Computational Toxicology Specialty Section (CTSS)

Newsletter: Fall 2019

2019-2020 CTSS Executive Committee

President
Lisa D. Beilke, MSPH, PhD, DABT, ERT

Vice President
David Szabo, PhD, DABT

Vice President-Elect
Catrin Hasselgren, PhD

Secretary
Joel M. Cohen, ScD, DABT

Treasurer
Mark Gosink, PhD

Past President
David R. Woolley, PhD, DABT, ERT

Councilors
Nigel Greene, PhD
Minjun Chen, PhD

Postdoctoral Representative
Position open

Graduate Student Representative
Linlin Zhao, MS

President's Letter

The 2018/2019 CTSS year flew by! It was marked with increased section membership, a number of endorsed symposia, a CTSS-organized CEP session and a great attendance at our annual luncheon. We are very appreciative of our sponsors (Lhasa Limited, Leadscope, AstraZeneca, SimulationsPlus and Genentech) for their generous contributions this past year, without them, many of our events/activities would not be possible.

I am also pleased to report that the CTSS has a new Endowment fund, the Yves Alarie Endowment fund, which will be registered in 2020-2021.

As noted in previous communications, the CTSS was pleased to announce a webinar series dedicated to computational toxicology for CTSS members, with the first webinar (An Introduction to in silico Toxicology) held on September 20, 2019. This series promises to be an exciting addition to the CTSS and of great value to members.

It is also that time of year when we are soliciting nominations for several open positions to the CTSS leadership team. Open positions include VP-Elect, Treasurer, Councilor, and Postdoc 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 board member.

Last but certainly not least, I would like to take this opportunity to thank the CTSS leadership team who have worked very hard this year to make all these activities/events possible. They are an amazing team to work with, and I very much appreciate all the efforts they've made in making this specialty section so successful!

I look forward to seeing everyone in Anaheim, CA at the next Annual Meeting and hope you can attend the CTSS luncheon that is being planned.

Warm regards,

Lisa Beilke

What is Computational Toxicology?

Computational toxicology is a multi-disciplinary science that requires understanding of:

- Computational sciences
- Statistics
- Chemistry
- Systems biology
- Exposure science
- Risk assessment and risk management

Provided there is a sufficient database of information, almost any toxicological endpoint can be modelled using computational toxicology software. The approaches used and the endpoints analyzed are as diverse as the users employing these methods. Examples of these include pathways, systems and tissue modelling, cheminformatics, big data methodologies for analysis of information, screening of chemicals, and uncertainty analysis. In addition, computational models have been used to calculate potential toxicokinetic and pharmacokinetic parameters.

At present, there is regulatory acceptance of the use of computational toxicology models in replacement of the reverse bacterial mutation (Ames) assay for impurities in pharmaceuticals, estrogen activity of environmental chemicals, and read-across for a variety of toxicological endpoints.

- The Computational Toxicology Specialty Section (CTSS) remains on strong financial footing thanks to our members, corporate sponsors and the SOT organization.
- CTSS's coffers currently stands at **$5K** despite a significant increase in SOT meeting costs. Our group was also able to give out **over $4K** in individual awards and as well as provide a **$500 donation** to the American Society for Cellular and Computational Toxicology (ASCCT).
- External financial support last year was provided by generous donations from **AstraZeneca UK Ltd**, **Leadscope, Inc.** and **Lhasa Limited**. This year, both **Simulations Plus, Inc.** and **Genentech, Inc.** have donated to our specialty section. It is with the help of our donors that we are able to give back to the computational toxicological community.
- **Accordingly, we wish to thank all our sponsors for their generosity**.

Meeting and Reception Highlights

The annual reception lunch was held on March 13, 2019 with approximately 100 people in attendance, and was called to order by then presiding President Dr. David Woolley. The CTSS Executive Team kicked things off by first thanking our sponsors (Lhasa Limited, Leadscope, AstraZeneca, Simulations Plus and Genentech) for their generous contributions. Dr. Lisa Beilke then discussed membership updates - of the 164 total members, most are from industry, followed by academia, government, software developers, and consultants. A summary of financials was provided by Treasurer Dr. Mark Gosink, followed by details on the forthcoming Yves Alarie Endowment Fund presented by Vice President-Elect Dr. David Szabo. Councilor Dr. Nigel Greene submitted requests for symposia ideas for the 2020 Annual Meeting, and Dr. Szabo and Dr. Catrin Hasselgren requested proposals for the 2019-2020 CTSS webinar series. After meeting and recognizing the three award winners, outgoing President David Woolley thanked the CTSS Leadership team for their support and wished incoming president Lisa Beilke the very best for the future.

