

**ACS Division of Chemical Information (CINF)**  
**Annual Report 2016**  
**Division Highlights**

**CINF Mission**

The ACS Division of Chemical Information (CINF) is committed to promoting the generation of, access to, and use of the world's knowledgebase in chemistry and the related sciences. The Division fosters the sharing of expertise in science informatics, information technology, and librarianship to ensure members benefit from the experience of others and are able to improve the dissemination and utilization of scientific information. We do this through innovative, high quality programming, education, career mentoring, collaboration and outreach, and recognition of excellence.

**CINF Membership**

CINF is a small division with more than 2000 members of diverse education and career interests, from information professions to publishing and to librarianship. The membership is made up by the professionals who work to acquire, process, manage, disseminate and preserve information, to support the information needs from all practicing chemists worldwide. In 2016, ACS survey shows that around half of CINF members are employed in industry, and the other half work for higher education, governments, foundations and other nonprofit organizations. As a service to all chemists, CINF having a broad professional scale and scope, actively engage in collaboration with other ACS technical divisions, including AGFD, ANYL, BIOL, BIOT, CHED, ENVR, COMP, MEDI, I&EC, ORGN, PHYS, PMSE and POLY, as well as sister associations, the Chemistry Division of the Special Libraries Association, Chemical Structure Association Trust and the Division of Computer-Information-Chemie of the German Chemical Society.

**National Meetings**

CINF hosted 21 symposia, 171 presentations in the spring meeting in San Diego and 15 symposia, 97 presentations in the fall meeting in Philadelphia. Topics ranged broadly including patent information for drug design, chemistry information literacy, modeling spectrophotometric titration data, Cheminformatics education and research, altmetrics analysis, 3D structure-based design, crystallographic informatics, hierarchical cluster analysis, electronic laboratory notebooks, novel neurotechnologies, brain chemistry and chemical structure visualization among other cutting edge research topics. The symposia engaged a large group of researchers who are interested in chemical data, information sharing and information technologies. These presentations were also good educational seminars that installed students with information literacy skills. CINF also held its luncheons that invited outstanding speakers to present their work. Dr. Christopher Tubbs from Conservation Education Division at the San Diego Zoo, Institute for Conservation Research and Dr. James Voelkel, Curator of Rare Books in Othmer Library of Chemical History, Resident Scholar in Beckman Center for the History of Chemistry, Chemical Heritage Foundation gave presentations during the luncheons in 2016 spring and fall meetings. In addition, CINF co-sponsored the Welcoming Reception & Scholarships for Scientific Excellence Posters in the two national meetings with Journal of Chemical Information & Modeling, ACS Publications, EPA National Center for Computational

Toxicology, Genentech, Journal of Cheminformatics, PerkinElmer, Thieme Chemistry and Wiley ChemPlanner.

CINF hosted its first Data Summit in the spring meeting co-sponsored by Journal of Chemical Information & Modeling (ACS Publications), Chemical Semantics, Dotmatics, MestReLab Research and tranSMART Foundation. The theme, Computers in Chemistry, was fitting for this lineup consisting of five full days of symposia focusing on core chemical information trends, data standards, knowledge representation, national and international initiatives aimed at defining policy and infrastructure, etc.

### **Outreach, education and publications**

CINF keep in touch with its members via different channels. For those who are not able to make the trip to national meetings, CINF publishes the Chemical Information Bulletin before and after each national meeting. The bulletin features the meeting symposia, committee reports, interviews and other items free available for CINF members and beyond. In addition, CINF periodically publishes book reviews, business meeting reports and annual reports that keeps members updated with innovation in chemical information and CINF division business. CHMINF-L listserv reaches a wider audience of chemical information professionals. CINF members use this listserv for reference questions and broader discussions on chemical information topics. CINF also has its Bylaws updated. ACS Committee on Constitution and Bylaws (C&B) has certified Division's bylaws which were voted on and approved by C&B member in July 2016. The new bylaws, effective on August 4, 2016, are available on CINF website <http://www.acscinf.org/content/complete-list-0>.

CINF hosts free webinars on its cinfacs YouTube channel. In the CINF webinar of January 2016, Diane Graves introduced EDUCAUSE, a program and community focus on analysis, advocacy, community building, professional development, and knowledge creation to support the transformative role that IT can play in higher education. Also, CINF has been active on social media, such as Twitter. #acscinf has its tweets monthly. News announcements and conference reflections are popular tweets and some of them were retweeted, liked and forwarded to a number of individuals in and outside ACS.

The Book *Frontiers in Molecular Design and Chemical Information Science - Herman Skolnik Award Symposium 2015* was published in October 2016. Herman Skolnik Award Symposium, held in Boston at the ACS National Meeting in Fall 2015. The symposium included presentations covering the areas of molecular fingerprinting and similarity analysis, virtual screening methodologies, QSAR, and visualization and graphical analysis of large chemical data sets and the application of these methods to drug discovery. The editor, Dr. Jurgen Bajorath was the awardee of the symposium for his contributions in these areas. Current CINF chair, Dr. Rachelle J. Bienstock was the co-editor of this book.

