

Computational Toxicology Specialty Section (CTSS)

Society of Toxicology | 2023-2024 Officer Team

Fall 2023



CTSS Member Highlights

We want to feature our members!

Scientific Accomplishments. Please send information on any of your publications, book chapters, presentations at local/national/international meetings, and any other milestones. Photos and images are welcome.

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?" This series hosts columns (which will be featured in upcoming newsletters) authored by the members of CTSS who would like to share about exciting projects or publications, 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 Councilor [Joel Cohen](#) with your news!

WHAT'S NEW

WEBINAR SERIES WAS A HIT

Offered 6 webinars in 2022-2023

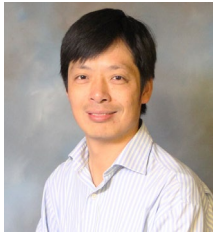










Recordings are available on [CTSS website](#)

MEMBERSHIP IS GROWING

Since 2019, our membership has grown from 164 to **254!**

Diverse membership drawing from: government (~13%), academia (~13%), consulting (~15%), and industry (~37%), among other sectors

2023-2024 Executive Council

<p><u>President</u></p> <p>Minjun Chen, PhD</p> <p>US FDA/NCTR</p>		<p><u>Past President, Councilor</u></p> <p>Nigel Greene, PhD</p> <p>AstraZeneca.</p>	
<p><u>Vice President</u></p> <p>Kevin Cross, PhD</p> <p>Instem</p>		<p><u>Councilor</u></p> <p>Lisa Truong, PhD, MBA</p> <p>Oregon State University</p>	
<p><u>Vice President-Elect</u></p> <p>Fjodor Melnikov, PhD</p> <p>Genentech, Inc.</p>		<p><u>Councilor</u></p> <p>Joel M. Cohen, ScD, DABT</p> <p>Gradient</p>	
<p><u>Secretary</u></p> <p>Holly Mortensen, PhD</p> <p>US EPA</p>		<p><u>Treasurer</u></p> <p>Alessandro Brigo, PhD, ERT, DABT</p> <p>F Hoffmann-La Roche AG</p>	
<p><u>Postdoctoral Representative (term ended September 2023)</u></p> <p>Emily Golden, PhD</p> <p>Johns Hopkins University</p>		<p><u>Postdoctoral Representative</u></p> <p>Heather Ciallella, PhD</p> <p>Cuyahoga County Medical Examiner's Office and Regional Forensic Science Laboratory</p>	
<p><u>Graduate Student Representative</u></p> <p>Elena Chung</p> <p>Rowan University</p>			

CTSS VISIBILITY AT SOT 2023

At the 2023 SOT Annual Meeting in Nashville, TN, CTSS sponsored 7 scientific sessions

SPECIAL THANKS TO

OUR OUTGOING OFFICERS

Catrin Hasselgren | Anne Loccisano |
Adrian Green | Emily Golden

OUR SCIENTIFIC SESSION COMMITTEE

Minjun Chen | Adrian Green | Kevin Cross | David Szabo | Lisa Truong |
Falgun Shah

WELCOME TO OUR NEW EC MEMBERS

Joel Cohen, Holly Mortensen,
Heather Ciallella, and Elena Chung

CTSS MENTORSHIP PROGRAM HAS LAUNCHED

The CTSS mentorship program continues into its second year of supporting young scientists.

Second cohort: 28 mentor/mentee pairs (up from 13 pairs in the first cohort)

The program goal was to generate awareness of the various career plans and provide network opportunities

Able to commit one hour at least four times during the entire program? Interested in participating in the program? Contact

sotctss@gmail.com

More information is available on the [Computational Toxicology Specialty Section](#) website.

President's Letter

As we move beyond the pandemic and transition back to normal life, I sincerely hope that you and your loved ones are staying safe and in good health. The COVID-19 pandemic has underscored the crucial role of science and technology in safeguarding public health. It has disrupted our daily lives, highlighting the urgent need for innovative solutions to address health challenges more effectively. In this context, the interest in computational toxicology continues to surge within SOT. This accentuates not only its promise but also its indispensable role in expediting drug discovery, enhancing our understanding of toxicity, and facilitating the development of safer pharmaceuticals.

