Computational Toxicology Specialty Section (CTSS)

Society of Toxicology | 2025-2026

Winter 2026

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.

"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 the 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 Adrian Green with your news!

WHAT'S NEW

WEBINAR SERIES

Offered 6 webinars in 2024-2025

Recordings are available on CTSS website

Webinars in Q1/Q2 2026:

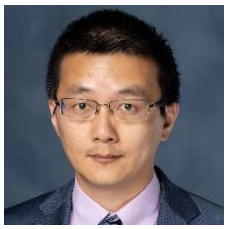
1) Virtual Control Groups & Virtual Omics Controls: Reducing Animal Use Without Sacrificing Rigor (Jan 21st)
2) Single-Cell Bioinformatics in Toxicology (May 20th)

MEMBERSHIP IS GROWING

Since 2019, our membership has grown from 164 to **265!**

Diverse membership drawing from government (~12%), academia (~20%), consulting (~18%), and industry (~35%), among other sectors

2025-2026 Executive Council

President **Fjodor Melnikov, PhD** Genentech, Inc.		**Past President, Councilor** **Kevin Cross, PhD** Instem	
Vice President **Alessandro Brigo, PhD, ERT, DABT** F Hoffmann-La Roche AG		**Councilor** **Adrian Green, PhD** Sciome, LLC.	
Vice President-Elect **Zhoumeng Lin, PhD** University of Florida		**Councilor** **Lennart Anger, PhD, ERT** Genentech, Inc.	
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Postdoctoral Representative **David Umbaugh, PhD** Genentech, Inc.		**Graduate Student Representative** **Pei-Yu Wu** University of Florida	

CTSS VISIBILITY AT SOT 2025

At the 2025 SOT Annual Meeting in Orlando, FL, CTSS offered 8 scientific and educational sessions

SPECIAL THANKS TO

OUR OUTGOING OFFICERS

Minjun Chen | Elena Chung | Heather Ciallella | Joel M. Cohen | Holly Mortensen

OUR SCIENTIFIC SESSION COMMITTEE

Fjodor Melnikov | Kevin Cross | Alessandro Brigo | Adrian Green | Zhoumeng Lin | Lennart Anger | Cody Robarts | Lisa Truong | David Umbaugh | Pei-Yu Wu

WELCOME TO NEW AND RETURNING EC MEMBERS

Zhoumeng Lin | David Umbaugh | Pei-Yu Wu | Lennart Anger | Cody Robarts

MENTORSHIP

SOT now provides centralized mentorship opportunities through the Mentor Match program on ToXchange. CTSS is working with other specialty sections to provide more tailored mentoring events during annual meetings.

Please look out for related invitations before the 2026 Annual Meeting in San Diego.

President's Letter

As has been the tradition in recent years, 2025 has once again presented a unique combination of opportunities and challenges. With the COVID era and it's travel restrictions and social limitations now far in the rearview mirror, new travel restrictions for government employees and budgetary shifts created unexpected barriers for the growing industry–academia–government partnerships that are vital to the annual SOT meeting. Yet, despite these hurdles, the 2025 SOT Annual Meeting in Orlando was a resounding success—providing an engaging forum for in-person scientific exchange and reinvigorating our cross-disciplinary community. During the meeting, CTSS hosted our annual reception and member gathering, celebrated this year's award recipients, and reviewed the accomplishments summarized in our annual report. We were delighted by the strong participation and the rich discussions across all reception and mentoring activities.

Looking at opportunities, advances in artificial intelligence (AI) technologies and large language model (LLM) applications have placed computational research in an excellent position to take on an even greater role within toxicology. The rapid growth of AI continues to propel computational toxicology forward at an extraordinary pace, as seen by the rising number of publications at the intersection of toxicology and data science. AI-driven tools are becoming central to how toxicologists compile, analyze, and interpret data. Large language models, initially developed for natural language processing, are now widely used to extract information from literature, curate and aggregate datasets, and learn from large-scale omics profiles. With sequencing costs continuing to decline, the volume of omics data is expanding rapidly and fueling the development of transcriptomics-based foundational models for biology and toxicology. Computational toxicologists are capitalizing on these opportunities by assembling large datasets from sources that were previously more difficult to consistently analyze and interpret at scale, such as preclinical animal studies. These and other data streams are being integrated to develop increasingly sophisticated computational models for toxicity prediction. Importantly, AI tools are also making it easier for scientists to begin coding, exploring, and learning from large datasets. We hope that in the coming years more toxicologists will be inspired to bring computational approaches to augment their work, even if only for parts of it.

