importance of representation and provenance for property data. For example, students can retrieve multiple results from a CASRN search for SiO_2 and see how and why these are aggregated into a single record. Or they can look at the various boiling points listed for benzene, then the sources to see where the data were acquired and under what context or conditions. Sunghwan also discussed the Cheminformatics Online Chemistry Course (OLCC) that was led by Robert Belford at University of Arkansas Little Rock in fall 2015 and fall 2017. This was developed to partly address the challenges of teaching cheminformatics at an undergraduate level. There is no appropriate textbook, it is not a well-established field, and there are few faculty with the requisite experience. The syllabus, online materials, and homework sets were prepared by experts (including Sunghwan and Leah McEwen), and the instruction was delivered simultaneously at multiple campuses. OLCC assignments relied heavily on PubChem for exercises on chemical structure representation and chemical searching online, and the course served as a good test case for incorporating PubChem in chemical information literacy activities.

Mindy Pozenel talked about a relatively new chemical information literacy project from CAS, an online tool aimed at sophomore-level organic chemistry classes to introduce them to real world research, cheminformatics, and the primary literature. CAS learned from focus groups that students were intimidated by the primary literature. They believe Chemistry Class Advantage can help ease students into searching the chemical literature and analyzing the research they do find, keeping them more interested and engaged. Each module or lesson begins with an introduction to the assigned article, followed by a series of questions. They are multiple-choice but are designed for critical thinking and require that the students read the article to answer them. When students get the correct answer, they can read a further explanation of why that answer was correct. The scoring is also based on how quickly they get the right answer. Students that select incorrectly get an explanation of why that answer is not correct, plus hints on what the right answer would be. The service is free to SciFinder account holders. After signing up, instructors answer some questions about the classes they teach, and then can select from a list of possible lessons that should map to their course topics. Mindy also shared feedback from a University of Virginia chemistry professor who has had a positive experience using Chemistry Class Advantage in her classes, and felt that her students have benefited from these exercises.

Elsevier's **Daniel Christe** discussed their recent efforts to build relationships with students, faculty, and librarians to better equip students to navigate the chemical information life cycle. Learning has evolved from a linear and constant journey to one that is more dynamic and influenced by multiple sources, and researchers need to reskill as technology and skills become obsolete. Daniel gave machine learning, robotics, and more data sharing as examples of where the future of chemistry is headed. He also referred to a 2015 George Whitesides essay in *Angewandte Chemie International Edition* where Whitesides noted that the traditional core chemical disciplines are focused more on iterative improvements rather than new discoveries. Daniel highlighted Elsevier's Research Sprints program, which incorporates learning experience design and scaffolded learning. Undergraduate teams used Reaxys or Knovel to develop solutions to questions related to real world challenges like corrosion management, while facilitators observed the groups to see where the students got stuck. Other initiatives include the ChemSearch Challenge, career professional development support for first-year graduate students, and programs for high school students to expose them to the scientific literature. Daniel also noted that Elsevier does need to consider researchers who do not have access to Reaxys or Knovel, and to support them as well. **Norah Xiao** also spoke about Reaxys. (Presentation)

Svetla Baykoucheva (University of Maryland, College Park) talked about her experiences using Qualtrics and SurveyMonkey to create online chemical information assignments for five undergraduate and graduate courses. This includes the first lab course for chemistry and biochemistry majors, and the last lab course taken by non-majors. This second course is the largest of the five, with 400-500 students who have to find physical properties of compounds and compare them with what they find in the primary literature. Students in each course get five to ten questions that require the use of SciFinder, Reaxys, advanced PubMed searching, and EndNote Online to complete. The questions are created to match the level and learning objectives of each course, and students are given ample time to complete them at their own pace. At the suggestion of some students, Svetla also created a series of QuickTime videos to support their assignment. She shared a few example questions with us, along with student feedback from a fall 2017 survey on the usefulness of these exercises. Most of questions are multiple-choice, with free-text questions where the students can paste references they exported from a database to an EndNote online bibliography. Svetla discussed some of the pros and cons of using SurveyMonkey and Qualtrics. While the former was easier to use, students could not get confirmations that their assignments had been submitted or save their work to return and complete at a later time. Qualtrics addressed both these concerns, but required more time on Svetla's part to create the assignments.

Susanne Redalje shared some recent information literacy successes at University of Washington, focusing on one materials science and engineering course. MSE 311 is a required, junior-level laboratory course that covers the tools of materials science information, including instrumentation, reading the scientific and technical literature, and introduction to library resources. She started meeting with this class in fall 2014 for ten 90-minute sessions, with five to six students in session (with 17 sessions this last fall). In consultations with the instructors, she established priorities for what should be covered to best support the class assignments, but was also given a lot of flexibility to develop the sessions. She focused on

research as process, the ethics surrounding the use of information, and finding and evaluating information. While Susanne did cover the importance of handbooks with curated data collections, she spent less time on actual database searching because interfaces change. She used a *Seattle Times* science series to lead a discussion on scholarly vs. popular sources. For another exercise, the research of local Nobel Prize winner David Thouless was the launching point for a discussion on how his work was covered in popular news sources, then the students looked at his original research and how other researchers have cited his work. The small group sizes allowed for a more personal teaching and learning experience, contributing to the success of these sessions, but even with 90 minutes, Susanne still has to find the right balance between covering a broader world view and more practical details and trying not to cram in everything she would love to cover. (Slides available upon request from curie at uw dot edu.)

Cornell University's **Leah McEwen** talked about several organic chemistry classes with embedded chemical information literacy activities. One is a freshman honors class that used a flipped model so that the students work on the assignment before they meet with Leah. It covered drawing compounds, arrow pushing, stereoisomers, literature searching, and creating chemical spreadsheets. She addressed any challenges the students had with the homework during their meeting. Then they had a quiz, followed by another homework assignment and library session, and then final class projects, either a poster or presentation. Leah also met with the first-year graduate students for two assignments, also completed in advance so that they can use the class time for more discussion. One assignment was on reaction searching, where students were required to use at least two databases and show their search schema, followed by the in-class review and presentations. The second assignment focused on literature searching, followed by group presentations and annotated bibliographies. As a new assignment, one for which they are still working on refining, the professor wanted to engage the students by studying the total synthesis of classic molecules. Leah highlighted the multiple trajectories of research paths for quinine and noted that total synthesis works well for literature searching assignments. The students map the synthetic pathways for different molecules for their presentations and bibliographies, identifying five to ten references that either highlighted great progress or introduced innovative methods for those pathways.

Ginger Schultz (University of Michigan) and **Ye Li** (formerly at Michigan, now at Colorado School of Mines) spoke about their use of intervention design. For her organic chemistry laboratory course, Ginger moved the curriculum from traditional experiments to problem-based learning where students worked in teams to find alternative methods to improve their reactions. She also wanted to encourage self-directed learning, so students would continue searching for information when they identified gaps in their knowledge, but she noticed problems with this part of the process. Students relied on Google but did not use it well: they cited sources without evaluating credibility or context, and they did not cite them properly or connect them to their laboratory work. Ginger realized that intervention design was needed to move the students' information-seeking skills from novice to more expert, while also reinforcing that information seeking is a progressive process and may not be finished after the initial search. Then Ye shared how they integrated the intervention throughout the quarter. It included pre- and post-assessment surveys about information seeking skills and what had been retained at the end of the quarter. Ye and Ginger also created three videos for this: what to look for when searching Google, evaluating information sources with the five W's (who, what, when, where, why), and databases to explore beyond Google (for this exercise, Reaxys). The videos were integrated with survey questions to check the students' understanding of the videos and test their ability to apply what they had learned. For example, when a flyer from a chemical company was the first Google result, what can students use from that source and what additional information is still needed? Comparing the pre- and longer-term post-survey results, the students reported using Reaxys and SciFinder more, while using fewer databases listed in the survey as "other." The students also reported an improved understanding of when to search for information in databases beyond Google. Ye and Ginger also conducted focus group interviews with five students, where they received additional feedback on how the exercises helped them place these learning skills in greater context. (Slides available upon request from yeli at mines dot edu.)