The 2023 Annual Meeting in Nashville marked another resounding success. During the event, we hosted our annual reception for members where we presented awards and reviewed the annual report. The Computational Toxicology Specialty Section (CTSS) continued its valuable contributions to the SOT Scientific Program for the meeting. In 2023, we sponsored four symposiums and workshop scientific sessions, along with three educational sessions. These sessions covered a wide array of computational topics, such as artificial intelligence, machine learning, predictive toxicology, big data, New Approach Methods (NAMs), Adverse Outcome Pathways (AOP), and cross-functionality. The increasing interest in computational toxicology is evident from the growing number of endorsement requests we received.

In addition to the SOT program, CTSS continues its sponsorship of a webinar series aimed at showcasing our members' achievements and providing education on computational toxicology. Notably, we recently hosted a seminar titled "ToxAlcology - The Future of Toxicology is AI," featuring Professor Thomas Hartung in August. In September, we also hosted another exciting seminar featuring our top three abstract winners. Topics covered included data fusion for exposome target interaction prediction, predictive toxicity screening of novel odorants, and the prediction of discontinued neurological drugs from off-targets. Additionally, we will be co-sponsoring a seminar with the Drug Discovery Specialty Section on AI GAN models for drug discovery. These webinars were recorded and are available on the [CTSS website](#) as valuable resources. If you have suggestions for future topics or are interested in nominating yourself or someone else as a speaker, please don't hesitate to reach out to us; we are always eager to hear your thoughts and ideas.

CTSS takes pride in recognizing the achievements of our fellow members over the past year and is delighted to offer a variety of awards, all of which can be found on our website. We strongly encourage each of you to consider applying for the Best Publication Award and Best Abstract Awards to highlight your most impactful

NEW PROCESS

UPCOMING AWARDS DEADLINES

DECEMBER 31, 2023

- PAPER OF THE YEAR
- TOP 10 BEST ABSTRACT AWARDS
- YVES ALARIE DIVERSITY AWARD

JANUARY 7, 2024

STUDENT & POSTDOC AWARDS

SUBMIT APPLICATIONS VIA CTSS WEBSITE

JOIN OUR LINKEDIN GROUP

Stay up to date with the latest news and events



Treasurer's Report

- 2023 financial support received from six sponsors
- Provided over \$5,000 in awards in 2022-2023
- After all expenses, the CTSS balance is \$23,998.

research from the past year. For young scientists, we have the Yves Alarie Diversity Award for Trainees and Young Investigators, Elsevier Postdoctoral Awards, and the annual CTSS Student Award.

We deeply appreciate the pivotal role played by our young scientists. In addition to the awards mentioned earlier, we also sponsor a mentorship program, which includes a face-to-face reception at the Annual Meeting. This program is now in its second year, and we are thrilled to see the growing interest among our members and young individuals. Last year, we successfully paired 13 mentors with mentees, and this year, we have already enrolled 28 mentees. However, we currently face a shortage of mentors. I wholeheartedly encourage you to consider contributing to the mentorship of these young minds, as they are the ones who will carry the torch forward. For more information, please visit [our website](#).

We would like to seize this opportunity to express our heartfelt gratitude to our sponsors, including Instem, Lhasa Limited, Genentech, Multicase, Roche, and Elsevier, for their generous contributions over the past year. Without their support, many of our past and upcoming events, activities, and awards would not have been possible. If you or your institute are interested in becoming a sponsor, please visit the [CTSS website](#) for more information.

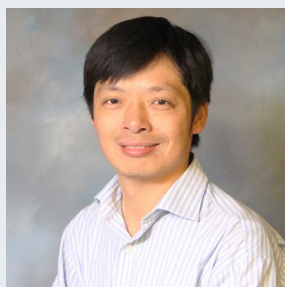
As we approach the time of year when we actively seek nominations for several open positions within the CTSS leadership team, I extend a warm invitation to those of you who are passionate about contributing your expertise, time, and energy to this organization. If you are a member in good standing of CTSS and SOT, please consider joining our outstanding team as a CTSS officer. This year, the open positions include VP-Elect, Treasurer, Councilor, and Postdoc Rep.

