



Computational Toxicology Specialty Section (CTSS)

Newsletter: Winter 2020

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David Edmondson, PhD

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President's Letter

I hope that everyone is staying safe and healthy in the midst of all of the uncertainty that we are experiencing this year. Although we will not have the opportunity to meet face-to-face at the SOT 2021 Annual Meeting in Orlando, we will have the opportunity to try something new and engage *virtually*, still honoring award winners, presenting our work, navigating the scientific program, and importantly, catching up with colleagues. We will likely see many changes in the coming months, but I remain optimistic and flexible, as I hope all of you are, as we embrace a new way to communicate and collaborate in our collective pursuit to advance the field of computational toxicology.



CTSS Officers have been working all year for you! We were successful at obtaining endorsement for two CTSS driven symposia in the upcoming SOT scientific program, increasing our section membership, and initiating our 2020-2021 CTSS Webinar Series. The webinar series is dedicated to broadcast the application of our members' accomplishments as well as educate fundamental concepts and celebrate discoveries. The first webinar honored the great work of three CTSS 2020 award winners. This series promises to continue to be an exciting addition to CTSS, while the recorded sessions are of great value to our members for reflection and continual improvement. We do hope you dial-in to a session, engage the speaker(s), and even nominate yourself or a colleague to be part of next year's webinar series. We are always looking for opportunities to support you as a valuable member.

We are very appreciative of our sponsors (Pfizer, Lhasa Limited, Leadscope, MultiCASE, and FDA) for their generous contributions this past year; without them, many of our past and upcoming events/activities/awards would not be possible. The CTSS continues to identify new mechanisms to recognize and give back to the CTSS membership, and we are proud to announce that the CTSS Endowment Fund is now fully sustainable. *The Yves Alarie Diversity Award for Trainees and Young Investigator Endowment Fund* will be available every year for a qualified candidate, including this coming 2020-2021 award cycle. However, this year we established another mechanism to recognize our members and their top scientific achievements, the *10 Best SOT-CTSS Abstract Awards*. This award is open to all members, and please don't forget to send us your accepted abstracts for consideration.

It is also that time of year when we are soliciting nominations for several open positions to the CTSS leadership team. This year, open positions include VP-Elect, Secretary, Councilor, and Postdoctoral Rep. If you are passionate about contributing your expertise, time, and effort to this organization and are a member with good standing of CTSS and SOT, please consider becoming a CTSS Officer.

I would like to take this opportunity to thank the CTSS leadership team who have worked so very hard this year to make all these activities/events possible. I learn and grow every time we get together, and they are a dedicated, brilliant, and fun team. I very much appreciate all the efforts they have put in to make this specialty section so successful! I am truly honored and thankful to work with you all!

I look forward to seeing everyone virtually at the upcoming 2021 Annual Meeting in March, and I hope you can attend our virtual CTSS annual reception.

Warm regards,

David Szabo

2020 Member Highlights

We want to feature you, our CTSS members!!!!

Scientific Accomplishments. Any time of year, please send us information on any of your publications, book chapters, presentations at local/national/international meetings and any other milestone. Photos and images are always welcomed.

New Section: "What's New in Computational Toxicology?" We are looking for authors who would like to contribute to our newly started series entitled "What's new in computational toxicology?". The series hosts columns authored by the members of the CTSS who would like to share about exciting projects they are working on, or published about, maybe new trends in toxicology pertaining to their area of expertise, impressions on meetings they attended and that were of interest to them and their group, etc. The column is to be between 1,000-4,000 characters (including spaces) long; 1 to 2 figures can be included at the author's discretion as long as there are no intellectual property conflicts.

Please contact our postdoctoral representative David Edmondson (David.edmondson@cchmc.org) with your news!



Congratulations: 2020 Member Accomplishments!!!

Past Continuing Education Courses (2020)

<https://www.toxicology.org/events/am/AM2020/continuing-education.asp>

Introduction to Open-Access Computational Toxicology Tools

Chair: Agnes Karmaus, Integrated Laboratory Systems, Inc.; and Nicole Kleinstreuer, NIEHS/NICEATM.

Lung Function: It's Not Just Breathing

Chairs: Andrew Gow, Rutgers, The State University of New Jersey; and Angie Groves, University of Rochester Medical Center.

Past Presentations (2020)

"Predicting Nitrosamine Activity from Structure-Activity Relationships", Kevin Cross, Leadscope Inc., Nitrosamines Impurities Forum Americas, Informa, 26 August 2020.

