11th Annual Meeting of the American Society for Cellular and Computational Toxicology

Shifting the Paradigm to Next-Generation (Quantitative) Risk Assessment

Sheraton Chapel Hill Chapel Hill, NC October 19-21, 2022



American Society for Cellular and Computational Toxicology

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New for 2022: Full program and all abstracts can be accessed *via* Oxford Abstracts

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About the American Society for Cellular and Computational Toxicology

The American Society for Cellular and Computational Toxicology (ASCCT) is a scientific society dedicated to the promotion of toxicology testing and research that reduces and replaces the use of animals.

Toxicology testing is currently undergoing a paradigm shift from a primarily observational, whole animal-based science to a predictive, mode-of-action-focused discipline. This shift has been spurred by factors as diverse as concern for the animals used in tests, logistical difficulties in assessing growing inventories of substances, and a better understanding of the interaction between chemistry and human biology at the molecular level.

The National Academies, the nation's premier scientific advisory body, recommended in 2007 nothing short of a complete overhaul in the way chemicals, pharmaceuticals, and pollutants are routinely assessed for potential hazardous effects in its report Toxicity Testing in the 21st Century: A Vision and a Strategy. Since the publication of this report, momentum has begun to build, bringing together a diverse set of organizations and scientific disciplines. The Physicians Committee for Responsible Medicine and the Institute for In Vitro Sciences formed the ASCCT in 2010 to harness this momentum and foster cooperation and dialog among North American scientists, regulators, and nongovernmental organizations from the pharmaceutical, chemical, pesticide, and consumer product sectors.

MISSION

The Society aims to provide an organized forum for discussion of cellular (in vitro) and computational toxicology approaches especially as replacements for animal-based toxicology methods. Through its meetings and activities, the Society will facilitate the development, acceptance, and routine use of cellular and computational methods through open dialog between industry, academic, advocacy, and regulatory scientists. The Society strives to include the participation of young scientists to promote their contributions to the field.

GOALS

- Facilitate the development, acceptance, and routine use of cellular and computational methods.
- Increase the routine application and use of computational and in vitro methods for prioritization, classification, and risk assessment purpose
- Foster open dialog between industry, academic, advocacy, and regulatory scientists throughout North America.
- Include the participation of young scientists to promote their contributions to the field.
- Strengthen cooperation between cosmetic, pharmaceutical, and chemical industry scientists and professionals.



ASCCT 11th Annual Meeting:

Shifting the Paradigm to Next-Generation (Quantitative) Risk Assessment

October 19-21, 2022 Chapel Hill, N.C.

President's Message

Dear colleagues,

On behalf of the American Society for Cellular and Computational Toxicology (ASCCT) and the Annual Meeting Organizing Committee it is my distinct honor to welcome you to our 11th Annual Meeting.

The ASCCT is a growing scientific society that provides a forum for the discussion and promotion of cellular and computational toxicology approaches, especially as replacements for in vivo toxicology methods. By fostering cooperation and dialog among individuals from the pharmaceutical, chemical, pesticide, and consumer product sectors and those working in academia, government, or nongovernmental organizations, the ASCCT offers a unique opportunity to openly discuss how these methods can advance the science of toxicology and contribute to protection of human health.

Toxicology is the science of poisons: a scientific discipline at the cross-roads of biology, chemistry, pharmacology, and medicine, focused on the study of the adverse effects of chemical substances on living organisms with an ultimate goal and purpose to protect human -and ecological- health. As our understanding of the interactions between xenobiotics and biology deepens and the technological frontiers of in vitro and computational methods advances, the science of toxicology is undergoing a transformation from an observational and descriptive science using in vivo approaches to an in vitro and in silico discipline.

The main tenet of toxicology is that the dose makes the poison (Paracelsus, 1538) – and thus, to protect human and ecological health from adverse effects of chemicals, we must limit exposures. To achieve this goal, toxicological data needs to be operationalized via the risk assessment process. In other words, for any given agent, the body of evidence available must be integrated into a framework to convert that wealth of information into a reference value – a daily oral dose or air / water concentration – that is expected to protect individuals (or ecosystems) exposed at or below that value. However, the risk assessment process has relied upon in vivo data since its inception, and we are now faced with the challenging task of finding scientifically robust and meaningful ways to use the totality of data available, and the best available data, of which an ever-growing fraction is computational or cellular-based in nature.