Our final speaker, **Charity Lovitt** from University of Washington Bothell, shared her work with embedding chemical information literacy in the general-chemistry sequence. The chemistry majors in their program receive this in their second- and third-quarter general chemistry labs, one upper-division course, and later

once more if they take undergraduate research. There are also some required general education courses with information literacy components, including a science writing course. Charity identified four goals for the assignment given to the second-quarter students, across six lab sections: identifying different types of resources, evaluating reliability using the five W's, using four tools to find and evaluate chemical information, and citing sources using ACS formatting. She also took into account the department's goals for their students as well as the ACRL Framework. The activity was delivered as a Word document that the students could complete and submit within five days. They started with learning about the types of resources, then selected one of four vitamins to search in Google and evaluate the sources retrieved. Next, they searched for their vitamin in Wikipedia, looking at both the entry and one of the sources cited. This was followed by a similar search using ChemSpider. After a quick exercise where they are asked to locate the library's chemistry research guide and their librarian, the students were given an opportunity to reflect on the experience. Charity asked the students what tools they would recommend for a relative who had questions about a chemical and why, and which tools they would use to find physical properties for that chemical. Charity and her colleagues only just received the preliminary data to begin reviewing, but so far the data indicate that most students found the activity at least moderately helpful, with similar results when asked about where they felt they gained on skills such as identifying reliable sources. Going forward, Charity hopes to get the data coded for the last question about reflecting, and then look for ways to see if the students retain these skills into the next quarter, and what can be done to integrate information literacy into other classes. (Slides available upon request from lovittc at uw dot edu.)

DISCUSSION

After the presentations we had a 20-minute Q&A for the attendees and speakers. Some of the highlights:

- Ashley mentioned that the SSML has just been introduced for Microsoft, and that we can now serve as "ambassadors" to promote its implementation. Human readers can also be used, if they can read the chemistry.
- Mindy was asked about how instructors can keep track of their students using Chemistry Class Advantage. They can use email, or integrate it into their learning management system. Librarians can also be added as "class assistants".
- One attendee asked why some of the speakers focus on Google and/or Google Scholar for their instruction. Adrienne, Charity, and Ye start with these, because that's what the students already know, and they would lose the students if they told them to disregard Google. Then they can discuss Google's limitations and the advantages of searching more specialized chemistry databases, from structure searching to greater ease of finding more credible sources. Google and Google Scholar are also freely available.
- On the question of whether the ACRL Framework had too much librarian jargon, Charity said that it resonated with her right away, along with Progress Oriented Guided Inquiry Learning (POGIL). Ginger had not heard of the Framework until Ye told her about it.
- The speakers were also asked more questions about their experiences with scaffolding. Adrienne said that for them the scaffolding started as multidisciplinary, which they then customized for the chemistry courses. Ye stressed that the relationship-building between instructors and librarians is essential.
- The last discussion topic centered on the inequality of information resources. We were reminded that Information Competencies for Chemistry Undergraduates identifies free resources, and that so many of the presenters focused their training on searching Google and other free resources because they do not know what their students will have access to once they leave that institution. They have also shifted the focus to teaching research as process, evaluating information and understanding the research cycle. Adrienne added that showing her students what Georgia Gwinnett College has compared with University of Georgia is an authentic way to demonstrate that "information has value".
- The final comment was an appreciation from one attendee that for presenters and attendees alike, assessment is still one of our biggest challenges.

Notes by Teri M. Vogel

Enhance Discovery: Share Chemical Structures

Vincent Scalfani at the University of Alabama is working with chemistry graduate students and faculty to create machine-readable chemical structure data files (SDFs) alongside submitted theses and dissertations. These SDFs contain the key synthesized substances from the thesis or dissertation and include the associated chemical connection tables, local identifiers, names, SMILES, and InChI line notations. The SDFs are then shared on our institutional repository (D-space) alongside the original thesis or dissertation, and more broadly on PubChem, allowing for greater management, discoverability, and reuse of the chemical structure data. Additionally, graduate students are taught to do indexing and the data is verified by the authors. PubChem provides reports on new structures to PubChem as well as identifying structures that are not a part of the CAS registry.

Greg Banik spoke about issues related chemical structure drawing and available tools. Chemists have been drawing two-dimensional versions of three-dimensional molecules for over a century and a quarter; however, interpretation by computer software has been less accurate. A remaining issue is the depiction of chemical structures with implicit stereochemical information using generally-accepted drawing conventions that humans understand but software does not (for example, in SpectraBase, thymidine has 18 total spectra with different representations of stereochemistry). Things to note include that SpectraBase is a now free through Bio-Rad and that the KnowItAll Stereochemistry toolkit helps with this issue and is free to academic institutions.

Suzanna Ward spoke about the Cambridge Structural Database (CSD) which contains over 915,000 small molecule crystal structures (43% organic; 57% metal-organic; 56% single component; 89% non-polymeric). One key aspect of CCDC workflows is integration with publisher workflows that aim to associate data and article from submission through peer review to publication. A second important aspect is the assignment of standardized chemical connectivity and two-dimensional structural information from the atomic coordinates in the deposited files using the knowledge in the CSD. One is now able to add ORCID information to submissions and preserve data authorship by identifying the data producer during the submission process. The data are also able to be published through “CSD Communication”; depositors can allow the data to be shared after one year if it has not been published. Depositors also have the opportunity to link to raw data, chemical interpretation of structures can be downloaded, and the identifiers can be sent to author to include in a manuscript.

Jian Zhang spoke about PubChem a public data repository in the field of chemical information which includes bioactivity data for tested chemical substances. PubChem’s upload system accepts several chemical structure annotations format including SDF (mol), smiles, and InChI string. The system archives structure drawings, known as substances, at the same time to standardize all chemical entities into compounds which are unique in the database. The submission form is for one compound at a time. The NLM PubChem Data submission policy allows for an “on-hold” date to be set up to a year.

Guy Jones from the Royal Society of Chemistry introduced a new data publishing route via the EPSRC National Chemical Database Service to allow researchers to deposit and publish machine-readable chemical structure files and associated spectra under open licenses, in association with a research publication or as an independent dataset. Each submitted structure is validated using the Chemistry Validation and Standardization Platform (CVSP) and assigned a shareable DOI, alongside associated spectra and metadata.

Martin Hicks from the Beilstein Institute spoke about chemical structures and their purpose. In scientific literature, chemical structures often serve as metadata to a larger set of experimental results. Current issues with structures including resonance, tautomers, conformers, and a lack of interoperability going between formats means that they are not good for data-driven analysis, or for building models to predict, understand, and elucidate. To solve these issues, we must enable reliable interoperability by standardizing current formats and making them open. There must be an affordable infrastructure to

support electronic notebooks (ELNs), structure-drawing programs, and repositories. Users should have "pods" on which to store their information that they could transfer to third parties.

