

Computational Toxicology Specialty Section (CTSS)

Society of Toxicology | 2021-2022

Fall 2022



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 milestone. Photos and images are 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?" 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 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

WHAT'S NEW

WEBINAR SERIES WAS A HIT

Offered 9 webinars in 2021-2022

Recordings are available on CTSS website

MEMBERSHIP IS GROWING

Since 2019, we our membership has grown from 164 to **238!**

~56% members are employed in government or consulting







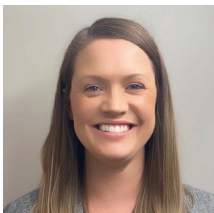
CTSS VISIBILITY AT SOT 2022

At the 2022 SOT National Meeting in San Diego, CA, CTSS offered 6 scientific symposiums

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 [Anne Loccisano](#) with your news!

2022-2023 Executive Council

<p><u>President</u></p> <p>Nigel Greene, Ph.D</p> <p>AstraZeneca</p> 	<p><u>Past President, Councilor</u></p> <p>Catrin Hasselgren, Ph.D</p> <p>Genentech, Inc.</p> 
<p><u>Vice President</u></p> <p>Minjun Chen, Ph.D</p> <p>USFDA/NCTR</p> 	<p><u>Councilor</u></p> <p>Lisa Truong, Ph.D, MBA</p> <p>Oregon State University</p> 
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<p><u>Secretary</u></p> <p>Fjodor Melnikov, Ph.D</p> <p>Genentech, Inc.</p> 	<p><u>Postdoctoral Representative</u></p> <p>Adrian Green, Ph.D</p> <p>NC State University</p> 
<p><u>Treasurer</u></p> <p>Alessandro Brigo</p> 	<p><u>Graduate Student Representative</u></p> <p>Emily Golden, M.F.S.</p> <p>Johns Hopkins University</p> 

SPECIAL THANKS TO..

OUR OUTGOING OFFICERS

David Szabo | Patricia Ruiz

OUR SCIENTIFIC SESSION COMMITTEE

Minjun Chen | Emily Golden | Adrian Green | Patricia Ruiz | Sandrine Chebekoue | Nigel Greene

ELENA CHUNG FOR HER HELP ON THE NEWSLETTER!

WELCOME TO NEW EC MEMBERS

Lisa Truong and Alessandro Brigo

CTSS MENTORSHIP PROGRAM HAS LAUNCHED

To support young scientists, the CTSS mentorship program was launched.

First cohort: 13 mentors:mentees

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

Able to commit 1 hour at least 4 times during the entire program? Interested in participating in the program?

Contact sotctss@gmail.com

UPCOMING AWARDS DEADLINES

DECEMBER 31, 2022

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

JAN 7, 2023

STUDENT & POST DOC AWARDS

SUBMIT APPLICATIONS TO:
SOTCTSSAWARDS@GMAIL.COM

Presidents Letter



As we emerge from the pandemic and begin to return back to normal life, things continue to be filled with uncertainty. Planning remains challenging and a requires everyone to be adaptable to an environment where in-person and virtual participation in meetings and events have become commonplace. I hope you are continuing to stay safe and healthy as we continue to deal with the aftermath of a global pandemic.

The 2022 Annual Meeting held in San Diego was a highly successful event and marked the return to "in person" sessions and talks. The CTSS sponsored six scientific sessions at the March meeting and we also hosted an annual reception for our members where we presented awards and went through the annual report. We are in the midst of preparations for next year's annual meeting in Nashville and we are hopeful that we will be able to meet many more of you in person. The tentative scientific program for the meeting is very exciting! There will be at least four symposia and workshops that are sponsored by the CTSS in 2023 along with two Continuing Education courses. These will cover a wide array of topics such as case studies of the successful applications of Artificial Intelligence in predictive toxicology, understanding the concept of similarity and its applications to risk assessment, the roles and responsibilities of developers and users in Computational Toxicology and data visualization to enhance scientific communication. The interest in computational toxicology continues to increase and this can be seen by the number of requests for endorsement we received again this year.

Increased interest in computational approaches is also apparent by the continued interest on the CTSS Webinar series. This webinar series is dedicated to highlighting our members' accomplishments as well as education around Computational Toxicology. We sponsored another six webinars, either alone or with other specialty sections. Our most recent webinar, was co-sponsored with the American Association of Chinese Toxicologists (AACT) and featured Dr Alexandre Ribeiro speaking on "Artificial Intelligence Enables Structural Toxicity Testing for Endpoint and Multiple-Timepoint Assays". The majority of our past webinars are recorded sessions and are available on the SOT website and are a great resource. If you have suggestions for future topics or are interested in nominating yourself or someone else as a speaker, please don't hesitate in reaching out to us, we are always interested in hearing your thoughts and ideas.