Last but certainly not least, I want to take this opportunity to give my earnest gratitude to the dedicated CTSS leadership team. They have worked tirelessly throughout the year to make all these activities and events possible. They are an exceptional team to collaborate with, and I genuinely appreciate the tremendous efforts they've invested in ensuring the success of this specialty section.

I eagerly anticipate meeting everyone in Salt Lake City, UT, at the next Annual Meeting and hope you can attend the CTSS Annual Reception, which is currently being planned for Tuesday evening.

Warm regards,

Minjun Chen



Sponsors



CTSS Yves Alarie Diversity Award

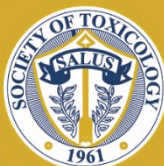
For Trainees & Young
Investigators

**Applications are
being accepted now!
Deadline: December
31, 2023**



This SOT Endowment was established in July 2019 by his students, friends, colleagues, and family. Dr. Alarie, a longtime member of SOT, has made significant contributions to the fields of inhalation toxicology and computational toxicology. During his career as a Professor at the University of Pittsburgh, he advised, trained, encouraged, and supported many students in the field of toxicology.

This award provides \$2,500 to a motivated trainee or young investigator from an under-represented group who is working in the field of computational toxicology and shares Dr. Alarie's passion for science. The award must be used for the professional development of the trainee/young investigator.



SOT | Society of
Toxicology
ENDOWMENT
Investing in the Future ...

HIGHLIGHT: Scientific Accomplishments of Our Membership

Over 500 peer-reviewed papers published by members of CTSS!

- Bajard L.; Adamovsky O.; Audouze K.; Baken K.; Barouki R.; Beltman J.B.; Beronius A.; Bonefeld-Jørgensen E.C.; Cano-Sancho G.; de Baat M.L.; Di Tillio F.; Fernández M.F.; FitzGerald R.E.; Gundacker C.; Hernández A.F.; Hilscherova K.; Karakitsios S.; Kuchovska E.; Long M.; Luijten M.; Majid S.; Marx-Stoelting P.; Mustieles V.; Negi C.K.; Sarigiannis D.; Scholz S.; Sovadinova I.; Stierum R.; Tanabe S.; Tollefsen K.E.; van den Brand A.D.; Vogs C.; Wielsøe M.; Wittwehr C.; Blaha L. (2023) "Application of AOPs to assist regulatory assessment of chemical risks – Case studies, needs and recommendations" *Environmental Research* doi: 10.1016/j.envres.2022.114650 <https://pubmed.ncbi.nlm.nih.gov/36309218/>
- Borghoff S.J.; Cohen S.S.; Jiang X.; Lea I.A.; Klaren W.D.; Chappell G.A.; Britt J.K.; Rivera B.N.; Choski N.Y.; Wikoff D.S. (2023) "Updated systematic assessment of human, animal and mechanistic evidence demonstrates lack of human carcinogenicity with consumption of aspartame" *Food and Chemical Toxicology* doi: 10.1016/j.fct.2022.113549 <https://pubmed.ncbi.nlm.nih.gov/36493943/>
- Cayley, A.N.; Foster, R.S.; Brigo, A.; Muster, W.; Musso, A.; Kenyon, M.O.; Parris, P.; White, A.T.; Cohen-Ohana, M.; Nudelman, R.; Glowienke, S. (2023) "Assessing the utility of common arguments used in expert review of in silico predictions as part of ICH M7 assessments." *Regulatory Toxicology and Pharmacology* doi:10.1016/j.yrtph.2023.105490 <https://pubmed.ncbi.nlm.nih.gov/37659712/>
- Chien H.-T.; Prior H.; Andrews L.; van Aerts L.; Cauvin A.; Clarke D.O.; Datta K.; Dempster M.; Dybdal N.; Freebern W.; de Haan L.; Herzyk D.; Hey A.; Kissner T.; Kronenberg S.; Leach M.W.; Lee D.; Schutte K.; Sewell F.; Trouba K.; Ulrich P.; Weir L.; van Meer P. (2023) "Re-evaluating the need for chronic toxicity studies with therapeutic monoclonal antibodies, using a weight of evidence approach" *Regulatory Toxicology and Pharmacology* doi: 10.1016/j.yrtph.2022.105329 <https://pubmed.ncbi.nlm.nih.gov/36592682/>
- Chou W.-C.; Lin Z. (2023) "Machine learning and artificial intelligence in physiologically based pharmacokinetic modelling" *Toxicological sciences* doi: 10.1093/toxsci/kfac101 <https://pubmed.ncbi.nlm.nih.gov/36156156/>
- Cross, K.P.; Myatt, G.J.; Johnson C. (2023) "Use of in silico protocols to evaluate drug safety, in QSAR in Safety Evaluation and Risk Assessment", H. Hong ed., Academic Press. ISBN: 9780443153402
- Cross, KP; Myatt, G.J. (2023) "The Use of Machine Learning to Support Drug Safety Prediction, in Machine Learning and Deep Learning" *Computational Toxicology*, H. Hong ed., Springer. <https://link.springer.com/book/10.1007/978-3-031-20730-3>
- Cross, K.P.; DeMarini, D.M. (2023) "Analysis of Chemical Structures and Mutations Detected by *Salmonella* TA98 and TA100 " Mutations Research/Fundamental and Molecular Mechanisms of Mutagenesis doi:10.1016/j.mrfmmm.2023.111838 <https://pubmed.ncbi.nlm.nih.gov/37804576/>
- Dawson D.E.; Lau C.; Pradeep P.; Sayre R.R.; Judson R.S.; Tornero-Velez R.; Wambaugh J.F. (2023) "A Machine Learning Model to Estimate Toxicokinetic Half-Lives of Per- and Polyfluoro-Alkyl Substances (PFAS) in Multiple Species" *Toxics* doi: 10.3390/toxics11020098 <https://pubmed.ncbi.nlm.nih.gov/36850973/>