"Overview of In Silico Models for Acute Toxicity Prediction and Study Design", Glenn Myatt, Leadscope, Inc. Northern California Regional Chapter on the Society of Toxicology. SOT 2020 Webinar Series, Nov. 2020.

"Results, the Importance of Expert Review, How to Perform an Expert Review", Catrin Hasselgren, Genentech, Northern California Regional Chapter on the Society of Toxicology. SOT 2020 Webinar Series, Nov. 2020.

"Developing Mechanism-Based Models for Complex Toxicology Study Endpoints Using Standardized Electronic Submission Data", Dan Russo, ORISE/FDA, Kevin Cross, Leadscope, Kevin Snyder, FDA, ACT, Nov 2020.

In silico methods to assess the toxicity of extractables, leachables and degradants. Candice Johnson, Leadscope, Inc., Extractables & Leachables USA, Virtual Event, 26-28 October 2020.



Scientific Accomplishments (cont.)

Publications from our CTSS members (2020)

[Integrating adverse outcome pathways \(AOPs\) and high throughput in vitro assays for better risk evaluations, a study with drug-induced liver injury \(DILI\)](#) KK Khadka, **M Chen**, Z Liu, W Tong, D Wang. *ALTEX-Alternatives to animal experimentation* 37 (2), 187-196

[The landscape of hepatobiliary adverse reactions across 53 herbal and dietary supplements reveals immune-mediated injury as a common cause of hepatitis](#) J Zhu, **M Chen**, J Borlak, W Tong. *Archives of Toxicology* 94 (1), 273-293

[Skin sensitization in silico protocol.](#) Candice Johnson, Ernst Ahlberg, Lennart T. Anger, **Lisa Beilke**, Romualdo Benigni, Joel Bercu, Sol Bobst, David Bower, Alessandro Brigo, Sarah Campbell, Mark T.D. Cronin, Ian Crooks, **Kevin P. Cross**, Tatyana Doktorova, Thomas Exner, David Faulkner, Ian M. Fearon, Markus Fehr, Shayne C. Gad, Véronique Gervais, Amanda Giddings, Susanne Glowienke, Barry Hardy, **Catrin Hasselgren**, Jedd Hillegass, Robert Jolly, Eckart Krupp, Liat Lomnitski, Jason Magby, Jordi Mestres, Lawrence Milchak, Scott Miller, Wolfgang Muster, Louise Neilson, Rahul Parakhia, Alexis Parenty, Patricia Parris, Alexandre Paulino, Ana Theresa Paulino, David W. Roberts, Harald Schlecker, Reinhard Stidl, Diana Suarez-Rodriguez, **David T. Szabo**, Raymond R. Tice, Daniel Urbisch, Anna Vuorinen, Brian Wall, Thibaud Weiler, Angela T. White, Jessica Whritenour, Joerg Wichard, **David Woolley**, Craig Zwickl, Glenn J. Myatt, (2020). *Regulatory Toxicology and Pharmacol.*, 116:1-22.

[Management of pharmaceutical ICH M7 \(Q\)SAR predictions – The impact of model update.](#) **Hasselgren C**, Bercu J, Cayley A, **Cross K**, et al. *Regulatory Toxicology and Pharmacology*. 2020. 118:103807

[Exploring Mechanistic Toxicity of Mixtures Using PBPK Modeling and Computational Systems Biology.](#) **Ruiz P**, Emond C, McLanahan ED, Joshi-Barr S, Mumtaz M. *Toxicol Sci*. 2020;174(1):38-50.

[CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity.](#) Kamel Mansouri, Nicole Kleinstreuer, Ahmed M. Abdelaziz, Domenico Alberga, Vinicius M. Alves, Patrik L. Andersson, Carolina H. Andrade, Fang Bai, Ilya Balabin, Davide Ballabio, Emilio Benfenati, Barun Bhatarai, Scott Boyer, Jingwen Chen, Viviana Consonni, Sherif Farag, Denis Fourches, Alfonso T. García-Sosa, Paola Gramatica, Francesca Grisoni, Chris M. Grulke, Huixiao Hong, Dragos Horvath, Xin Hu, Ruili Huang, Nina Jeliakova, Jiazhong Li, Xuehua Li, Huanxiang Liu, Serena Manganelli, Giuseppe F. Mangiatordi, Uko Maran, Gilles Marcou, Todd Martin, Eugene Muratov, Dac-Trung Nguyen, Orazio Nicolotti, Nikolai G. Nikolov, Ulf Norinder, Ester Papa, Michel Petitjean, Geven Piir, Pavel Pogodin, Vladimir Poroikov, Xianliang Qiao, Ann M. Richard, Alessandra Roncaglioni, **Patricia Ruiz**, Chetan Rupakheti, Sugunadevi Sakkiah, Alessandro Sangion, Karl-Werner Schramm, Chandrabose Selvaraj, Imran Shah, Sulev Sild, Lixia Sun, Olivier Taboureau, Yun Tang, Igor V. Tetko, Roberto Todeschini, Weida Tong, Daniela Trisciuzzi, Alexander Tropsha, George Van Den Driessche, Alexandre Varnek, Zhongyu Wang, Eva B. Wedeby, Antony J. Williams, Hongbin Xie, Alexey V. Zakharov, Ziyi Zheng, and Richard S. Judson. *Environ Health Perspect*. 2020;128(2):27002.