Antony John Williams from the Environmental Protection Agency spoke about sharing chemical structure with peer-reviewed publications. In chemistry research, the majority of chemical structure data associated with scientific publications remains locked up in document form, primarily in PDF files or on webpages. While finding articles is easy, extracting data and especially structures is still difficult to achieve. To address obstacles in chemical structure sharing, US EPA National Center for Computational Toxicology (EPA-NCCT) scientists use a combination of cheminformatics applications and online repositories to distribute chemical structure data associated with their publications. EPA-NCCT chemical structure data are amenable to indexing, and distribution is shared and highlights the benefit of open data sharing for modeling, data integration, and research impact.

Christopher Grulke from the Environmental Protection Agency spoke about the DSSTox database. In environmental chemistry, the class of substances referred to as Unknown, Variable composition, Complex reaction product or of Biological origin (UVCB) cannot be represented with a single structure, making accurate characterization difficult. The results shared via chemical databases often include questionably-mapped structures associated with names or registry numbers that indicate a UVCB. The EPA's DSSTox project has started employing Markush representations to represent UVCBs. Markush representation yields a new set of problems, including difficulty with determining uniqueness, storage format limitations, and inconsistencies in different software's representations. It has, however, allowed linking of a UVCB with the associated chemical components which can be auto-enumerated. It also provides depictions of the substance, and the linkage of research results which increases the efficiency of collecting information associated with all components of a UVCB from within EPA databases.

Emma Schymanski, also from the Environmental Protection Agency, spoke about curating and sharing structures and spectra. In the environmental community, the use of high-mass-accuracy non-target mass spectrometry methods has been increasing in popularity, combined with the reliance on open data sources. Candidate structures are often retrieved with either exact mass or molecular formula from large resources and suspect lists can be used to perform efficient annotation. Libraries can then be used to increase the confidence in identification. Metadata in the form of exposure, hazard, reference, and data source information is useful in helping to identify substances of high environmental interest. Sharing structural linkages between these resources requires curation, yet many datasets arise from scientists and regulators with little training. This talk focused on curation efforts to map spectral libraries (e.g. MassBank.EU, mzCloud) and suspect lists from the NORMAN Suspect Exchange to unique chemical identifiers associated with the US EPA CompTox Chemistry Dashboard. Additionally, these curation efforts support worldwide exchange of suspect and are cross-annotated internationally.

Aurora Costache presented ChemAxon's solution for better storage and exchange of information on molecular structures and properties by discussing two new file formats: ChemAxon Extended SMILES and Marvin Document (MRV). ChemAxon Extended SMILES is a line notation which extends the well-known SMILES notation with features which are not represented in the regular SMILES strings. On the other hand, the MRV (Marvin Document) file format based on the open source CML (Chemical Markup Language) format, provides the ability to store all the molecular structure information, all the relevant query information, rendering parameters, text, and graphical elements. Both file formats from ChemAxon are human-readable text formats that allow users to check the stored information without any additional converters.

Marc Nicklaus discussed the NCI CADD Group's web server CACTUS: a "small molecule centric" tool for connecting chemical structures. The Chemical Identifier Resolver (CIR) provides conversions of an input structure identifier into another structure identifier, ranging from identifiers such as InChI[Key] through structure drawings to molecular properties such as molecular weight. CIR can be used via a web form or URL API. The Chemical Structure Lookup Service (CSLS) provides links to the occurrence of an input structure in around 100 databases. These services can help work with structure files and notations,

thereby aiding chemistry students, educators, researchers, and librarians in their sharing and discovery of chemical structures.

Notes by Kortney Rupp

Presidential Symposium shines spotlight on safety data sharing successes and challenges

The Chemical Information Division (CINF) of the American Chemical Society (ACS) organized a symposium and panel discussion for the 255th ACS National Meeting and Exposition in New Orleans dedicated to chemical safety data sharing. Cosponsors included the Division on Chemical Health and Safety (CHAS) and Corporate Associates (CA), and the Committee on Chemical Safety (CCS). We were thrilled that ACS President Peter Dorhout designated this a Presidential Event, providing expanded publicity, support to external speakers, and refreshments during our break.

I had the privilege of chairing and speaking at this session and introducing a terrific lineup of speakers: Mark Jones of Dow Chemical, Carlos Toro of ACS Publications, John Rumble of R&R Data Services, Thomas Zoeller of the Chemical Safety Board (CSB), Irene McGee of Covestro with Bradford Johnson of the American Chemistry Council (ACC), Dr. William Tolman of Washington University (formerly at University of Minnesota), Steve Addlestone of Eastman Chemical, and Ralph Stuart of Keene State College and current chair of the ACS Committee on Chemical Safety.

We learned about the important collaboration Dow created with academia to share safety from both the Dow and the University of Minnesota perspectives, and how graduate students at university put their insights from Dow into practice by, among other things, establishing Learning Experience Reports that are shared following incidents and near misses. We found out the details behind the ACS's new publication obligations that authors include safety information in their manuscripts where unusual hazards have been encountered, and the important role reviewers will have to play to implement the policy. We heard about the extensive collection of safety data in the *CRC Handbook of Chemistry and Physics*, and the role of the expert in creating authoritative content. Our CSB speaker had formerly been at the National Transportation Safety Board (NTSB), so we heard a case study from the airline industry that examined the various data-sharing steps that this industry took to reduce accidents, and the realization that efficiency and safety are in fact compatible goals. From the ACC folks, we learned how a seeming plateau in process safety improvement spurred the organization to implement a safety improvement initiative that incorporates sharing of safety experiences in new forums and workshops across member companies to achieve continuous improvement in safety. Finally, the Eastman Chemical speaker discussed the legal landscape surrounding formal incident investigations for serious accidents, and how that data end up being shared.

The morning was full of interesting insights. Some highlights included:

- Sharing safety data is possible, but it often requires the leaders of a company or institution to insist on the concept and overrule the more risk-averse legal teams.
- The "fresh eye" approach was one great suggestion to improve safety culture and make safety more personal; that is, if I tell you what I am doing, and you tell me what you are doing, not only can we watch out for each other, but we will gain an outside perspective that can spot a potential problem.
- A 2016 paper in the *Journal of Chemical Health and Safety* (https://doi.org/10.1016/j.jchas.2015.10.001) reviewed 726 journals from 28 publishers and found that 41% of these journals' ethics guidelines did not address safety, and only 8% of the author guidelines did.
- Students at the University of Minnesota are finding that the safety culture they have been cultivating is helping them get jobs, because industry is looking for new employees to already be steeped in safety culture.

I left this symposium both enthusiastic and frustrated. On the plus side, everyone seemed to agree that sharing of safety information was a worthy aspiration that should be fostered and promoted, but despite this acknowledged greater good, we did not manage to see a clear path to eliminate the barriers that are keeping people from sharing: from embarrassment, to fear, to "not my job" attitudes.

Towards the end of the session, the topic of ethics and legal aspects of not sharing safety data came up, but we were unable to pursue this further. To continue this conversation, CINF, in conjunction with CHAS,

is planning a symposium for San Diego in fall 2019 that will delve into the ACS Core Value of Professionalism, Safety and Ethics, with a focus on ethical aspects of safety data sharing. I welcome your ideas for potential speakers.