In June 2016, ACS Executive Director Tom Connelly issued a challenge to the chemistry community to consider the Society's role in safety. Leah McEwen, the CINF safety liaison, presented a statement, engaged in the concerns of chemical safety and addressed the

additional questions. The questions include if ACS Publications and CAS should increase safety content and considerations in the publications and online information; how CINC ensure that all ACS content (print, virtual, video) not only conforms to safety best practices, but actively promotes best practices; how ACS might increase its programming related to safety at our national and regional meetings; if there an analogous role for ACS in chemical laboratory safety; since ACS approving bachelor's degree chemistry programs involves an examination of safety policies and procedures, if there are ways to measure various institutions' underlying safety cultures; if ACS partner with other organizations to promote tools that will help institutions strengthen their safety programs; and if ACS should include safety explicitly within its core values.

XCITR: Explore Chemical Information Teaching Resources was a repository for exploring and sharing chemical information teaching resources. XCITR was created by Gary Wiggins at Indiana University in the mid-1980's, and was developed to meet the need for an international repository of chemical information educational material. In 2016, XCITR website has been archived by Stanford University library. XCITR is a hub in which librarians, instructors and information providers deposited and accessed important and useful teaching materials. It is now searchable on Stanford's catalog and documents are viewable and downloadable.

### **Awards & Recognition**

The division established the Herman Skolnik Award in 1976 to recognize outstanding contributions to and achievements in the theory and practice of chemical information science. The Award is named in honor of the first recipient, Herman Skolnik. In 2016, Steve Bryant and Evan Bolton received the Herman Skolnik award. They are being recognized for their outstanding contribution: the creation of the needed computer and software systems to make PubChem information easily web accessible to biomedical researchers.

In 1989, the Division established the annual Student Scholarship Award to recognize chemists pursuing graduate studies in information, library, or computer science, leading to a career in chemical information. Allison Langham, student of Library and Information Studies at the University of Wisconsin-Madison, has been selected as the 2016 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."

Val Metanomski Meritorious Service Award is to recognize outstanding contributions to the Division. The CINF Awards committee unanimously approved the nomination of Leah Rae McEwen for the 2016 Val Metanomski Meritorious Service Award. Leah is cited in the nominating letter "for her outstanding contributions to the division" including six years as Secretary, also serving as Program Chair, and Education Chair.

CINF Scholarship for Scientific Excellence is designed to reward graduate and postdoctoral students in chemical information and related sciences for scientific excellence and to foster

their involvement in CINF. The winners were announced in the Welcoming Reception & Scholarships for Scientific Excellence Posters co-sponsored by a number of other ACS divisions in annual meetings. Wilian Augusto Cortopassi from Chemistry Research Laboratory, University of Oxford in Oxford, UK, Iva Lukac from School of Pharmacy and Biomolecular Sciences at John Moores University in Liverpool, UK and Yu-Chen Lo from Department of Chemistry and Biochemistry at University of California, in Los Angeles, California won in 2016 spring meeting. Mojtaba Haghightlari, Department of Chemical and Biological Engineering, University at Buffalo, George Van Den Driessche from Department of Chemistry, Bioinformatics Research Center at North Carolina State University and Nathanael Kazmierczak from Department of Chemistry & Biochemistry at Calvin College won the award in the fall meeting.

In August of 2016, CINF Division received the "Salutes to Excellence" plaque from ACS immediate Past-President Diane Grob Schmidt for supporting her presidential programming during the period 2014-2016. CINF is one of the ten divisions that received this award.

### **Innovative Project Grant**

CINF division submitted grant application for ACS Divisional Activities Committee funds titled "Division of Chemical Information Web Platform Development". The grant sponsored a web interface design, content organization, web structure building and user experience optimization. This project will enhance the communication of CINF division, and engage members and general audience with rich resources, programming and activities.

### **Challenges & Opportunities**

CINF is a small and specialized community as broadly geographically distributed. Networking happens traditionally during national meetings twice a year, however, the members need more frequent and accessible networking venue outside the national meetings. Traditionally members use virtual communication, such as online conference and phone meeting. But, the virtual communication technologies only rely on member's home institute facilities and network, without receive any help from ACS. CINF has a need of effective networking and communication venues from current technology tools and support system from ACS.

Chemical information is essential for practicing chemists on their daily bases. However, CINF as a division of chemical information has not received enough recognition within the ACS communities. For instance, CINF members' jobs are not reflected as a field of specialization on ACS job board for its members. Also, the majority category of CINF membership demographic reports is "others" for job title, industry, departments, etc.

Division members are volunteers who have full-time professional work to support the chemical enterprise, are involved in ACS primarily for chemical information interests. Yet, the volunteer services on executive board and in committees requires significant time and efforts. CINF has difficulty to find volunteers to run in elections and for committee functionary positions. Since CINF vision consists of information management professionals, it is suggested that some

volunteering efforts could be applied in closer collaboration with ACS infrastructure to help solve these problems for CINF.

There are both opportunities and challenges to enhance quality of collaboration efforts, across technical divisions and ACS local sessions, across professional associations and scientific organizations. CINF has worked together with ACS divisions and outside on programs and symposia in national meetings, as well as, in webinars web presentations, publications, awards and grants. The executive committee members thrive to to establish and foster relations across board. Also, CINF has raised awareness of the interdisciplinary and global collaborations. In 2016 fall meeting, CINF executive board has discussed using social media for a broader outreach, and improvement plan for CINF web platform.