As we are entering this new scientific era and as these data streams continue to mature, we need to successfully integrate them into risk assessment. This is why this year's meeting is focused on fostering discussion on how we can harness the full potential of the advancements in cellular and computational toxicology to improve and strengthen chemical risk assessment. The collegial atmosphere of our Annual Meeting creates the perfect forum for this task with a setting that is conducive to dialog, idea sharing, and the exchange of information and perspectives. Together, we can help facilitate the development, acceptance, and routine use of cellular and computational methods for prioritization, classification, and ultimately risk assessment.

Therefore, we have gathered leaders in the field and look forward to your participation to the vibrant and lively scientific sessions on ecotoxicology, developmental neurotoxicity, and next generation risk assessment, a CE course on weight of evidence and risk assessment, flash presentations and poster sessions, our Awards Ceremony, as well as a mentor mixer and reception. We look forward to hearing from you as we work together to shift the paradigm to next-generation (quantitative) risk assessment.

Sincerely,



Marie C. Fortin, ASCCT President

WEDNESDAY, OCTOBER 19th, 2022

12:00-12:45	Arrival, Registration	
12:45-1:00	Welcome Marie Fortin, ASCCT President	
1:00-2:30	Next Generation Risk Assessment Dr. Marie Fortin, Dr. Laura Langan Oral Presentations	
	1:00-1:30 [OR-01] Next Generation Risk Assessment – Accelerating the Paradigm Shift Gavin Maxwell Unilever Safety & Environmental Assurance Centre, Bedford, United Kingdom	
	1:30-1:50 [OR-02] Feasibility of Achieving a Modern Paradigm for Agrochemical Carcinogenicity Assessment <u>Gina Hilton</u> ¹ , Raffaella Corvi ² , Mirjam Luijten ³ , Jyotigna Mehta ⁴ , Douglas Wolf ⁵ ¹ PETA Science Consortium International e.V., Stuttgart, Germany. ² European Commission, Joint Research Centre (JRC), Ispra, Italy. ³ National Institute for Public Health and the Environment (RIVM), Centre for Health Protection, Bilthoven, Netherlands. ⁴ ADAMA Agricultural Solutions Ltd, Reading, United Kingdom. ⁵ Syngenta Crop Protection LLC, Greensboro, NC, USA	
	1:50-2:10 [OR-03] Identification of Changes in Biological Activities and BioMAP® Toxicity Signatures Following Treatment of BioMAP Platform Human Cell-based Disease Models with Per- and Polyfluoroalkyl Substances Jennifer I. Drake¹, Sheryl P. Denker¹, Katie Paul-Friedman², Keith A. Houck², Sharlene Velichko¹,³, Antal Berenyi¹, Ellen L. Berg¹,⁴, Diane Werth¹ ¹Eurofins Discovery, St. Charles, MO, USA. ²Center for Computational Toxicology and Exposure, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC, USA. ³Natera, Austin, TX, USA. ⁴InSitro, South San Francisco, CA, USA	
	2:10-2:30 [OR-04] Profiling Mechanisms That Drive Acute Oral Toxicity in Mammals and Its Prediction via Machine Learning Sanjeeva Wijeyesakere, Dan Wilson, Tyler Auernhammer, Amanda Parks, Sue Marty The Dow Chemical Company, Midland, MI, USA	
2:30-3:30	Ecotoxicology Dr. Enrica Bianchi Oral Presentations	
	2:30-3:00 [OR-05] Next Generation Ecotoxicity Testing Dan Villeneuve Environmental Protection Agency, Duluth, USA	
	3:00-3:20 [OR-06] Expanding High-Throughput Chemical Hazard Evaluation to Ecotoxicology-Relevant Species With a Rainbow Trout Gill Cell Line Felix Harris ^{1,2} , Johanna Nyffeler ^{1,3} , Christopher Schaupp ^{4,3} , Steven Lasee ^{4,3} , Clinton Willis ¹ , John Nichols ⁴ , Brett Blackwell ⁴ , Kevin Flynn ⁴ , Dan Villeneuve ⁴ , Joshua Harrill ¹ 1US EPA CCTE, RTP, NC, USA. ² ORAU, Oak Ridge, TN, USA. ³ ORISE, Oak Ridge, TN, USA. ⁴ US EPA CCTE, Duluth, MN, USA	