Notes by Carmen Nitsche

Workflows & Cheminformatics

Greg Landrum, of KNIME, assisted with organizing and presiding over a packed, standing room only symposium (in a very small room!) discussing the increasing significance of workflows and their applications for chemistry data analysis.

The symposium opened with a presentation by **Katrina Lexa**, Denali Therapeutics, who discussed the development and application of open-source web tools for medicinal chemistry compound screening applications in a small drug-discovery company environment. She discussed using SMINA, RDKIT, and CHEMALOT for docking, shape, and strain energy calculations. Also discussed was development of an open-source tool for tracking novel compound proposals within a project. The workflows developed for ligand modeling and design tracking are available on GitHub.

Thomas Luechtefeld, Underwriter Labs and Johns Hopkins University, presented the UL Cheminformatics Toolbox (ULCT), tools for toxicology and cheminformatics to address regulatory needs in the European REACH program. The Toolbox was built using chemical-similarity-based approaches and publicly-available toxicology data from nearly 10,000 chemicals registered under REACH.

Valery Tkachenko, Science Data Software, gave a presentation on chemical processing and support for different chemical formats and validation of these formats using RDKIT, Indigo, and Open Babel in a workflow.

Anthony Bradley, Diamond Light Source, discussed the use of workflows for high-throughput screening of fragments using an x-ray synchrotron sources. They have developed Collaborative Computational Project (CCP) CompMedChem (http://www.ccp-cmc.org/) to facilitate user access to computational chemistry tools for *in silico* small molecule compound design.

Sunghwan Kim, PubChem, presented the different available programmatic access routes to its data, including Entrez Utilities (E-Utilities or E-Utils), PubChem Power User Gateway (PUG), PUG-SOAP, PUG-REST, and PUG-View. There is also a PUG_XML based PubChem-specific XML schema and an RDF REST Interface, PubChem RDF.

Dr. Greg Landrum gave a presentation on KNIME, an open source workflow software with over 2000 nodes which provide for data analytics and interactive analysis, available for free download at http://www.knime.org/knime-introductory-com. KNIME makes it easy for the user to integrate with other software tools. There is a KNIME server with REST-based web services, and capabilities can be added to KNIME including creating new nodes, and integrating Python and/or R code, and calling out to external command-line applications. A case study was presented with use of KNIME for the rapid elimination of swill in Pan Assay Interference compounds (PAINS) files and an example processing a hit list of compounds using the available RDKit tools within KNIME.

Paul Sanschagrin, Cambridge Crystallographic Data Centre, discussed using Python to access the CSD. The CSD Python API can read and write molecules and provide search capabilities for structure similarity, fingerprints, SMARTS searching, 2D diagram generation and GOLD docking. CCDC tools can be used with https://plot.ly, Jupyter notebooks, iPython shell, py3Dmol, and many third-party Python libraries and modules, and with workflow tools. Paul presented an application of using the CSD Python API to build a basic web-based tool for data analysis.

Paul Hawkins, OpenEye, presented, Floe, a cloud-based cheminformatics and drug discovery workflow tool. Because it is “in the cloud”, workflows can easily be shared across and between organizations. An example using Floe with Psi4, an open-source quantum-chemistry application (http://www.psicode.org) combined with molecular dynamics (MD) simulation for free energy calculations, followed by enumeration of virtual ligands with omega generating conformers and FastROCS for shape similarity, was presented.

Erin Davis presented Schrodinger's LiveDesign for combining tools and datasets across platforms. **Travis Hesketh**, Optibrium, discussed automated workflows for processing downloads from ChEMBL to generate datasets, filling in tautomer, stereochemistry and descriptors (tools for 3D descriptors can be used and are available from scikit-learn.org). The resulting sets can then be used for QSAR models.

Lei Jia, Amgen, discussed the use of Pipeline Pilot (Commercial Workflow Product: Daussault Systems) protocols for full workflows, from retrieving compound and assay data from internal data warehouses to physiochemical property calculation, predictive ADME modeling, managing compound design ideas, and data processing. The Pipeline Pilot workflows of data are output to Spotfire for visualization and analysis.

Frederik van den Broek, Elsevier, discussed automating Matched Molecular Pair Analysis (MMPA) which compares molecules that differ only by a single chemical transformation. Using workflow tools (Reaxys has KNIME nodes), he was also able to integrate disparate tools (i.e. Swissbioisostere, KNIME Earlwood, and Vernalis analysis tools) with reactivity and solubility data from Elsevier's Reaxsys for MMPA.

Gerhard Ecker, Department of Pharmaceutical Chemistry, University of Vienna, Wien, Austria, discussed the development of BCRP inhibitors using an Open PHACTS decision tree model and workflows to identify privileged scaffolds in a drug repurposing application. He presented ToxPHACTS, which is based on a KNIME workflow for toxicological read across.

Kamel Mansouri, presented a KNIME workflow developed in conjunction with the National Center for Computational Toxicology at the EPA for automated preparation of large collections of chemical structures and associated chemical data for the development of QSAR models. The workflow uses up to four provided chemical identifiers, including chemical names, CAS RNs, SMILES, and MolBlocks, and performs a series of operations on the 2D structures, including desalting, stripping stereochemistry, standardizing tautomers and nitro groups, correcting valence, neutralizing (when possible), and removing duplicates. All workflows, data, and models are open-source and freely available on GitHub (https://github.com/kmansouri).

The final speaker for the session was **Jana Gurinova**, Department of Pharmaceutical Chemistry, University of Vienna, Vienna, Austria, who gave a presentation on combining web services and databases using a KNIME workflow for an integrated view of a protein family, as well as a starting point for a selection of a homology model template. The workflow began with a complete multiple sequence alignment web service, (Clustal Omega), passed to iTOL, a web service capable of visualizing phylogenetic trees, followed by identification of conserved domains and visualization with annotation of phylogenetic tree as the output. Annotations are derived from DisGeNET (diseases), DrugBank (drugs), and SureChEMBL (patents), and topology information is retrieved from UniProt.

The day-long symposium was an amazing presentation of a wide variety of new workflow tools available and their applications and integration with databases and available API tools.

Notes by Rachelle Bienstock

Fragrances, Food & Cheminformatics

A symposium discussing the development of computational and cheminformatics databases and methods specifically for application in the food and fragrance industries was an appropriate new topical area of exploration for a CINF symposium, in accordance with the theme for the New Orleans meeting "Food, Energy and Water". **Jack Bikker**, International Fragrances and Flavors, assisted with organizing a superb group of expert speakers who illuminated attendees on developments and applications of cheminformatics to foods and fragrances.

Jose L. Medina-Franco, Universidad Nacional Autónoma de Mexico, Mexico City, Mexico, opened the symposium with "Global structure diversity and chemical space of food chemicals", where he presented methods for exploring chemical space diversity and scaffolds within a variety of food-related resources (FDA CFSAN, EU Food Improvement Agents, FAO/WHO JECFA) integrated within PubChem. Dr. Medina-Franco presented and discussed the development of data analysis tools, PUMA, https://www.difacquim.com/d-tools for activity landscape analysis and Consensus Diversity Plots.