- Faramarzi S, Kim M.T., Volpe D.A., Cross K.P., Chakravarti S and Stavitskaya L (2022), Development of QSAR models to predict blood-brain barrier permeability. *Front. Pharmacol.* 13:1040838.
<https://doi.org/10.3389/fphar.2022.1040838>
- Natsch A.; Kleinstreuer N.; Asturiol D. (2023) "Reduced specificity for the local lymph node assay for lipophilic chemicals: Implications for the validation of new approach methods for skin sensitization" *Regulatory Toxicology and Pharmacology* doi: 10.1016/j.yrtph.2023.105333 <https://pubmed.ncbi.nlm.nih.gov/36608925/>
- Liu A.; Seal S.; Yang H.; Bender A. (2023) "Using chemical and biological data to predict drug toxicity" *SLAS Discovery* doi: 10.1016/j.slasd.2022.12.003 <https://pubmed.ncbi.nlm.nih.gov/36639032/>
- Pognan F.; Beilmann M.; Boonen H.C.M.; Czich A.; Dear G.; Hewitt P.; Mow T.; Oinonen T.; Roth A.; Steger-Hartmann T.; Valentin J.-P.; Van Goethem F.; Weaver R.J.; Newham P. (2023) "The evolving role of investigative toxicology in the pharmaceutical industry" *Nature Reviews Drug Discovery* doi: 10.1038/s41573-022-00633-x
<https://pubmed.ncbi.nlm.nih.gov/36781957/>
- Seal S.; Carreras-Puigvert J.; Trapotsi M.-A.; Yang H.; Spjuth O.; Bender A. (2022) "Integrating cell morphology with gene expression and chemical structure to aid mitochondrial toxicity detection" *Communications Biology* doi: 10.1038/s42003-022-03763-5 <https://pubmed.ncbi.nlm.nih.gov/35999457/>
- Stucki A.O.; Barton-Maclaren T.S.; Bhuller Y.; Henriquez J.E.; Henry T.R.; Hirn C.; Miller-Holt J.; Nagy E.G.; Perron M.M.; Ratzlaff D.E.; Stedeford T.J.; Clippinger A.J. (2022), "Use of new approach methodologies (NAMs) to meet regulatory requirements for the assessment of industrial chemicals and pesticides for effects on human health" *Frontiers in Toxicology* doi: 10.3389/ftox.2022.964553 <https://pubmed.ncbi.nlm.nih.gov/36119357/>
- Trejo-Martin, A., et. al., (2022), "Use of the Bacterial Reverse Mutation Assay to Predict Carcinogenicity of N-Nitrosamines", *Regulatory Toxicology and Pharmacology* 135, <https://doi.org/10.1016/j.yrtph.2022.105248>.
- van der Zalm A.J.; Barroso J.; Browne P.; Casey W.; Gordon J.; Henry T.R.; Kleinstreuer N.C.; Lowit A.B.; Perron M.; Clippinger A.J. (2022), "A framework for establishing scientific confidence in new approach methodologies" *Archives of Toxicology* 96(11). Doi: 10.1007/s00204-022-03365-4
<https://pubmed.ncbi.nlm.nih.gov/35987941/>
- Wohlleben W.; Mehling A.; Landsiedel R. (2023) "Lessons Learned from the Grouping of Chemicals to Assess Risks to Human Health" *Angewandte Chemie - International Edition* doi: 10.1002/anie.202210651
<https://onlinelibrary.wiley.com/doi/full/10.1002/anie.202210651>
- Zwickl, C.M.; Graham, J.; Jolly, R.; Bassan, A.; Ahlberg, E.; Amberg, A.; Anger, L.T.; Barton-Maclaren, T.; Beilke, L.; Bellion, P.; Brigo, A.; Cronin, M.T.D.; Custer, L.; Devlin, A.; Burleigh-Flayers, H.; Fish, T.; Glover, K.; Glowienke, S.; Gromek, K.; Jones, D.; Karmaus, A.; Kemper, R.; Piparo, E.L.; Madia, F.; Martin, M.; Masuda-Herrera, M.; McAtee, B.; Mestre, J.; Milchak, L.; Moudgal, C.; Mumtaz, M.; Muster, W.; Neilson, L.; Patlewicz, G.; Paulino, A.; Roncaglioni, A.; Ruiz, P.; Suarez, D.; Szabo, D.T.; Valentin, J.P.; Vardakou, I.; Woolley, D.; Myatt, G. (2022) "Principles and Procedures for Assessment of Acute Toxicity Incorporating In Silico Methods." *Comput Toxicol* doi: 10.1016/j.comtox.2022.100237
<https://pubmed.ncbi.nlm.nih.gov/36818760/>



