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Letter from the Editor

Due to the COVID-19 epidemic, the American Chemical Society has taken the unprecedented step of cancelling the spring national meeting. This means that there are no technical program or committee reports in this issue, making it much shorter than normal.

There was, in fact, some discussion as to whether to publish the spring and summer issues of the *Chemical Information Bulletin* this year. We have decided that there was enough material submitted to justify publication. The Lucille M. Wert scholarship winner for 2020 has been announced, and there is a call for applications for Chemical Structure Association Trust grants for 2021. Bob Buntrock has another book review for us, and we have a current list of CINF office holders at the end.

Finally, we would like to acknowledge those that have made the presentations (oral or poster) available on the ACS SciMeetings platform ([https://www.acs.org/content/acs/en/meetings/national-meeting/scimeetings.html](https://www.acs.org/content/acs/en/meetings/national-meeting/scimeetings.html)). A list of CINF contributions to that platform, as of May 9, 2020, is given on the next page.

Submitted by David Shobe
Presentations available on ACS SciMeeting
(https://www.acs.org/content/acs/en/meetings/national-meeting/scimeetings.html)
As of May 9, 2020.

1. Richard T Cupitt, Charlotte Slavick, Gregory D. Koblentz, Stefano Costanzi, “Structurally annotated lists of chemicals from international frameworks for the control of chemical weapons and precursors”.

2. Gerhard Ecker; Stefanie Kickinger; Anna Seiler, “Proteochemometric modeling of GABA transporters”.

3. Alexey A. Lagunin et al., “Predicting synergism of anti-HIV drug pair combinations”.


5. Jennifer Hemmerich; Florentina Troger; Barbara Füzi; Gerhard F. Ecker, “Using machine learning methods and structural alerts for prediction of mitochondrial toxicity”.

6. Alexey A. Lagunin, “Predictions of pairs of drugs with synergistic activity against leukemia cell lines based on NCI-ALMANAC data”.

7. Philip Barnett, “STN to the rescue: When SciFinder is not sufficient”.


9. Sarah E. Hosler; Jacquelyn S. Fetrow, “Clustering of the phosducin protein family and its functionally relevant groups”.

10. Matthew Whitman, “Extracting an empirical intermetallic hydride design principle from limited data via interpretable machine learning”.


12. Ethan Evans, “Using machine learning to predict human health from biofluid-based metabolomics”.

13. Annie Zeidman-Karpinski; Jimmy Murray; Elliott Freeman; Melissa Galvan; Samantha Ehlers; Eowyn Boosinger, “Student library employees make the makerspace safe!”


15. Neelam Bharti; Shailendra Singh; Aastha Singh, “3D printing in library makerspace: Health and safety concern”. 
16. Milad Salem; Arash Keshavarzi Arshadi; Jiann Shiun Yuan, “Application of deep learning in purchasing compound libraries for non-target based drug discovery”.

17. Lutz Weber, Konstantin Kruse, Timo Böhme, Claudia Bobach, Stephen Boyer, “Using chemical ontologies to create molecular prediction systems for any molecular property”.

18. Shailendra Singh; Andrew Lawson, “Are you ready to have a laser cutter in your makerspace? Think again!”

19. Ekaterina Sosnina, “Multitask prediction using techniques of recommender systems”.


21. Beihong Ji; Matthew Brock, “Generation of druglike molecules with generative adversarial networks (GANs)”.


23. Leah R McEwen; Michael Boruta, “Associating live analytical data to synthetic chemistry experiments: Applying FAIR principles across the scientific experimentation lifecycle”.

24. Dmitri Kireev, “AI-driven 3D design for orphan targets from big PDB/SAR data”.

25. Mihyun Kim; Surendra Kumar; Cheongyun Jang, “Target-based vs inverse target-based drug discovery: Machine learning assisted balance between in-house compounds and commercial screening compounds”.