While AI applications in toxicology still have substantial room to grow, interest in computational toxicology continues to rise, as reflected in the increasing number of scientific sessions focused on computational methods and seeking CTSS endorsement. This year, CTSS endorsed 15 proposed sessions, 6 of which were accepted for inclusion in the 2026 scientific program. The accepted sessions were weighted toward workshops and continuing education courses—highlighting the growing

AWARDS DEADLINES

DECEMBER 1
- YVES ALARIE DIVERSITY AWARD

DECEMBER 31
- PAPER OF THE YEAR
- TOP 10 BEST ABSTRACT AWARDS - STUDENT

- ELSEVIER POSTDOC AWARDS

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Stay up to date with the latest news and events

SCAN ME

Treasurer's Report

2025 financial support received from six sponsors

Provided over $4,000 in awards in 2024-2025

After all expenses, the CTSS balance is $26,441

appetite among SOT members to learn computational methods. These included:

- Toxic Insights Unlocked: Leveraging Machine Learning and Advanced Image Analysis to Transform the Science of Toxicology
- Toward AI-Enabled Digital Biomarkers: Improving the Predictivity of Toxicology in the 21st Century
- This Is Real: How AI Can Actually Be Used in Hazard and Risk Assessments
- AI in Toxicology: Navigating Promise, Pitfalls, and Practical Implementation

In addition to the SOT program, CTSS—often in collaboration with other specialty sections—continues to expand its webinar series, which remains one of our most valued outreach and educational initiatives. Recent and upcoming webinars include:

- Virtual Control Groups & Virtual Omics Controls: Reducing Animal Use Without Sacrificing Rigor
- Expanded Decision Tree: US FDA's Food Chemical Toxicity
- Data Interoperability in Toxicology: A Framework for Source-to-Outcome Assessment
- The Annual Computational Toxicology Paper of the Year and CTSS Award Winners Presentations

Recordings of most webinars will continue to be available through the SOT ToXchange website. We welcome suggestions for future topics and speaker nominations—your ideas directly shape the direction of our scientific programming.

CTSS is proud to recognize the achievements of our members through a series of awards designed to highlight excellence in the field and support students and early-career scientists. We strongly encourage our early-career members to apply for the Yves Alarie Diversity Award, the Elsevier Postdoctoral Award, and the Student Award. We also hope to see recently published work and SOT abstracts submitted for the Paper of the Year and Best Abstract awards. This year, we continued our tradition of featuring awardees in dedicated webinars that showcase their scientific contributions.

Most importantly, CTSS and the leadership team remain immensely grateful to our generous sponsors. Their continued support enables our participation in mentoring events at the annual SOT meeting, offsets the costs of the CTSS reception, supports our webinar series, and funds the

Sponsors

awards that define our mission. If you or your institution is interested in becoming a sponsor, please visit the CTSS website for additional information.

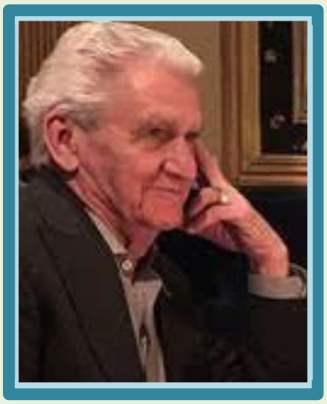
Finally, I want to express my heartfelt gratitude to the dedicated CTSS leadership team, whose commitment and tireless efforts—including reviewing award nominations and session proposals, organizing in-person events and webinars, and continually engaging with the computational toxicology community—make all our accomplishments possible. I look forward to reconnecting with all of you at the 2026 Annual Meeting in San Diego and to another exciting year of growth in AI-enabled, data-rich toxicology.

Best regards,

Fjodor (Yodi) Melnikov

CTSS Yves Alarie Diversity Award

For Trainees & Young Investigators



This SOT Scholarship Fund Endowment was established in July 2019 by his students, friends, colleagues, and family. Dr. Alarie, a longtime member of the 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.