[Exploring current read-across applications and needs among selected U.S. Federal Agencies.](#) Patlewicz, Lizarraga, Rua, Allen, Daniel, Fitzpatrick, Garcia-Reyero, Gordon J, Hakkinen P, Howard AS, Karmaus A, Matheson J, Mumtaz, M, Richarz AN, **Ruiz P**, Scarano L, Yamada T, Kleinstreuer N. 2019. *Regul. Tox Pharm*. 106:197-209.

[Development of Improved QSAR Models for Predicting the Outcome of the in vivo Micronucleus Genetic Toxicity Assay.](#) Lidiya Stavitskaya, Jae Wook Yoo, Naomi L Kruhlak, Curran Landry, **Kevin P Cross**, Alexander Sedykh. *Regulatory Toxicology and Pharmacology*, June 2020.

[Whole-brain R1 predicts manganese exposure and biological effects in welders.](#) **Edmondson D**, Yeh C-L, Helie S, Dydak U. *Archives of Toxicology* 2020, 94:3409-3420



Treasurer's Report and Acknowledgement

- This year the CTSS received **\$11,500** in financial support from Pfizer, Inc., Leadscope, Inc., Lhasa Limited, and MultiCASE Inc.
- Thank you to Dr. Nigel Greene for donating his stipend from his Continuing Education course at last year's meeting.
- Because of our sponsors, the CTSS was able to give out **\$4500** in awards.
- After expenses, the CTSS still has a balance of over \$27K. Unfortunately, part of this financial success was due to the lack of SOT meeting expenses.

Future Sponsors

CTSS now offers the opportunity for several levels of sponsorship:

Bronze: \$500 - \$999

Silver: \$1000 - \$1499

Gold: \$1500 - \$2499

Platinum: \$2500+

Current Sponsorship

Platinum



Gold



Silver



Awards / Endowment

Recognition of CTSS award winners of 2020:

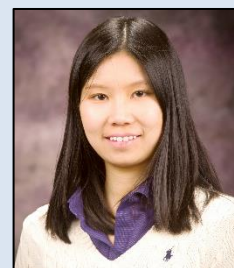
AstraZeneca Student Travel Award - \$1250

Dr. Mary Davis-Schleiff from University of Arkansas for Medical School for the SOT abstract "**Bioactivation of halogenated aromatic drugs as a precursor to drug-induced hepatotoxicity**". The awardee will receive \$750 fund for travel cost with an additional monetary prize of \$500. The poster for this work is available here: https://files.abstractsonline.com/CTRL/BE/C/BC5/C13/9AB/42B/1B8/B8E/1C1/005/5F5/22/a1250_1.pdf



AstraZeneca Postdoctoral Travel Award - \$1250

Dr. Zhenzhen Shi from Emory University for the SOT abstract "**Computational Identification and Analysis of Nonmonotonic Concentration Responses in Tox21 Estrogen Receptor Assays**". The awardee will receive \$750 fund for travel cost with an additional monetary prize of \$500. The poster for this work is available here: http://files.abstractsonline.com/CTRL/4D/E/64F/B66/D69/418/EBB/4F2/914/EA7/2B8/4A/a3390_1.pdf



Paper of the Year Award - \$1500

Kapil Khadka (pictured), Minjun Chen, Zhichao Liu, Weida Tong, Dong Wang for their publication titled "**Integrating Adverse Outcome Pathways (AOPs) and High Throughput In Vitro Assays for Better Risk Evaluations, a Study with Drug-Induced Liver Injury (DILI)**". The awardee will receive \$750 fund for travel cost with an additional monetary prize of \$750. The paper is available here: <https://www.altex.org/index.php/altex/article/view/1337>



New this year!