Recognition of the three award winners of 2019:

- **AstraZeneca Student Travel Award:**

  David A. Edmondson (Purdue University) for SOT abstract: "*Whole-brain R1 Mapping Predicts Mn Accumulation in the Human Brain: A Support Vector Machine Approach*"

- **AstraZeneca Postdoctoral Travel Award:**

  Timothy E H Allen (Univ. of Cambridge, UK) for SOT abstract: "*Combining Structural Alerts and Machine Learning Algorithms to Predict Human Molecular Initiating*"

- **Paper of the Year Award:**

  John F. Wambaugh, Michael F. Hughes, Caroline L. Ring, Denise K. MacMillan, Jermaine Ford, Timothy R. Fennell, Sherry R. Black, Rodney W. Snyder, Nisha S. Sipes, Barbara A. Wetmore, Joost Westerhout, R. Woodrow Setzer, Robert G. Pearce, Jane Ellen Simmons, and Russell S. Thomas, "*Evaluating In Vitro-In Vivo Extrapolation of Toxicokinetics*", Toxicological Science, 2018, 163(1): 152-169.

The CTSS will continue to offer the paper of the year award and student/postdoc award in 2020. Please check the SOT website for the detail.

Annual Report

Officers	2018-2019	2019-2020
President:	David R. Woolley	Lisa D. Beilke
Vice President:	Lisa D. Beilke	David Szabo
Vice President-Elect:	David Szabo	Catrin Hasselgren
Secretary:	Sudin Bhattacharya	Joel Cohen
Treasurer:	Mark Gosink	Mark Gosink
Past President	N/A	David R. Woolley
Councilors:	Catrin Hasselgren	Nigel Greene
	Nigel Greene	Minjun Chen
	Minjun Chen	
PDA Representative:	Suzanne Martos	open
GSLC Representative:	Fjodor Melnikov	Linlin Zhao

- 2019 CTSS Reception was held in Baltimore, MD during the SOT Annual Meeting, with approximately 100 people in attendance. Topics covered at the meeting included thank yous to our sponsors, membership, finances, endowment fund, symposia ideas, CTSS webinar series and awards/presentations.
  - CTSS Proposed Webinar Series (details are in the *Upcoming Events* section)
    - Title: Computational Toxicology Methods and Approaches
    - Title: Computational Methods in Next-Generation Risk Assessment of Consumer Products
    - Title: US FDA Experience in the Regulatory Application of (Q)SAR Modeling
    - Title: Big Data & Artificial Intelligence - a new kid on the block in toxicological safety sciences
  - CTSS Endorsed Symposia
    - 11 proposals for various symposia, CE/Informational sessions, and workshops were reviewed and the following were endorsed:
      - SYM-25: Mechanistic Read-Across of Chemical Toxicants Based on Big Data, Artificial Intelligence, and Critical Validations
      - SYM-10: Dealing with Uncertainties in Novel Approach Methods (NAM) – based Safety Testing
  - CTSS mugs were given out to members at the 2019 luncheon

- The CTSS will hold their annual luncheon meeting at the 2020 SOT Annual Meeting in Anaheim, CA.

- **CTSS WEBINAR SERIES 2019-2020:**

  1. An Introduction to in silico Toxicology
  Speakers: Dr. Donna MacMillan, Lhasa & Dr. Glenn Myatt, Leadscope September 20, 2019, 11am-noon EDT (1 hour)

  2. US FDA Experience in the Regulatory Application of (Q)SAR Modeling
  Speakers: Dr. Naomi Kruhlak, FDA CDER
  January 16, 2020, 11am-noon EST (1 hour)

  3. Computational Methods in Next-Generation Risk Assessment of Consumer Products
  Speakers: Dr. Steve Gutsell, Unilever
  April 16, 2020, 11am-noon EDT (1 hour)

  4. Artificial Intelligence in the Design of Safer Medicines – Science or Science Fiction?
  Speakers: Dr. Nigel Greene, AstraZeneca
  June 25, 2020, 11am-noon EDT (1 hour)

  Events information and update:
  http://www.toxicology.org/groups/ss/ctss/events.asp

- **Our new endowment fund - Yves Alarie Scholarship Endowment Fund**

  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.

The fund was established to acknowledge Dr. Yves Alarie, a pioneer and leader in the field of inhalation toxicology who laid the foundation for applying computational approaches to this field. While a classically trained toxicologist, he had the vision in the early 1970s to develop and apply computational toxicology tools for rapid screening of chemicals and to reduce the use of animals. Dr. Alarie has been an active member of SOT and has made many presentations at SOT meetings for over 50 years. At the time the fund was established, he held the position of Professor Emeritus in the Graduate School of Public Health at the University of Pittsburgh, where he held leadership positions, including Full Professor (1975–2002) and Chairman of the Industrial and Environmental Health Sciences Department (1978–1990). Dr. Alarie has made significant contributions to the field of Toxicology, through his research on the sensory irritating properties of airborne chemicals (Respiratory Depression 50% [RD50]) and the development of Quantitative Structure Activity Relationships (QSARs) for such irritants. Dr. Alarie has been a passionate graduate advisor for many Masters, Doctoral, and Post-Doctoral students at the University of Pittsburgh and has mentored the development of many young professors over the years.

Use the **online giving system**
(https://www.toxicology.org/endowment/contribute/EndowmentOnline.asp) or download the **Donation form**
(http://www.toxicology.org/endowment/docs/Endowment_Donor_form.pdf) to make a gift to the Yves Alarie Scholarship Fund.

- **Post your recent work related to computational toxicology:**

  Please contact our student representative Linlin Zhao (lz295@scarletmail.rutgers.edu) to post any new work in future CTSS newsletters.