26. Yulia Borodina; Tyler Peryea, “Representation of biopharmaceutical substances in the FDA global substance registration system and in the structured product labeling”.
Scholarships and Awards

Lucille M. Wert Student Scholarship

The Lucille M. Wert Student Scholarship is awarded annually and is designed to help persons with an interest in the fields of chemistry and information to pursue graduate study in library, information, or computer science. The CINF Awards Committee reviewed the applications during the spring ACS meeting and is very pleased to announce that the 2020 scholarship recipient is Dr. Winnie Ak Wai Li.

Winnie holds a B.Sc. in Chemistry from the Chinese University of Hong Kong. She is currently pursuing a Master of Library and Information Studies at the University of British Columbia. Winnie is eager to promote Open Science. Her study focuses on data services and information systems. Winnie is interested in designing user-centered information systems to support researchers to adopt Open Science practice. Congratulations to Winnie!

Submitted by Rajarshi Guha

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 2021.

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?

Applicants, age 35 or younger, who have demonstrated excellence in their chemical information related research and who are developing careers that have the potential to have a positive impact on the utility of chemical information relevant to chemical structures, reactions, and compounds, are invited to submit applications. 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; e.g. 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 2021 grant is April 16, 2021. Successful applicants will be notified no later than May 24, 2021.

Address for Submission of Applications: The application documentation can be mailed via post or emailed to: Bonnie Lawlor, CSA Trust Grant Committee Chair, 276 Upper Gulph Road, Radnor, PA 19087, USA. If you wish to enter your application by e-mail, please contact Bonnie Lawlor at chescot@aol.com prior to submission so that she can contact you if the e-mail does not arrive.
Chemical Structure Association Trust: Recent Grant Awardees

2020

Review of 2020 proposals is currently in process.

2019

Vinicius Alves, University of North Carolina Eshelman School of Pharmacy, Chapel Hill (USA), was awarded $2,572 to present his research paper entitled “Multi-Descriptor Read Across (MuDRA) as a novel computational approach for Chemical Toxicity Prediction” at the 10th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources that was held in Ionnina, Greece from June 23-27, 2019.

Guilian Luchini, Colorado State University, Fort Collins, CO, was awarded $1,399.00 to attend the American Chemical Society Meeting that was held August 24-29 in San Diego, CA, to present his research in applying often-overlooked corrections to DFT frequency calculations in an automated fashion.

Roi Rutenberg, Chemistry Department at Stanford University, Stanford, CA, was awarded $2,072 for travel to visit the University of Illinois, Chicago in order to model molecular dynamic (MD) simulations at the Kral group as part of his research related to retrieving information about pEtN cellulose’s chemical structure as an individual compound, as well as a partner in future chemical reactions.

Monika Szabo, Monash Institute of Pharmaceutical Sciences, Monash University, Victoria, Australia, was awarded $2,000.00 for travel to attend two conferences at which she presented her research on drugs for myelofibrosis. The conferences were: EFMC-ASMC’19 International Symposium on Advances in Synthetic and Medicinal Chemistry - Athens Greece; September 1-5, 2019, and the 20th SCI/RSC Medicinal Chemistry Symposium-Cambridge UK; September 8-11, 2019.

2018

Stephen Capuzzi, Division of Chemical Biology and Medicinal Chemistry at the University of North Carolina Eshelman School of Pharmacy, Chapel Hill, NC, was awarded a grant to attend the 31th ICAR in Porto, Portugal on November 6-15, 2018, where he presented his research entitled “Computer-aided Discovery and Characterization of Novel Ebola Virus Inhibitors”.

Christopher Cooper, Cavendish Laboratory, University of Cambridge, UK, was awarded a grant to present his current research on systematic, high-throughput screening of organic dyes for co-sensitized dye-sensitized solar cells. He presented his work at the Solar Energy Conversion Gordon Research Conference and Seminar held June 16-22, 2018 in Hong Kong.
Mark Driver, Chemistry Department, University of Cambridge, UK, was awarded a grant to offset costs to attend the 7th EUChEMS conference where he presented a poster on his research that focuses on the development and applications of a theoretical approach to model hydrogen bonding.