Next, **Jian Zhang**, PubChem, discussed the development of PubChem, as a chemical information hub, with the integration of food-related chemical information from several resources including FDA CFSAN, EU Food Improvement Agents, and FAO/WHO JECFA. Dr. Zhang presented methods for data access and downloading of data, including direct URL access (https://pubchem.ncbi.nlm.nih.gov/cmpound/cid), Pub_View RESTful API access and programmatic access.

Suzanna Ward of the Cambridge Crystallographic Data Centre (https://www.ccdc.cam.ac.uk) discussed the data available through the Cambridge Structural Database (CSD). She then looked at the overlap of the CSD with various other databases including the Pesticides Properties DataBase (PPDB, (https://sitem.herts.ac.uk/aeru/ppdb). She then went on to look at some of the tools that are available from the CCDC alongside the CSD, including solid form analysis, crystal packing, conformer generation, hydrogen bonding propensity, and full interaction maps, and explored how these could be used in the food and fragrances industry.

Joel Mainland, Monell Chemical Senses, University of Pennsylvania, Department of Neurosciences, talked about structure predictions of odor properties of molecules, in light of the fact that there are no known solved structures of olfactory receptors, and the DREAM Olfaction Challenge sponsored by Sage Bionetworks. He discussed using a Random Forest Model for predictions and general properties which correlate with odor that can be used for predictive models, such as the prediction that large nonvolatile compounds have no odors as compared to smaller compounds and that small, very polar molecules do not interact with the olfactory receptor.

Martin Slater, Cresset Discovery Services, presented the use of molecular fields to dissect fragrance properties and the correlation of small fragrance molecules to the Cresset electronic force field (their own force field) and shape. There are 400 Olfactory G-coupled protein receptors (GPCR), and Dr Slater presented how molecular similarity could be related to odor perception.

Jack Bikker, International Flavors and Fragrances, discussed the application of machine learning using molecular descriptors (ECFP4, FCFP6, FCFP4, Dragon) and models (Random Forest, R regression SVM, RF, Bayes, JMP, QSPR) for prediction of odor intensity. He also discussed predictions of environmental fate regarding aerobic aquatic biodegration.

Tamsin Mansley, Optibrium, discussed the use of physicochemical properties for multiparameter optimization and the development of an Auto-Modeler QSAR Modeling Builder based on a training data set and PLS, RBF, GPS and RF models.

Prakash Madhav presented predictions of color stability at Procter and Gamble based on two-dimensional descriptors and recursive partitioning methods.

Rachelle Bienstock closed out the session discussing the modeling of Sudan dyes and implications of their toxicity as an adulterant in food products, and the molecular modeling of Sudan-dye/DNA-adduct formation.

The session was very well attended and very comprehensive in covering a wide range of topics related to databases, cheminformatics and structure and property predictive methods for use in the development of molecules for specific food and fragrance applications with specific odors and properties.

Notes by Rachelle Bienstock

Preview of Fall 2018 Meeting

The fall Boston program for CINF promises to be a large and an outstanding one.

We have over 174 submitted abstracts, and the program will feature many special-topic and invited-speaker symposia, including the CINF Herman Skolnik Symposium on Tuesday (Prof. Dr. Gisbert Schneider, Inst. f. Pharmazeutische Wiss. ETH Zürich, awardee).

There will be eight full-day (including days with symposia in two halves in two days) and six half-day oral symposia, as well as a CINF Poster Session Sunday evening and a Sci Mix poster session.

We will have triple tracking: three concurrent sessions are scheduled on both Sunday and Wednesday. Below is a summary of the preliminary CINF program scheduled for the Fall 2018 Boston meeting, August 19-23, 2018. The Program Committee welcomes input and suggestions for future symposia and programming. We meet Saturday afternoons prior to the ACS national meeting, but feel free to email me with any programming suggestions (rachelleb1@gmail.com).

Sunday, August 19, 2018, will feature:
Chemical Structure Searching for Patent Information (Cosponsored by CHAL and CPRM) (AM & PM)

Chemoinformatic Approaches to Enhance Drug Discovery Based on Natural Products (AM & PM)

Reporting & Reproducibility of Chemistry Research Data (Cosponsored by ETHX and ORGN)
Financially supported by Chemical Structure Association Trust; IUPAC Committee (AM & PM)

CINF Poster Session (Poster) 6:00 - 8:00pm (EVE)

Monday , August 20, 2018, will feature:
Ethics of Data Sharing (Cosponsored by ETHX) (AM)

Publishing Chemical Data (Cosponsored by ETHX and ORGN) (AM & PM)
Financially supported by Chemical Structure Association Trust and IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)

Where are the Standards: Biologics Registration & HELM Representation of Biologics: Informatics Standards & Challenges (PM)

Sci-Mix Poster Session, 8:00 - 10:00pm (EVE)

Tuesday, August 21, 2018, will feature:
Chemistry Librarians of the Future (CHED) (AM & PM)

Skolnik Symposium: *De Novo* Design (Invited) (Prof. Dr. Gisbert Schneider, Inst. f. Pharmazeutische Wiss. ETH Zürich, awardee) (AM & PM)

Wednesday, August 22, 2018, will feature:
Machine Learning Scoring Functions (AM)

Move Away from the Lamppost & Find Druggable Targets (AM)

Semantics in Chemistry Vocabulary & Terminology (AM)

Drug Discovery: Cheminformatic Approaches (PM)

Reaction Analytics (PM)

The More the Merrier: Combine Drugs Together (PM)

Thursday , August 23, 2018, will feature:
Drug Discovery: Cheminformatic Approaches (Cosponsored by AGRO) (AM)

Reaction Analytics (AM)

Submitted by Rachelle Bienstock, CINF Program Chair

Committee Reports

Report from the Council Meeting held on March 21, 2018

The Council of the American Chemical Society met in New Orleans, LA on Wednesday, March 21, 2018 from 8:00 am until approximately 12:00 pm in the Grand Ballroom A-D of the Hilton New Orleans Riverside Hotel. Below are highlights from the meeting.

Nominations and Elections

President-Elect

The Committee on Nominations & Elections (N&E) had identified four nominees for the office of 2019 ACS President-Elect. They were as follows: Harmon B. Abramson, Luis A. Echegoyen, Thomas T. Gilbert, and Mary Virginia Orna. By electronic ballot, the Council selected Luis A. Echegoyen and Thomas R. Gilbert as the candidates for 2019 President-Elect. These two candidates, along with any candidates selected via petitions, will stand for election in the fall national election.

Other Elections

The Committee on Nominations and Elections announced the list of nominees to represent District I and District V on the Board of Directors for the term 2019-2021. Nominees for District I are Mary K. Carroll, Katherine L. Lee, Gerard F. Parkin, and Laura E. Pence. Nominees for District V are John E. Adams, Mark C. Cesa, Joseph A. Heppert, and Catherine H. Middlecamp. Ballots were emailed to the voting councilors in the two districts and the results were announced at the council meeting in New Orleans and in *Chemical & Engineering News.* By internet ballot, the councilors from these districts selected Katherine L. Lee and Laura E. Pence as District I candidates; and John E. Adams and Joseph A. Heppert as District V candidates. Ballots will be distributed on or before October 1 to all ACS members in District I and District V for election of a director from each district.

