



American Society for Cellular and Computational Toxicology

8th Annual Meeting of the ASCCT

*Computational Toxicology:
Peeking into the Clouds while Keeping our Feet on Solid Ground*

September 24-26, 2019

Montgomery Ballroom
Gaithersburg Doubletree by Hilton
Gaithersburg, Md

Tuesday, September 24

7:00: Pre-meeting mentoring event
Gaithersburg Doubletree Hotel Bar

Wednesday, September 25

8:30: Registration & Coffee

9:00: Welcome and Introduction
Erin Hill, President, ASCCT

9:10: Protocols describing the combined use of experimental data and *in silico* results for the assessment of toxicological endpoints
Glenn Myatt, Leadscope

10:00: Session I

1. Whole transcriptome extrapolation and mechanism of action analysis: Tunicamycin case study
Ruchir Shah, Sciome
2. Good decisions require good data: Creating curated and structured resources for toxicology
Shannon Bell, ILS, Inc

BREAK and Poster Viewing

3. Characterizing the GPCR-ome target profile of emerging chemical agents with PRESTO-TANGO
Tyler DP Goralski, Combat Capabilities Development Command Chemical Biological Center
4. Multi-label model for toxicity prediction
Xiu Huan Yap, Wright State University

5. Quantitative in vitro to in vivo extrapolation using microphysiological systems: Towards predictive toxicological assessment for inhaled reduced risk products
Aditya Reddy Kolli, Phillip Morris International

12:00: Lunch [Doubletree Restaurant]

1:00: Poster session

2:00: Session II

1. Tiered-testing strategies and the use of new approach methodologies Under the amended Toxic Substances Control Act
William Irwin, US EPA
2. ReCAAP: Carcinogenicity case study waivers for food-use pesticide registration
Gina Hilton, PETA International Science Consortium
3. Beyond the barrier: A readily-adoptable in vitro model for exploring the effects of inhaled toxicants beyond the epithelium
Samantha C. Faber, University of North Carolina Chapel Hill
4. Development of a high-throughput iPSC-derived Liver-on-a-Chip for hepatotoxicity detection
Ryan M Reddinger, Mimetas BV

3:30: BREAK and Poster Viewing

4:00: International Collaboration

- 4:00 – 4:15: A new society for alternatives in India
Mohammad A. Akbarsha, General Secretary, Society for Alternatives to Animal Experiments– India
- 4:15 – 4:30: Establishment of the Asian Consortium for Three Rs supported by ASCCT
Hajime Kojima, JSAAE
- 4:30 – 4:45: 2020 congresses: ESTIV2020 and WC11
Mathieu Vinken, ESTIV President
- 4:45 – 4:55: The International Conference on QSARs (QSAR2020)
Grace Patlewicz, US EPA, Conference chair

5:00: Business Meeting

- Elections, finances, other business
- Cooperation with other societies

5:30: Awards Ceremony & Poster Reception

Thursday, September 26

8:30: Coffee & Networking

9:00: The march toward big data in toxicology: Striking a balance between machine learning and mechanistic modeling
Nicole Kleinstreuer, NICEATM

9:50: Session III

1. Toxicological mechanistic inference: Generating mechanistic explanations for adverse outcomes
Ignacio Tripodi, University of Colorado, Boulder
2. An integrated approach to testing and assessment of chemical mixtures in the environment: The advent of Adverse Outcome Pathway footprinting
Jason C. Lambert, US EPA
3. The GARD platform: Cutting-edge technology using genomics and machine learning to test for various toxicological endpoints
Joshua Schmidt, Senzagen, Inc.

10:50: BREAK

11:00: Computational Tools Showcase

Presenter	Affiliation	Tool
Ignacio J. Tripodi	University of Colorado, Boulder	DAStk: Differential ATAC-seq toolkit
Kamel Mansouri	Integrated Laboratory Systems, Inc.	OPERA QSAR models
Barry Hardy	Edelweiss Connect	SaferSkin
David Filipovic	Michigan State University	PyPK for PBPK modeling
Tom Luechtefeld	Insilica	Sysrev.com
Nancy Baker	Environmental Protection Agency	Abstract Sifter
Adam Lee	DuPont	Chemical Awareness Toolkit
Shannon Bell	ILS/NICEATM	Integrated Chemical Environment (ICE)
Maggie Coombs	Lhasa Limited	Multiple
T.J. Bozada	ToxTrack	Chemchart Enterprise

12:00: Panel Discussion: Comp Tox: Data and methodology quality and transparency

Moderator:

David Allen, Integrated Laboratory Systems, Inc.

Panelists:

Nicole Kleinstreuer, NICEATM

Glen Myatt, Leadscope, Inc.

Thomas Hartung, Johns Hopkins University/CAAT

Kristie Sullivan, PCRM

David Filipovic, MSU

1:00: Meeting Ends

POST-MEETING HANDS-ON TRAINING IN COMPUTATIONAL METHODS

Offered by the PCRM

Separate registration requested

1:00 PM - 5:30 PM

Gaithersburg Doubletree by Hilton

The training will feature short summaries of key tool features followed by rotating demos with opportunities to try out the models and/or hands-on exercises. Agenda and registration for this session can be found at www.ascctox.org/meetings. Lunch will be served.

Thank you to the meeting sponsors