HIGHLIGHT: Selected Scientific Accomplishments of Our Membership

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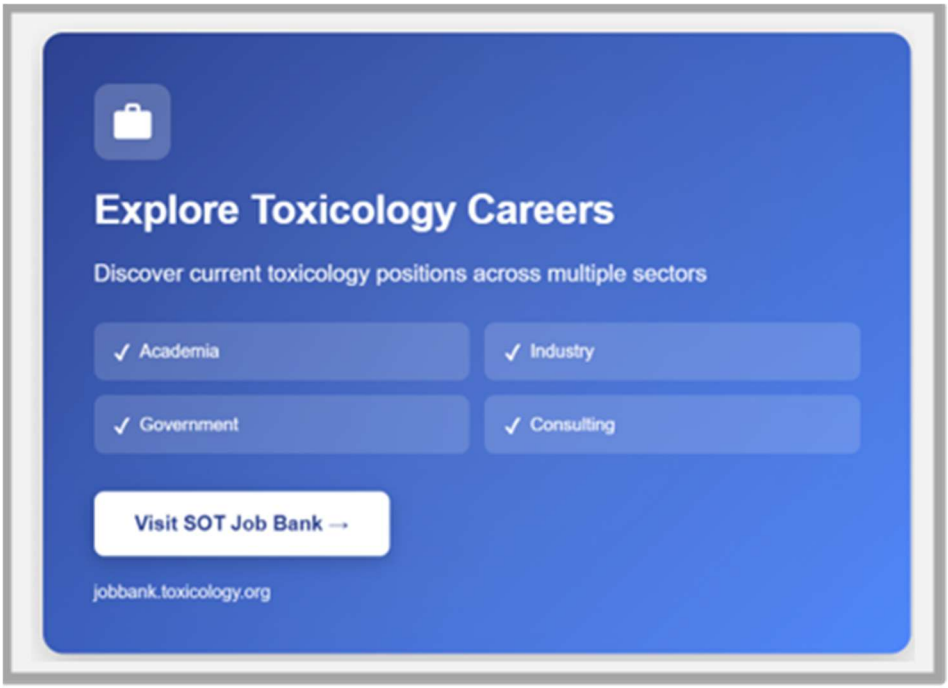

2025 CTSS Awards

CTSS PAPER OF THE YEAR AWARD

AYOOLUWA OLUBANIWA (NATIONAL CENTER FOR TOXICOLOGICAL RESEARCH, US FDA)

Drug interaction with UDP-Glucuronosyltransferase (UGT) enzymes is a predictor of drug-induced liver injury | PMID: 39024247

CTSS ELSEVIER POSTDOCTORAL TRAVEL AWARD

XUELIAN JIA (TULANE UNIVERSITY)

ABSTRACT 4077 POSTER BOARD – PK576: APPLICATION OF MACHINE LEARNING AND MECHANISTIC MODELING TO PREDICT INTRAVENOUS PHARMACOKINETIC PROFILES IN HUMANS

CTSS STUDENT TRAVEL AWARD

DIANA GARNICA ACEVEDO (THE GEORGE WASHINGTON UNIVERSITY)

ABSTRACT 4010 POSTER BOARD – PJ504: *IN SILICO* MODEL FOR BINARY READILY-BIODEGRADABLE PREDICTION IN SMALL MOLECULES

2025 Yves Alarie Diversity Award Winner

Jessie Chappel

The University of North Carolina at Chapel Hill

SOT Abstract 3406 Poster Board – J537: Interpretable Machine Learning to Understand Wildfire Toxicity: Bridging Chemicals, -Omics, and Health Outcomes via Symbolic Regression with Novel Feature Scoring

2025 CTSS Top 3 Poster Awards

Zhicheng Zhang (University of Florida)

Elena Chung (Rowan University & Tulane University)

Paul Kruse (US EPA)

2025 CTSS Abstract Awards

Ayooluwa Olubamiwa, US FDA

Oyemwenosa Avenbuan, UNC-Chapel Hill

Ricardo Scheufen Tieghi, UNC Chapel Hill & NIEHS

Nada Daood, Rowan University

Chi-Yun Chen, University of Florida

Han-Hsuan Tsai, Texas A&M University

Reception at 2025 SOT Meeting

Many thanks to all those who attended the CTSS annual reception at SOT this past year in rainy Orlando Florida. During the event, we hosted our annual reception/meeting for members, where we presented our newly elected slate of officers, awards for outstanding research and reviewed the annual report. The Computational Toxicology Specialty Section (CTSS) continued its valuable contributions to the SOT scientific program for the meeting and remains financially on solid ground.

In 2025, 3 Continuing Education courses and 5 symposia from CTSS were included in the program. Symposia topics ranged from, "Recent Advances in Exposure Predictions", "Leveraging AI and Genomics in Gene and Therapies", "Challenges of NAM-Based Toxicokinetic Assessment", "Principles of *In Silico* Methodologies for Chemical Safety Assessment", to "Unlocking the Power of Read-Across for Safety Assessment".

CTSS proudly recognizes the achievements of our fellow members of the past year and continues offering a variety of awards to highlight their accomplishments. In 2025 these included: Ayooluwa Olubaniwa PhD, US FDA/NCTR CTSS Paper of the Year, "Drug interaction with UDP-Glucuronosyltransferase (UGT) enzymes is a predictor of drug-induced liver injury, *Hepatology* 2024", Elena Chung, Rowan and Tulane University, CTSS Paper of the Year runner-up, Xuelian Jia PhD, Tulane University, CTSS Elsevier Postdoctoral Award, and Dian Garnica Acevedo, George Washington University, CTSS Student Travel Award. The year's best CTSS poster awards included: Zhicheng Zhang PhD, University of Florida (1st), Elena Chung, Rowan and Tulane University (2nd) and Paul Kruse PhD, US EPA (3rd).