2023 CTSS Awards

CTSS PAPER OF THE YEAR AWARD



**FJODOR MELNIKOV
(GENENTECH INC.)**

Toward Quantitative Models in Safety Assessment: A Case Study to Show Impact of Dose-Response Inference on hERG Inhibition Models." *Int J Mol Sci.* 2022, 24: 635.

CTSS STUDENT TRAVEL AWARD

**TONG WANG
(ROWAN UNIVERSITY)**

**ABSTRACT 3094 POSTER BOARD - P199:
INTEGRATING STRUCTURE ANNOTATION AND
MACHINE LEARNING APPROACHES TO
DEVELOP GRAPHENE TOXICITY MODELS**



CTSS STUDENT TRAVEL AWARD

**ELENA CHUNG
(ROWAN UNIVERSITY)**

**ABSTRACT 3083 POSTER BOARD - P188:
INTEGRATING HIGH-THROUGHPUT
TOXICOKINETICS DATA AND KNOWLEDGE-
BASED DEEP NEURAL NETWORK (K-DNN)
METHODOLOGY TO ADVANCE A
COMPUTATIONAL ADVERSE OUTCOME
PATHWAY FRAMEWORK FOR ASSESSING
HEPATOTOXICITY**



2023 Yves Alarie Diversity Award Winner



Chao Ji, PhD, EIT

Indiana University Bloomington

SOT Abstract 3210 Poster Board -
P327: Integrating Bayesian Statistical
Models to Mitigate Environmental
Health Risks