N&E also announced the election of directors-at-large that will be conducted in the fall. The candidates for a 2019-2021 term are Frank D. Blum, Lee H. Latimer, Ingrid Montes and Angela W. Peters. N&E also announced that Susan M. Schelble received 142 votes to Rick Ewing's 128 votes to fill a vacancy on the Committee on Committees (ConC) for a full two-year term (2018-2019).

ACS Dues for 2019

Council voted to accept the recommendation from the Committee on Budget and Finance with regard to the 2019 membership dues (an increase of $4.00, from $171 to $175). The increases to ACS dues are based upon an escalator defined in the ACS Bylaws (Bylaw XIII, Section 3,a). The dues are calculated by multiplying the base (current) rate "by a factor which is the ratio of the revised Consumer Price Index for Urban Wage Earners and Clerical Workers (Service Category) for the second year previous to the dues year to the value of the index for the third year previous to the dues year, as published by the United States Department of Labor, with the fractional dollar amounts rounded to the nearest whole dollar".

Base rate 2018: $171.00

Change in the Consumer Price Index, Urban Wage Earners, Services Category:

	December 2017 CPI-W (Services):	$305.191
	December 2016 CPI-W (Services):	$297.480
	Change in CPI-W Index:	2.59%
2019 Dues, fully escalated:	$171.00 x 1.0259 =	$175.43
2019 Dues, rounded:		$175.00

Petitions for Vote

Petition on the Composition of Society Committees

Society committees, which are the Committee on Budget and Finance (B&F), and the Committee on Education (SOCED), are composed of councilors and non-councilors. Committee appointments are made adhering to the requirement that two-thirds (2/3) of the committee members are qualified voting councilors. The Society's Bylaws also require the chair and vice-chair of Society committees to be councilors. B&F requires members with significant budget and financial experience and expertise. SOCED strives for a balance of members with expertise across many facets of chemical education. They include chemical education researchers as well as active educators at four-year colleges and universities, graduate schools, two-year colleges, and high schools. Councilors who are educators at two-year colleges or high schools are few in number. To comply with the Society's Bylaws, it is not unusual for an active, contributing member of a Society committee to be removed from the committee member roster as a result of a change in status from councilor to non-councilor. It is also not unusual for a non-councilor to be removed from the committee member roster because of another committee member undergoing a change in status from councilor to non-councilor. This petition changes the councilor requirement of Society committee members from at least two-thirds (2/3) to a majority in order to provide for greater flexibility in member appointments and continuity of committee membership. This petition also removes the councilor requirement for the chair and vice-chair of a Society committee. Committee members with expertise and strong leadership abilities should not be disqualified to serve as chair or vice-chair because of status as a non-councilor.

The Council approved the above Petition which will change the requirement for councilors on Society committees from at least two thirds (2/3) to a majority, and remove the requirement that the chair and vice-chair of a Society committee must be councilors.

Petition for Election of Committee Chairs

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

Council did not approve the above petition.

Approval of the Distribution Formula for Division Funding

The purpose of the revision is to encourage and financially reward divisions to more fully participate in ACS regional and international meetings. The current formula provides no incentive for participation in either category of meeting. ACS national meetings are the only type of meeting for which divisions receive a financial incentive. The Committee on Divisional Activities (DAC) seeks to change that with this proposal, which it thinks will more fully advance the mission of the Society. While the committee's primary concern is ACS divisions, DAC believes this proposal will also result in even more vibrant and successful ACS regional meetings, as well as ACS international meetings.

DAC proposes to reduce from 62.5% to 50% the amount it allocates to divisions for their performance at ACS national meetings. The 12.5% created from this change would be allocated in the following manner: 7.5% would be directed at division participation in ACS regional meetings and 5% in ACS international meetings. More specifically, the 7.5% directed at ACS regional meetings would reward divisions based on the number of division members registered for regional meetings (5%), and the number of half-day sessions divisions contribute to regional meetings (2.5%).

The proposed formula was not approved and was recommitted to the committee.

Petitions for Consideration

Petition of Affiliation with Other Technical Organizations

This petition proposes to add DAC and the Committee on Local Section Activities (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 Committee on Constitution and Bylaws (C&B), in approving the affiliation of divisions and local sections with other technical organizations. DAC: (vii) acting for the Council, in collaboration with the C&B, in approving the affiliation of divisions with other technical organizations. (6/1/73) LSAC: (xi) acting for the council, in collaboration with the C&B 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. The proposed Bylaw amendment accomplishes the petitioners' goal of adding the approval from the Committees on Divisional Activities and Local Activities for the affiliation of divisions and local sections with other technical organizations, since these approvals are already included in their respective duties elsewhere in the Bylaws. 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 Committee on Membership Activities, which has primary substantive responsibility for the petition. Comments and suggestions may be sent to bylaws@acs.org.

Petition to Rename and Remove Restrictions for International Chemical Sciences Chapters

The first proposal is to allow all instances of "International Chemical Sciences Chapters" in the Constitution and Bylaws to be also known as "International Chapters." This is to help streamline the ACS Governing Documents without changing current, Council-approved chapter bylaws. The second proposal addresses 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 (2/3) approval. Bylaw IX was written more than 25 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 United States or abroad; ACS award recipients, editors, authors, donors, and national or 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 financial implications of this petition are still being assessed. The Final Statement of Financial Impact will be available per Article XVIII, Sec. 2, d, which states in part, "The Chair of the Society Committee on Budget and Finance shall prepare a financial impact statement which also shall appear in the Council agenda when action is to be taken on the petition."

Recommendation to Continue Committees

The Committee on Committees (ConC) is required to review ACS Committees every five years and either recommend that they continue or recommend dissolution. This is standard at all Council meetings. The Council approved the recommendation that the Committee on Ethics be continued, and that the Committees on Publications and on Younger Chemists also be continued contingent upon approval by the Board of Directors.

Reports from Committees

Budget and Finance

In 2017, ACS generated a net from operations of $28.6 million, which was $4.8 million higher than 2016. Total revenues were $553.1 million, increasing 5.0% or $26.4 million over 2016. Expenses ended the year at $524.5 million, which was $21.6 million or 4.3% higher than the prior year. This was 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 can be found at www.acs.org. At the bottom, click "About ACS", then "ACS Financial Information". There you will find several years of the Society's audited financial statements and IRS 990 filings.

Membership

The ACS ended 2017 with over 150,000 members. While this means that ACS remains the world's largest scientific society, this number represents a continuing decline in overall membership for the sixth year in a row. The Committee on Membership Affairs is committed to working with Council, the Board of Directors, the Committee on Budget and Finance, ACS staff, and other stakeholders to halt this trend and return ACS to a growing and engaged membership.

New Orleans Meeting Attendance

As of Monday, March 19, 2018 attendance at the 2018 spring National ACS Meeting stood as follows:

Attendees	8,470
Students	6,432
Exhibitors	877
Expo only	301
Guests	505
Total	16,585

Spring National Meeting attendance 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: 1	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 (as of Monday, March 19, 2018)

Attendance at the three most recent spring national meetings held in New Orleans has been as follows: 2008 (13,454), 2013 (15,473) and 2018 (16,585).

Actions of the Board of Directors

The Board's Executive Session

The ACS Board of Directors met in executive session March 16-17, and considered a number of key strategic issues and responded with several actions.