We look forward to seeing you all at SOT in San Diego, CA, for our annual CTSS meeting and reception on **Wednesday, March 25th, 2026, 6:00-7:30 PM at the Marriott Marquis Marina, San Diego Ballroom C.**

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

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PPG Foundation on behalf of Heather Burleigh-Flayer

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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 2024-2025

2025 Membership Total: 239

Key Outcomes in 2024 – 2025:

A. Of a total of 21 CTSS sponsored/co-sponsored sessions, 8 were accepted for inclusion in the 2025 SOT annual meeting scientific program.

B. Visibility of the specialty section has been greatly elevated due to the interest in Artificial Intelligence and rapid progress in computational toxicology.

Activities:

A. 2025 SOT Annual Meeting Activities (e.g., courses, scientific sessions, or virtual receptions):

Computational Toxicology Specialty Section Reception
Date and Time: Monday, March 17th, 2025, from 6 pm – 7:30 pm ET
Summary: The CTSS reception included a brief welcome by the CTSS President, highlights of the 2024-2025 events and accomplishments, recognition to sponsors and supporters were described and an award ceremony followed. The event attracted about 100 participants.

B. 2025 Awards Information:

CTSS Paper of the Year Award
"Drug interaction with UDP-Glucuronosyltransferase (UGT) enzymes is a predictor of drug-induced liver injury" *Hepatology*. 2025, 81(5),1512-1521. PMID: 39024247
Ayooluwa Olubamiwa (US FDA)

CTSS Paper of the Year Award (runner-up)
"Hybrid non-animal modeling: A mechanistic approach to predict chemical hepatotoxicity, *Journal of Hazardous Materials*. 2024, 471,134297. PMID: 38677119
Elena Chung (Rowan University & Tulane University)

The Yves Alarie Diversity Award - Jessie Chappel (The University of North Carolina at Chapel Hill)

CTSS Elsevier Postdoc Award – Xuelian Jia (Tulane University)

CTSS Elsevier Student Award – Diana Garnica Acevedo (The George Washington University)

Best SOT-CTSS Abstract Awards - Zhicheng Zhang (University of Florida); Elena Chung (Rowan University & Tulane University); Paul Kruse (US EPA)

Top 10 SOT-CTSS abstract awards - Ayooluwa Olubamiwa (US FDA), Oyemwenosa Avenbuan (UNC-Chapel Hill), Ricardo Scheufen Tieghi (UNC-Chapel Hill & NIEHS), Nada Daood (Rowan University), Chi-Yun Chen (University of Florida), Han-Hsuan Tsai (Texas A&M University)

C. Other Educational Activities Conducted

Expanded Decision Tree: US FDA's Food Chemical Toxicity Screening Tool (Co-sponsored with FSSS)
Date: December 4th, 2025
Duration: 1 hour
Speaker: Szabina Stice (US FDA)

2025 Computational Toxicology Paper of the Year and CTSS Award Winners Presentations
Date: December 3rd, 2025
Duration: 1.5 hours
Speaker 1: Ayooluwa Olubamiwa (PharmQuest LLC)
Speaker 2: Xuelian Jia (Rowan University)
Speaker 3: Diana P. Garnica Acevedo (George Washington University)
Speaker 4: Jessie Chappel (University of North Carolina at Chapel Hill)

Data Interoperability in Toxicology: Supporting Source-to-Outcome Assessment (Co-sponsored with RASS)
Date: November 12th, 2025
Duration: 1.5 hours
Speaker: David E. Hines (RTI International)

Don't Miss the Mark! How Secondary Pharmacology Can Affect Pharmaceutical Drug Development
(Co-sponsored with DDTSS and with British Toxicology Society Discovery Toxicology Specialty Section)
Date: December 5th, 2024
Duration: 1 hour
Speaker 1: Jean-Pierre Valentin (UCB Biopharma SRL)
Speaker 2: Friedemann Schmidt (Sanofi)

Opportunities to Harness AI and Machine Learning in Drug Discovery Toxicology (Co-sponsored with RSESS)
Date: December 3rd, 2024
Duration: 1 hour
Speaker: Yodi Melnikov (Genentech)

CTSS 2024 Award Winner Presentations
Date: November 14th, 2024
Duration: 1.5 hours
Speaker 1: Lauren Koval (University of North Carolina at Chapel Hill)
Speaker 2: Paul Kruse (US EPA)
Speaker 3: Nada Daood (Rowan University)