2023 CTSS Top 3 Poster Awards

Kai Wang, University of Michigan

Isaac Mohar, Gradient

Mohan Rao, Neurocrine

2023 CTSS Abstract Awards

Louis Groff, US EPA

Mark Cronin, Liverpool John Moores
University

Brianna Paisley, Eli Lilly

Martyn Chilton, Lhasa Limited

Kimberly To, Inotiv

Anders Wallqvist, US Army

Liang Xu, US FDA/NCTR

Reception at 2023 SOT Meeting

CTSS hosted another successful luncheon and awards ceremony on March 22nd, 2023. A warm welcome to our newly elected leaders to ensure the future success of CTSS. We express our appreciation to the past CTSS officers for their contributions.

Reviewing our 2022-2023 year, we recognized the successful events and remarkable accomplishments of CTSS and its members. We hosted and co-hosted educational webinars and will continue to hold webinars in the future. Our webinars are recorded and posted on the [CTSS website](#). CTSS proudly continued a mentorship program, connecting 28 mentees and mentors, more than double the number from the prior year. In addition, CTSS would like to thank everyone who joined us in our SOT 2023 science symposia, as well as those who submitted session proposals for SOT 2024. Learn more from our CTSS committee members by contacting us at sotctss@gmail.com.

We always invite volunteers who would like to contribute to the vibrancy of CTSS and its committees. Please submit your nominations to [Minjun Chen](#). Follow CTSS on LinkedIn to develop your network and get up to date on the latest CTSS news, events, and highlights.

May this year bring new goals, new achievements, and new inspirations! Once again, CTSS thanks all our sponsors, speakers, scientific session committee members, and volunteer organizers for their continued commitment. We eagerly look forward to seeing you at the 2024 SOT Annual Meeting in Salt Lake City. CTSS will be hosting an evening reception on Tuesday, March 12th.



**63RD ANNUAL MEETING
& ToxExpo • March 10–14, 2024
SALT LAKE CITY, UTAH**

Endowment Fund Donors

Yves Alarie

Yves Alarie in memory of Gunnar D. Nielsen

Yves Alarie in memory of Micheline Alarie

Rosalind C. Anderson in honor of Yves Alarie

Craig S. Barrow

The BP Foundation on behalf of Daniel Goon

Dennis Bridge

Heather D. Burleigh-Flayer

Daniel J. Caldwell in honor of Yves Alarie

Mary and Bill Conner

Alison C. P. Elder in honor of Yves Alarie

Francis Michael Esposito

Jeffrey S. Ferguson in honor of Dr. Yves Alarie

Thomas Glaab in honor of Yves Alarie

GlaxoSmithKline Foundation on behalf of Jeffrey Ferguson

Daniel Goon in honor of Dr. Yves Alarie

Barbara J. Henry in honor of Yves Alarie

Andree Hertz in memory of Micheline Alarie

Marianne Hirkulich in honor of Yves Alarie

Johnson and Johnson Matching Gifts Program on behalf of Daniel J. Caldwell

Laurel E. Kane in honor of Yves Alarie

Lawrence Keller

Amy L. Kennedy in honor of Dr. Yves Alarie

Dolores E. Malek in honor of Yves Alarie

Francine Matijak

Razzak Memon

Sunanda and Koustubh Oka in honor of Dr. Yves Alarie

Kate Okabayashi in honor of Yves Alarie

PPG Foundation

PPG Foundation on behalf of Heather Burleigh-Flayer

Gurcharan (Ghona) K. Sangha in honor of Dr. Yves Alarie

Anonymous donor in honor of Yves Alarie

Michelle and Ken Schaper

Maryanne F. Stock in honor of Yves Alarie

Dietrich A. Weyel

King Lit Wong in honor of Yves Alarie

Annual Report 2022-2023

2022 Membership Total: 234

Key Outcomes in 2022–2023:

A. Members of the CTSS committee were involved in the development of several proposals for the 2023 Annual Meeting to further the uptake and awareness of computational toxicology at SOT. In total, CTSS sponsored nine sessions, of which, seven were accepted for inclusion in the 2023 Scientific Program.