I would like to take the opportunity to thank our sponsors (Elsevier, US FDA, Genentech Inc, Instem, SOT) for their generous contributions this past year; without them, many of our past and upcoming events/activities/awards would not be possible. The CTSS has a number of awards that are listed on our website for SOT Annual Meeting attendees, as well as the *The Yves Alarie Diversity Award for Trainees and Young Investigator Endowment Fund* which is only available to apply by our membership. Elsevier will again be sponsoring a *Postdoctoral Award* as well as a *CTSS Student Award*, both of which are awarded annually.

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GROUP

Stay up to date with the
latest news and events



Treasurer's Report

- 2022 financial support received from FDA & Elsevier
- Provided over \$7,000 in awards in 2021-2022
- After all expenses, the CTSS balance is \$24,471

Sponsors



SOT



It is also the time of year when we are soliciting nominations for several open positions to the CTSS leadership team. This year, open positions include VP-Elect, Councilor, Secretary, Postdoctoral Representative, and Graduate Student Representative. 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. On that note, I would also like to thank my fellow CTSS Officers, who I am incredibly grateful for and happy to work with. This is a wonderful group of people who are full of ideas and energy.

We are all experiencing uncertainty and unpredictability right now. Despite this, I remain hopeful that I will see many of you in Nashville and I look forward to meeting you!

Warm regards,

Nigel Greene

Sponsors



[CTSS Yves Alarie Diversity Award](#)

For Trainees & Young Investigator

Applications are being accepted now!

Deadline: December 31, 2022



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 that 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: Scientific Accomplishments of Our Membership in the Journal of Toxicological Sciences

Over 420 peer-reviewed papers published by members of CTSS!

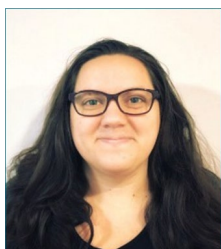
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2022 CTSS Awards

CTSS PAPER OF THE YEAR AWARD



HEATHER CIALLELLA
(RUTGERS UNIVERSITY)

"REVEALING ADVERSE OUTCOME PATHWAYS FROM PUBLIC HIGH-THROUGHPUT SCREENING DATA TO EVALUATE NEW TOXICANTS BY A KNOWLEDGE-BASED DEEP NEURAL NETWORK APPROACH." *ENVIRON. SCI. TECHNOL.* 2021, 55, 10875–10887

2022 Yves Alarie Diversity Award Winner



Linlin Zhao, PhD

Genentech, Inc.

SOT Abstract 4026: Poster Board - P724: Application of a Matrix Factorization Method for Kinase Data to Support Safety Profiling.

2022 CTSS Abstract Awards

Alexandre Borrel from Silent Spring Institute (Abstract no. 4671)

M. T. Smith from UC Berkeley (Abstract no. 4031)

Mark D. Nelms from RTI International (Abstract no. 4673)

Candice Johnson from Instem (Abstract no. 4658)

Rachael E. Tennant from Lhasa Limited (Abstract no. 4646)

Martyn L. Chilton from Lhasa Limited (Abstract no. 4015)

A. Tandon from Sciome LLC (Abstract no. 4680)

CTSS STUDENT TRAVEL AWARD

XUELIAN JIA
(RUTGERS CENTER FOR COMPUTATIONAL AND INTEGRATIVE BIOLOGY)

ABSTRACT NO 4662: POSTER BOARD - P708: MECHANISM-DRIVEN MODELING OF DRUG-INDUCED LIVER INJURY USING STRUCTURAL ALERTS AND AN OXIDATIVE STRESS SCREENING ASSAY"



CTSS POSTDOCTORAL AWARD

DR. ADRIAN GREEN
(NORTH CAROLINA STATE UNIVERSITY)

ABSTRACT 1146: LEVERAGING HIGH-THROUGHPUT SCREENING DATA, DEEP NEURAL NETWORKS, AND CONDITIONAL GENERATIVE ADVERSARIAL NETWORKS TO ADVANCE PREDICTIVE TOXICOLOGY



Reception at 2022 SOT Meeting

CTSS geared up for another round of excitement with our “Veritas Ex Machina”-themed reception/luncheon and awards ceremony on March 30th, 2022. 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 2021-2022 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 announced a mentorship program connecting 13 mentees and mentors. In addition, CTSS would like to thank everyone who joined us in our SOT 2022 science symposia. Please send your proposals for symposia for the 2023 SOT meeting and turn your idea into an on-site conference. Learn more from our CTSS committee members 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 Nigel Greene. 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, and volunteer organizers for their continued commitment. We eagerly look forward to seeing you at the SOT annual meeting 2023 in Nashville, TN.