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

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

2017

Jesus Calvo-Castro: University of Hertfordshire, England, was awarded a grant to cover travel to present his work at the Fifth International Conference on Novel Psychoactive Substances to be held in Vienna, Austria from August 23-23, 2017. He works on the development of novel methodologies for the in-the-field detection of novel psychoactive substances (NPS), where chemical structure and information play a crucial role.

Jessica Holien: St. Vincent’s Institute of Medical Research, Fitzroy, Victoria, Australia, was awarded a grant to cover travel to present her work at the 2017 Computer-aided Drug Design (CADD) Gordon Research Conference scheduled to take place July 16-21, 2017 in Mount Snow, VT, USA. She is a postdoctoral researcher at St. Vincent’s and is responsible for a range of computational molecular modeling, including: compound database development, virtual screening, docking, homology modeling, dynamic simulations, and drug design.

Submitted by Bonnie Lawlor
Book Review


Although this book was published in 2016, I thought it was worth reviewing now since it covers topics that are still “hot”. The book is a Festschrift for Blaise Cronin upon his retirement as Rudy Professor of Information Science at Indiana University. The editor, Cassidy Sugimoto, has been a frequent collaborator with Cronin on several books and articles. She points out that this is an unusual Festschrift in that it is not just laudatory but contains several chapters by those working in the two fields, exemplifying Cronin’s extensive participation in both. The forward was written by Eugene Garfield, and the 27 authors of the chapters (including Cronin himself) include famous names like Henry Small, Christine Borgman, and Howard White.

The 19 chapters are organized into six sections: Critical Informetrics (Cronin), Citation Theories (Small, Borgman), Statistical Theories, Authorship Theories (White), Knowledge Organization Theories, and Altmetric Theories. The last deals with the impact of altmetrics on scholarly research, knowledge, and publication.

The editor stresses that this is the beginning of a “conversation” on the topics but that, in addition to agreements, disagreements occur. For example, in Section I, Critical Informatics, Cronin criticizes searching for a unifying theory of citation, the theme of the rest of the sections, but does not elaborate on objectives for future research. The Festschrift is the beginning, but not the end, of the conversation. From our viewpoint five years in the future, the conversation is definitely ongoing.

In the Citation Theories section (II), the authors agree with Cronin that a unifying theory of citation is “nonsensical” and that multiple theories are needed. In Section III, Statistical Theories, definitions of “success” in relation to the number of citations are discussed, including Merton’s “Matthew Principle” (often restated as “he who has gets”). Success is defined as publication measured by citations and not stimulation of original research. The (in)famous common distributions of information (Zipf, Lotka, and Bradford) are discussed. A key chapter is titled, “From Matthew to Hirsch: a Success-Breeds-Success Story”.

In Section IV, Authorship Theories, Cronin’s publications on authorship in scientific publication are further discussed (Cronin coined “hyperauthorship” to describe increased numbers of authors in article bylines). In Section V, Knowledge Organization Theories, such organization in relation to databases is discussed. One chapter considers analysis of the process using books. Another considers semantic mapping.

In Section VI, Altmetric Theories, the societal impact of the increased use of such metric is discussed. Altmetrics are based on the responses to social media with different criteria than traditional citation...
metrics. One author posits that there are six additional reasons for citation in social media than the 15 possible motivations cited by Garfield in 1962. The true meaning of “impact” (originally “application to research”) and the expansion to societal needs are important, even revolutionary. An argument is made that altmetrics track research progress, not output. Once again, Cronin was way out ahead of the field.

Cited references conclude every chapter. Biographies of all contributors and an index conclude the book.

As the title suggests, the book largely concentrates on theories and less on pragmatics. Alternatives to the h-Index are not discussed, nor are the impacts of use and misuse of informetrics on personal practices such as hiring, firing, and career advancement. The book is recommended for all who are interested in these evolving aspects of citations and science communication in general.

Submitted by Bob Buntrock
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