B. The mentorship program was reviewed, and feedback from participants was favorable. The program was renewed in 2023. An SOT-sponsored reception was held at the Annual Meeting in Nashville for mentors and mentees to meet in person.

Activities:

A. 2023 SOT Annual Meeting Activities (e.g., courses, scientific sessions, or virtual receptions):

Tools Supporting Open Chemical Evaluations

(Continuing Education Course)

Date: Sunday, March 19, 2023

Chair: David Reig

Checking In on Adverse Outcome Pathways: Evolving Development, Evaluation and Application

(Continuing Education Course)

Date: Sunday, March 19, 2023

Chair: Kristie Sullivan

Making the Most of Your Data: How to Build Machine-Learning Models for Toxicology

(Continuing Education Course)

Date: Sunday, March 19, 2023

Chair: Nigel Greene

AI Buzz or Bliss: Case Studies for Successful Applications of Artificial Intelligence in Predictive Toxicology

(Symposium)

Date: Monday, March 20, 2023

Chair: Falgun Shah

Understanding the Concept of Similarity and Its Applications to Toxicological Research and Risk Assessment

(Workshop)

Date: Monday, March 20, 2023

Chair: Kamel Mansouri

OK, Google, How Do I Science? Roles and Responsibilities of Developers and Users in Computational Toxicology

(Roundtable)

Date: Monday March 20, 2023

Chair: Lyle Burgoon

Computational Toxicology I

(Poster Session, 38 Poster Presentations)

Date: Monday, March 20, 2023

Chair: Agnes Karmaus, Zhoumeng Lin

Computational Visualization Tools for Communicating Large, Complex Data

(Workshop)

Date: Tuesday, March 21, 2023

Chair: Matthew Martin

Computational Toxicology II

(Poster Session, 37 Poster Presentations)

Date: Tuesday, March 21, 2023

Chair: Qiran Chen, Colleen McLoughlin

Computational Toxicology Specialty Section Meeting

Date and Time: Wednesday, March 22, 2023 from 12:00 Noon-1:30 PM PT

Summary: The CTSS luncheon included a brief welcome by the CTSS President, highlights were announced regarding the 2021-2022 events and accomplishments, recognition to sponsors and supporters, and was followed by an award ceremony.

B. Top 3 Poster Awards

Kai Wang from University of Michigan, Ann Arbor, MI for the SOT Poster, "Data Fusion by Matrix Completion for Exposome Target Interaction Prediction" (Abstract No. 3077)

Isaac Mohar from Gradient for the poster, "Framework for *In Silico* Toxicity Screening of Novel Odorants" (Abstract No. 3698)

Mohan Rao from Neurocrine for the poster, "Computational Analysis of Discontinued Neurological Drugs without Defined Primary Target Pharmacology" (Abstract No. 3059)

C. Other Educational Activities Conducted

Overview of Bioinformatic Sequence Analysis and Applications in Toxicology

(Co-sponsored with SOT Arab Toxicologists Association Special Interest Group)

Date: December 6, 2022

Duration: 1 hour

Speaker 1: Dr. Ahmed Abdelmoneim, BVMS, MSc, PhD

Speaker 2: Dr. Tamer Mansour, MBChB, MS, PhD

Artificial Intelligence Enables Structural Toxicity Testing for Endpoint and Multiple-Timepoint Assays

(Co-sponsored with AACT)

Date: September 16, 2022

Duration: 1 hour 10 min

Speaker: Alexandre Ribeiro, PhD

Integrating mass spectrometry non-targeted analysis and computational toxicology to characterize chemicals

(Co-sponsored with MDCPSS)

Date: June 30, 2022

Duration: 1 hour

Speaker 1: Antony Williams

Speaker 2: Ron Brown

2022 Computational Toxicology Specialty Section Award Winner Presentations

Date: June 29, 2022

Duration: 1 hour

Speaker 1: Heather Ciallella

Speaker 2: Xuelian Jia

Speaker 3: Adrian Green

Speaker 4: Linlin Zhao