

Computational Toxicology Specialty Section

ANNUAL REPORT: 2020-2021

May 1, 2020 to April 30, 2021

I. Officers/Committees:

<u>Officers</u>	<u>2020-2021</u>	<u>2021-2022</u>
President:	David T. Szabo	Catrin Hasselgren
Vice President:	Catrin Hasselgren	Nigel Greene
Vice President-Elect:	Nigel Greene	Minjun Chen
Secretary:	Joel M. Cohen	Fjodor Melnikov
Treasurer:	Kevin Cross	Kevin Cross
Past President	Lisa D. Beilke	David T. Szabo
Councilors:	Lisa D. Beilke	David T. Szabo
	Minjun Chen	Patricia Ruiz
	Patricia Ruiz	Anne Elizabeth Loccisano

PDA Representative: David A. Edmondson Adrian James Green

Grad Student Representative: Emily Golden Emily Golden

Committees: Executive committee (chair: David Szabo), awards committee (chair: Minjun Chen), nominations committee (chair: David Szabo), Website Liaison (Joel Cohen), Outreach Liaison (chair: Nigel Greene), membership outreach (chair: Catrin Hasselgren)

II. 2020 Membership total: 245

III. Key Outcomes in 2020-2021:

- A. Members of the CTSS committee submitted two (both accepted) proposals for the 2021 Annual Meeting to further the uptake and awareness of Computational Toxicology at SOT
- B. Instated a new awards category for the top 10 SOT-CTSS abstracts

IV. Activities:

- A. **2021 SOT Virtual Annual Meeting Activities** (e.g., courses, scientific sessions, or virtual receptions):

Computational Toxicology Specialty Section Virtual Meeting

Date and Time: Tuesday, March 16, 2021 from 8:30 am – 9:30 am ET

Summary: The CTSS virtual event included a brief welcome from the CTSS President, highlights were announced regarding the 2020-2021 events and accomplishments, recognition to sponsors and supporters, and an award ceremony followed by awardee presentations.

- B. **2021 Awards Information:**

CTSS Paper of the Year Award

“A cross-industry collaboration to assess if acute oral toxicity (Q)SAR models are fit-for-purpose for GHS classification and labelling,” *Regulatory Toxicology and Pharmacology*, 2020 By Joel Bercu, Melisa J. Masuda-Herrera, Alejandra Trejo-Martin, Catrin Hasselgren,

Jean Lord, Jessica Graham, Matthew Schmitz, Lawrence Milchak, Colin Owens, Surya Hari Lal, Richard Marchese Robinson, Sarah Whalley, Phillip Bellion, Anna Vuorinen, Kamila Gromek, William A. Hawkins, Iris Van de Gevel, Kathleen Vriens, Raymond Kemper, Russell Naven, Pierre Ferrer, Glenn J. Myatt*

The Yves Alarie Diversity Award- Shagun Krishna, PhD (National Toxicology Program/NIEHS)

CTSS Student Award- Alexander Blanchette (Texas A&M University)

CTSS Postdoctoral Travel Award- Kiara Fairman (the FDA's National Center for Toxicology Research)

Best SOT-CTSS Abstract Awards - David Filipovic (Michigan State University), Suguna Dev Sakkiah and Ting Li (the FDA's National Center for Toxicological Research)

Top 10 SOT-CTSS abstract awards- Farida Akhtari and Shagun Krishna (NIEHS), Cathy Lester (Procter & Gamble), Robert Pullen III (Sanofi), David Rouquie (Bayer SAS), Elizabeth Shipp (Corteva Agriscience), Leihong Wu (the FDA's National Center for Toxicological Research)

C. Other Educational Activities Conducted (e.g., webinars, in person meetings):

CTSS Award Winners: Government and Academic initiatives with AOPs, Endocrine Predictions, and Deep Neural Network

Date: December 2, 2020

Duration: 1 hour

Speaker 1 : Sara Vliet, PhD, ORISE Postdoctoral Fellow, EPA

Speaker 2: Mary Schleiff, Doctor of Philosophy Candidate, University of Arkansas for Medical Sciences

Speaker 3: Dong Wang, Senior Statistician, FDA

Attendees: 113

Co-sponsored Webinar with CTPVSS – Advanced Tissue Imaging and AI Data Analysis: The Opportunities and Challenge for Application in Supporting Drug Discovery

Date: April 7, 2021

Duration: 1 hour

Speaker 1: Richard Goodwin, PhD, Head of Imaging & AI Imaging & Data Analytics, Clinical Pharmacology & Safety Sciences, AstraZeneca R&D

Speaker 2: Matthew Jacobsen, PhD, DipACVP, Director of Pathology Regulatory Safety Centre of Excellence, clinical Pharmacology & Safety Sciences, AstraZeneca R&D

Attendees: 112

Co-sponsored Webinar with IVAMSS - State of the Science: QSAR Modeling of Skin Sensitization

Date: March 19, 2021

Duration: 75 minutes

Speaker 1: Vinicius Alves, PhD, Researcher Assistant Professor, Division of Chemical Biology and Medicinal Chemistry, University of North Carolina at Chapel Hill

Speaker 2: Emily Golden, MS Graduate Student, Center for Alternatives to Animal Testing, Johns Hopkins University

Speaker 3: Glenn Myatt, PhD, CEO, Leadscope, Inc.

Attendees: 361

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

D. Communication Activities:

1. Newsletter publication frequency: Winter 2020
2. New or Significant Announcements/blogs:
3. Highlight of Website enhancements: The CTSS website has been maintained and updated as needed.
4. CTSS member participation on the SOT Specialty Section Collaboration and Communication Group (SS-CCG)

E. Mentoring activities: N/A

V. Feedback and Ideas:

A. In what ways is your group fostering and maintaining an inclusive environment?

CTSS requests for volunteers from our membership to participate on our many committees. This opportunity is open to all members.

B. How might SOT better support your group's activities (perhaps something the Society should be doing that we currently do not do, or do not do effectively, that would be of importance/benefit to the members of your component group?):

Note: If funding is listed, please provide detail on the membership need that the funding would support.

N/A

C. What is one thing that the Society is currently doing that impacts your component group that should be changed (e.g., stopped, modified, etc.)?

Mentoring sessions for students and postdocs are a universal goal for all Specialty Sections and request the Specialty Section Collaboration and Communication (SS-CCG) coordinate best practices for different session types. Further, recommend they work with SOT to establish a Specialty Section wide event at SOT Annual Meeting.

D. **What changes do your component group anticipate making in the way in which it operates in the coming year?**

N/A