**62nd Annual Meeting
& ToxExpo • Nashville, TN
March 19–23, 2023**

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

Annual Report 2021-2022

2021 Membership Total: 274

Key Outcomes in 2021 – 2022:

- A. Members of the CTSS committee submitted three (all accepted) proposals for the 2022 Annual Meeting to further the uptake and awareness of Computational Toxicology at SOT. In total CTSS sponsored 6 sessions in the 2022 scientific program.
- B. Instituted a new Mentorship program to support the development of junior scientists

Activities:

- A. **2022 SOT Annual Meeting Activities** (e.g., courses, scientific sessions, or virtual receptions):
Computational Toxicology Specialty Section Virtual Meeting
Date and Time: Wednesday, March 30, 2022 from 12 pm – 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. 2022 Awards Information:

CTSS Paper of the Year Award

“Revealing Adverse Outcome Pathways from Public High-Throughput Screening Data to Evaluate New Toxicants by a Knowledge-Based Deep Neural Network Approach”, Environ. Sci. Technol. 2021, 55, 10875–10887 by Heather L. Ciallella, Daniel P. Russo, Lauren M. Aleksunes, Fabian A. Grimm, and Hao Zhu

The Yves Alarie Diversity Award - Linlin Zhao, PhD (received whilst at Genentech Inc., currently at Amazon)

CTSS Student Award - Xuelian Jia (Rutgers Center for Computational and Integrative Biology)

CTSS Postdoctoral Travel Award - Adrian Green, PhD (North Carolina State University)

Best SOT-CTSS Abstract Awards - Yun Hao (University of Pennsylvania), Natalie Mesens (Janssen Pharmaceuticals), Mohan Rao (Janssen Pharmaceuticals)

Top 10 SOT-CTSS abstract awards - Alexandre Borrel (Silent Spring Institute), M. T. Smith (UC Berkeley), Mark D. Nelms (RTI International), Candice Johnson (Instem), Rachael E. Tennant (Lhasa Limited), Martyn L. Chilton (Lhasa Limited), A. Tandon (Sciome LLC)

C. Other Educational Activities Conducted

Co-sponsored Webinar with MDCPSS - Practical Application of Computational Models to Predict Release Kinetics and Toxicity of Compounds Released from Medical Devices

Date: June 2, 2021

Duration: 1.5 hours

Speaker 1: Rob Brown, Risk Science Consortium, LLC

Speaker 2: David Saylor, US Food and Drug Administration

Attendees: 189

CTSS Webinar - Application of in vitro and in silico data in predictive modeling of human organ toxicity

Date: June 23, 2021

Duration: 1 hour

Speaker: Ruili Huang, PhD, National Center for Advancing Translational Sciences, NIH

Attendees: 162

CTSS Webinar - Moving from One-Size-Fits-All to Fit-for Purpose TTC Values

Date: August 5, 2021

Duration: 1 hour

Speaker: Ron Brown, PhD, Risk Sciences Consortium

Attendees: 685

Joint CSS & CTSS Webinar - Integrating Computational Tools into Carcinogenicity Assessments

Date: December 14, 2021

Duration: 1 hour

Speakers: Mark Cronin, PhD, Liverpool John Moores University, Liverpool, UK & Federica Madia, PhD, Joint Research Centre, Ispra, Italy

Attendees: 240

Joint CSS & CTSS Webinar - Integrating Computational Tools into Carcinogenicity Assessments II

Date: February 15, 2022

Duration: 1 hour

Speakers: Emilio Benfenati, PhD, Istituto Negri, Milan, Italy & Raymond Tice, PhD, RTice Consulting, Hillsborough, NC, USA

Attendees: 248

CTSS Webinar - The Predictive Toxicogenomics Space (PTGS) Modeling Tool Captures Diverse Cellular and Organ Toxicity Mechanisms and Serves for *In Vitro* Model-Driven Prediction of Drug-Induced Liver Injury

Date: April 27, 2022

Duration: 1 hour

Speaker: Roland Grafström, Professor & Pekka Kohonen, PhD, Karolinska Institutet, Stockholm, Sweden

Attendees: 177