The Board's Committees

The Board of Directors received and discussed reports from its committees on Executive Compensation, Strategic Planning, Corporation Associates, Pensions and Investments, Professional and Member Relations, the Joint Board-Council Policy Committee Task Force on Governance Design, the Joint Board-Council Committee on Publications, and the Leadership Advisory Board. In particular,

- The Board received an extensive briefing and approved several recommendations from its Committee on Executive Compensation. The compensation of the Society's executive staff continues to receive regular review from the Board.

- On the recommendation of the Joint Board-Council Committee on Publications, the Board voted to approve the reappointments of Editors-in-Chief for several ACS journals. Those appointments will be announced in *C&EN* once the appointed individuals have been notified and arrangements for their continued service have been made.

- On the recommendation of the Committee on Professional and Member Relations, the Board approved a Society nominee for the 2019 King Faisal International Prize for Science, and screened lists of nominees for the 2019 Priestley Medal and the ACS Award for Volunteer Service. The Board will select the recipients of these latter two awards from the screened lists provided.

- The Board liaison to the Leadership Advisory Board gave an update on the history of the Advisory Board and the ACS Leadership Program and offered key observations and strategic questions regarding the direction of the program in light of future Society and member needs.

- The Board liaison to the Committee on Corporation Associates offered an update on the future design state of the committee in the context of the landscape for chemical corporations and professional societies.

- The co-chair of the Task Force on Governance Design offered brief comments on its written interim report and provided a preview of its planned presentation to the Councilor caucuses focusing on streamlining the Society's governing documents.

The Executive Director and CEO Report

The Board received an extensive report from the Executive Director and CEO on issues relating to the safety and professionalism core values of the Society, as well as on membership, ACS financial performance, operational excellence, and upcoming events and activities. He also led a discussion on the strategic direction of the Science History Institute (formerly the Chemical Heritage Foundation) and its ramifications for ACS. His direct reports then engaged in discussions with the Board on the activities, opportunities and challenges of the Education Division, Chemical Abstracts Service (CAS), and the ACS Publications Division.

Other Society Business

As is customary, the Board heard reports from the presidential succession on their current and planned activities for 2018. Several presidential symposia and events incorporating and supporting the meeting's theme of Food, Energy and Water were highlighted in those reports.

Board Resolution

Finally, the Board approved a resolution that recognizes and applauds the United Nations for proclaiming 2019 as the International Year of the Periodic Table, and pledged that the Society will do its utmost to recognize and participate in events celebrating this important scientific milestone and achievement.

The Board's Regular (Open) Session

The Board held a well-attended open session on March 18, which featured a presentation from Dr. Lisa M. Balbes (Balbes Consultants, LLC) on *Nontraditional Careers in Chemistry: Thinking Outside the Beaker.* She also introduced two alumni from the ACS Scholars Program, Brandon Presley and Isa Watson, who briefly shared their careers paths to date with the assembled audience.

Prior to the presentation, the Board Chair gave a report on Board actions and issues from its Executive Session March 16-17. Members of the presidential succession and the Executive Director & CEO also offered brief reports on their activities. The officers provided more extensive reports on their activities and/or future plans as part of their written and oral reports to the Council.

Resources on the Web

Committee Preference Forms	www.yellowbook.acs.org
Highlights of ACS Achievements	www.acs.org/acshighlights
Governing Documents	www.acs.org/bulletin5
Resources on mentoring	www.acs.org/grad
Guidelines & Recommendations on Teaching HS / Middle School Chemistry	www.acs.org/mshsguidelines
Career Consultant Program	https://goo.gl/2sppC9

At https://www.acs.org/content/acs/en/about/governance/councilors.html:

- Legal Resource Manual for Divisions and Local Sections (2nd Edition)
- Freedom to Meet Without Limitation

Submitted by the CINF Councilors: Bonnie Lawlor, Svetlana Korolev, and Andrea Twiss-Brooks

Book Review

*Elements of Ethics for Physical Scientists***,** Greer, Sandra C.; MIT Press, Cambridge, MA, 2017. 239p. xii, ISBN 978-8026203-688-7 (hardcover), $50.

Why am I reviewing a book on ethics for the *CIB*? Not exactly chemical information? Here are my reasons. I've already reviewed this book twice (disclosure, one was the 190-word terse review in CHOICE, a buy/no buy recommendation for academic librarians, the reason I got the book in the first place), the second for ChemEdX (which may not appear for some time), since book reviews are no longer accepted for *J. Chem. Educ.* Most importantly, it is a good book, recommended for use and for purchase for readers of the *CIB*, most of whom are technical librarians, scientists, or both. I think this is essential information for those groups of readers.

The book is a textbook, aimed at classes for physical scientists, both for standalone courses or course content in other collegiate science classes. Besides the physical sciences, the target audiences include engineering researchers but not those engaging in engineering practice. Ethics of biomedical scientists is better covered elsewhere, and bioethics is not covered (but references are given in an appendix).

All of these subjects are hot topics, and there are many current articles on them published in newspapers, magazines, and the original literature. Depending on your point of view, distrust of scientists and scientific research in many areas is prevalent among the lay public and politicians (some even call it a war on science). Scientists are often accused of being unethical and worse. These issues make this book and use of it very timely and a helpful contribution to successful scientific careers.

The author maintains that this book differs from others in that additional topics, not always discussed in other books, are included. These topics include the philosophy of both ethics and science, issues related to underrepresented groups in science, the use of science in controversial topics like weapons research, and the relationship of science to public policy.

The first two chapters cover the philosophy and history of ethics and science, and subsequent chapters deal with the practice of scientific research including hypotheses, observations, recording and storage of data, error analysis, and construction of models. The chapter "The Scientist and Justice" deals with authorship, predecessors and citation, reviewers and referees, journal editors and grant officers, and whistleblowers. Chapter 5 covers personal interactions including discrimination, career styles, work-life conflicts, and sexual harassment.

Science and society is discussed in Chapter 6, including public funding, basic and applied science, scientific literacy among the public, and controversial science. Examples of the latter include Haber's nitrogen fixation process, atomic bombs, and chemical warfare. Final advice on conducting science is given in a concluding chapter. Four appendixes and an index conclude the book.

The author says a print textbook is superior to an e-book since it fosters class discussion of the issues. Discussion questions and case studies conclude each chapter. Inquiry questions requiring further research are also included, as well as notes and lists of resources.

Rather than take the author's word for the distinctions cited, I searched for reviews both in CHOICE and books available in the Fogler Library at the University of Maine. From CHOICE I found *Ethics of Scientific Research* (1) and *Science and Technology Ethics* (2). The first was also found at Fogler and covers a variety of topics including history, objectivity, public good, uncertainty and errors, litigation, gender and racial issues, engineering design, and public health. All topics are similar to those in this reviewed book, but this book is more current by more than two decades. Also found in the library search was *Research Ethics: Cases and Materials* (3). Again, it's an older book (1994) and the research areas are broader and

include cases in the humanities. *Science and Technology Ethics* (2) is more recent, although still not particularly current. A more recent book is *Ethics in Science: Ethical Misconduct in Scientific Research* (4). Types of misconduct are discussed here as well as the effect on the public from examples such as MMR vaccine and autism, cold fusion, and fracking and pollution. Specific case studies include those of particular interest to chemists including Corey and Woodward, patent disputes, and Woodward and quinine.

I recommend purchase of this book for both scientists and science librarians as well as *Ethics in Science* (4), which is next on my voluminous list of reading.