Yves Alarie Scholarship Endowment Fund – \$2500

"Established in June 2019, the purpose of this fund is to encourage members of under-represented groups to pursue careers in toxicology, particularly with a focus on developing or applying computational toxicology methods and tools. The fund will be used to support the professional development of trainees who are members of groups under-represented in toxicology."

Sara M. Vliet for the abstract titled "**A Weight-of-Evidence Approach for Androgen Receptor Conservation Across Vertebrate Species**". Dr. Vliet is currently a postdoctoral fellow at Great Lakes Toxicology & Ecology Division, Center for Computational Toxicology & Ecology, U.S. Environmental Protection Agency. The poster is available here: https://files.abstractsonline.com/CTRL/27/4/C10/8F2/972/433/687/39E/908/247/CC6/F0/a4230_1.pdf



Please join us in congratulating our award/fellowship recipients!!!

Upcoming Awards:

The CTSS will continue to offer the paper of the year award and student/postdoc award in 2021. Please check the CTSS-SOT website for additional information.

<https://www.toxicology.org/groups/ss/ctss/index.asp>

Annual Report

Officers

2019-2020

2020-2021

President:
Vice President:
Vice President-Elect:
Secretary:
Treasurer:
Past President
Councilors:

PDA Representative:
GSLC Representative:

Lisa D. Beilke
David Szabo
Catrin Hasselgren
Joel Cohen
Mark Gosink
David R. Woolley
Nigel Greene
MinJun Chen
n/a
Fjodor Melnikov

David Szabo
Catrin Hasselgren
Nigel Greene
Joel Cohen
Kevin Cross
Lisa D. Beilke
MinJun Chen
Patricia Ruiz
David Edmondson
Emily Golden



Committees: Executive committee (chair: David Szabo), Awards committee (chair: Minjun Chen), Nominations committee (chair: Lisa Beilke), Website Liaison (Joel Cohen), Outreach Liaison (chair: Nigel Greene), Membership outreach (chair: Catrin Hasselgren), Endowment Fund (David Szabo), Symposia (Nigel Green), Webinars (David Szabo, Catrin Hasselgren)

○ CTSS Membership

- Total number CTSS members = **234 members strong**



○ CTSS Webinars Recorded on CTSS Webpage from 2019 and 2020

- First webinar was presented by Glenn Myatt, Leadscope, and Donna MacMillan, Lhasa on the topic “**Computational Toxicology Methods and Approaches**”.
- The second by Naomi Kruhlak, FDA CDER on “**US FDA Experience in the Regulatory Application of (Q)SAR Modeling**”.
- The third was initiated by CTSS and co-hosted with Risk Assessment Specialty Section by Steve Gutsell of Unilever on **Computational Approaches in Next Generation Risk Assessment of Consumer Products**.
- The fourth was initiated by CTSS and co-hosted with Drug Discovery Toxicology Specialty Section by Nigel Greene, Astra Zeneca, **Artificial Intelligence in the Design of Safer Medicines – Science or Science Fiction?**

CTSS Endorsed Symposia for 2020-2021

- Pre-Review: **10 sessions** requested CTSS pre-endorsement review
- Official Endorsement: **12 proposals** reviewed: Symposia, CE/Info, Workshops,
- The CTSS Committee determined primary endorsement of the following
 - **SYM-22: Industrial Application of Artificial Intelligence in Toxicology**
 - **SYM-10: Application of Computational genomic Approaches to Address Toxicity Mechanisms and Predictions**



Run for CTSS office!

Calling for Enthusiastic Colleagues to Serve!
Available positions for 2021:

Please send an email today to David Szabo at dszabo@ppg.com for more details or if you already decided to run for office, then simply send a short bio-sketch with an indication of which position you would like to run for by December 15, 2020! Thank you!



Want to present?

Are you interested in participating as invited speaker for our future CTSS webinars?

Do you have colleagues who might be a great fit? We welcome nominations, including yourself, for anyone with interest and expertise in computational toxicology, applications, methods development, and cutting-edge topics. Please submit your nominations (or yourself!) to Catrin Hasselgren at hasselgren.catrin@gene.com.

SOT Virtual 2021 Annual Meeting and ToxExpo

- All 59 accepted Symposia, Workshops, and other Scientific Sessions, plus the 14 Continuing Education courses, are expected to be presented as part of the Virtual Meeting.
- The accepted abstracts will be programmed into virtual Platform and Poster Sessions.



Save the dates!
March 12-26, 2021