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Submitted by Bob Buntrock

Sponsor Announcements

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The American Chemical Society, the Royal Society of Chemistry, and the German Chemical Society partner to support ChemRxiv

The American Chemical Society (ACS) entered into an agreement with the Royal Society of Chemistry and the German Chemical Society (GDCh) to jointly support the financial and strategic development of ChemRxiv.

Through the establishment of this strong international alliance, ChemRxiv is a truly global preprint server driven by researchers. Collaboration between the ACS, the Royal Society of Chemistry, and the GDCh ensures the sustainability of this service and its continued ability to meet the needs of the global chemistry community.

Launched in August 2017, ChemRxiv has posted over 300 preprints online, all of which are openly available. Authors working across all fields of chemistry are able to post their findings to the server ahead of formal peer review and publication. The service is free of charge, features a streamlined portal for direct and easy submission, and supports a wide variety of file formats, which enables readers to visualize and interact with data without the need for specialized software.

New features that have recently been added to ChemRxiv include a triage process that checks for plagiarism and other basic elements, while retaining its rapid posting time of less than two business days. In the coming months, ChemRxiv will debut a “Direct to Journal” transfer feature so that authors can easily submit their preprint directly from ChemRxiv to the journal of their choice.

Where can I learn more about ChemRxiv?

- View the FAQs
- Follow ChemRxiv on Facebook
- Follow ChemRxiv on Twitter

Other questions? Please contact Dr. Marshall Brennan, ChemRxiv Publishing Manager: mbrennan@chemrxiv.org.

Pace of Pharmaceutical Innovation Accelerates as Record Number of New Blockbuster Drugs Forecast to Hit the Market in 2018

Twelve new game-changing drugs predicted to achieve annual sales of >$1 billion by 2022, to the benefit of millions of patients around the world

PHILADELPHIA, USA. March 22, 2018 — Clarivate Analytics, the global leader in providing trusted insights and analytics to accelerate the pace of innovation, announced today the launch of its annual "Drugs to Watch" report. The analysis **identified 12 new drugs forecast to achieve annual sales of $1 billion or more (ie, blockbuster status) by 2022** using the Cortellis database, which includes information gathered from diverse sources including drug pipelines, patents, clinical trials, chemistry deals and company announcements. More blockbuster drugs have been predicted to launch in 2018 than in any other year since the Drugs to Watch report began in 2013.

The drugs forecasted to launch in 2018 cover a wide range of therapeutic areas—ie, type 2 diabetes, endometriosis, childhood epilepsy, hemophilia, HIV, migraine, opioid addiction and shingles. Noteworthy examples on this list include:

Drug & company	Disease & Impact
Aimovig (erenumab) Amgen (USA) Novartis (Switzerland)	**Migraine**: Migraine is the third most common disease in the world, with an estimated global prevalence of 14.7% (i.e., one in seven people).[1] Fewer than 50% of patients with migraine are satisfied with their current treatment. After little movement for many years, the migraine-prevention market is about to undergo a transformation with several new drugs, known as calcitonin gene-related peptide (CGRP) receptor inhibitor. Aimovig (erenumab) has the potential to contribute to the transformation of the migraine market in 2018.
Biktarvy (tenofovir alafenamide + emtricitabine + bictegravir) Gilead (USA)	**HIV infection**: 37 million people globally are living with HIV, 21 million of whom receive antiretroviral therapy.[2] While antiretroviral therapy does not cure HIV infection, it suppresses viral replication and allows an individual's immune system to strengthen and regain the capacity to fight off infections. Expanding access to antiretroviral treatment is at the heart of a new set of targets for 2020, issued by the WHO, which aim to end the AIDS epidemic by 2030.[2] Biktarvy offers an effective and simple treatment option for patients with HIV.

Ozempic (semaglutide) Novo Nordisk (Denmark)	**Type 2 diabetes**: More than 425 million people globally live with diabetes, 90% with type 2 diabetes. By 2045, this number is projected to rise to 629 million.[3] Despite competing in a crowded market, Ozempic represents a new treatment that helps patients effectively control their blood sugar and significantly reduces the health risks commonly associated with diabetes, such as strokes and heart attacks. It is forecast to perform well due to its superior efficacy and safety versus competitor products.
Shingrix (Zoster vaccine recombinant, adjuvanted) GlaxoSmithKline (UK)	**Shingles**: It's estimated around one in every four people will have at least one episode of shingles during their life.[4] The only vaccine to make the list is GSK's Shingrix (Zoster vaccine recombinant, adjuvanted), which is set to become the market-leading shingles vaccine.
Sublocade (once-monthly buprenorphine) Indivior (UK)	**Opioid dependence**: More than 15 million people are living with opioid dependence worldwide.[5] This disorder is ongoing and is rapidly evolving into a public health crisis, with the U.S. government declaring a public health emergency in late 2017. Sublocade looks set to disrupt the market for medication-assisted treatment to overcome opioid use disorder. It is administered via subcutaneous injection once a month by a healthcare provider and does not require a detox period, thereby addressing the limitations of other treatment options.

2018 is also expected to see the launch of the first FDA-approved cannabidiol-based drug (Epidiolex), potentially opening up a new market for cannabidiol-based medicines, and the first approved treatment option (Erleada) for men with castration-resistant prostate cancer whose cancer has not yet spread.

"Despite political and regulatory uncertainties in the USA and EU markets, the annual Drugs to Watch report 2018 shows that the pace of pharmaceutical innovation continues to accelerate," explained Mukhtar Ahmed, President, Life Sciences at Clarivate Analytics. *"2018 is on track to see many new potential game-changing drugs come to market, which will benefit the lives of millions of patients around the world."*

Data for this report were compiled from the Cortellis database, the premier source of life sciences competitive, clinical and regulatory intelligence and analytics which includes data gathered from diverse sources, including annual filings, drug pipelines, clinical trials, patents, chemistry, company announcements, deals and conferences.

ABOUT CORTELLIS

Cortellis delivers the unique insights needed to reduce risk and increase success across the drug development lifecycle from early discovery to commercialization and beyond. The Cortellis suite of solutions serves the needs of life science professionals with unmatched content, intelligent search, best-in class analytics and insightful visualization tools. For more information, visit www.clarivate.com/cortellis.

ABOUT THE DRUGS TO WATCH REPORT

The annual Drugs to Watch report was first published in 2013. Using data from Cortellis, the report aims to forecast which drug launches in a given year will achieve blockbuster status within five years of launch. Following an advanced analysis of this database, a shortlist of drugs is manually researched and evaluated by life-science experts at Clarivate Analytics, who review each drug in its individual context and assess clinical trial results, regulatory data, market data and regulatory designations for each drug.
The full report is available at: http://info.clarivate.com/drugstowatch2018

Follow us on Twitter: @Cortellis | #blockbusterdrugs2018

ABOUT CLARIVATE ANALYTICS

Clarivate Analytics is the global leader in providing trusted insights and analytics to accelerate the pace of innovation. Building on a heritage going back more than a century and a half, we have built some of the most trusted brands across the innovation lifecycle, including Web of Science, Cortellis, Derwent, CompuMark, MarkMonitor and Techstreet. Today, Clarivate Analytics is a new and independent company on a bold entrepreneurial mission to help our clients radically reduce the time from new ideas to life-changing innovations. For more information, please visit www.clarivate.com.

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