WEDNESDAY, OCTOBER 19th, 2022

3:30-4:30	Flash Poster Session Dr. David Allen, Ms. Kristie Sullivan Flash Posters
4:30-6:00	Poster Session I and Reception Poster Board Posters should be attended by presenters at the minimum between 4:45 pm - 5:30 pm.
6:00-6:30	Mentor Mixer, Reception Continued Please indicate if you'd like to participate as a mentor or mentee when you register. All are welcome to attend reception; additional activities will be offered for mentors and mentees.

THURSDAY, OCTOBER 20th, 2022

8:00-8:30	Coffee/Poster Viewing
	Poster Boards
8:30-10:30	Developmental Neurotoxicity Ms. Erin Hill, Dr. Sairam Jabba Oral Presentations
	8:30-9:00 [OR-07] The DNT in Vitro Battery on the Road to Regulation Ellen Fritsche
	IUF - Leibniz Research Institute of Environmental Medicine, Düsseldorf, Germany
	9:00-9:30 [OR-08] Application of DNT NAMs Data in Regulatory Scenarios Tim Shafer
	Environmental Protection Agency, Research Triangle Park, USA
	9:30-9:50 [OR-09] Neural Rosette ArraysTM for Quantitative High-Throughput Screening of Human Developmental Neurotoxicity Randolph Ashton ^{1,2,3} , Gavin Knight ^{2,3} , Nikolai Fedorchak ^{2,3} , Brady Lundin ^{2,3} , Rebecca Willett ^{1,4}
	¹ Neurosetta LLC, Madison, WI, USA. ² University of Wisconsin-Madison, Madison, WI, USA. ³ Wisconsin Institute for Discovery, Madison, WI, USA. ⁴ University of Chicago, Chicago, IL, USA
	9:50-10:10 [OR-10] Increasing the Dimensionality of Rapid Behavioral Screening in Planarians Danielle Ireland ¹ , Alexander Lehner ¹ , Ellen Adams ¹ , Luca Cerbin ¹ , Ameet Soni ¹ , Eva-Maria Collins ^{1,2} ¹ Swarthmore College, Swarthmore, PA, USA. ² Center of Excellence in Environmental Toxicology, University of Pennsylvania, Philadelphia, PA, USA
	10:10-10:30 [OR-11] In Vitro Developmental Neurotoxicity (DNT) Dosing Vehicles Nominally Impact Growth, Viability, and Phenotypic Profile of Human Neural Progenitor Cells Megan Culbreth, Kelly Carstens, Joshua Harrill CCTE, ORD, USEPA, Durham, NC, USA

THURSDAY, OCTOBER 20th, 2022

10:30-11:00	Break
11:00-1:00	Human Data for WoE Toxicology Dr. Stephen Edwards Oral Presentations 11:00-11:30 [OR-12] Characterizing Human Exposure to Contaminant Mixtures: New Sampling Tools to Support Exposome Research Heather Stapleton Duke University, Durham, USA 11:30-12:00 [OR-13] Utilizing Electronic Health Records to Understand Health Risks of Chemical Exposure Cavin Ward-Caviness Environmental Protection Agency, Research Triangle Park, USA 12:00-12:20 [OR-14] Leveraging Electronic Health Record Data for Environmental Health Research and WoE Toxicology Karamarie Fechol.*2, Stanley Ahalt.*3, Ashok Krishnamurthy!.3-4, Emily Pfaff*3, Lisa Stillwell*1, Hong Yi¹ ¹Renaissance Computing Institute, University of North Carolina at Chapel Hill, North Carolina, USA. ²Copperline Professional Solutions, Pittsboro, North Carolina, USA. ³Department of Computer Science, University of North Carolina at Chapel Hill, North Carolina, USA. *North Carolina Translational and Clinical Sciences Institute, Chapel Hill, North Carolina, USA. *Department of Medicine, University of North Carolina at Chapel Hill, Chapel Hill, North Carolina, USA. 12:20-12:40 [OR-15] Human 3D Liver Spheroids - the Smallest Functional Unit of the Liver as a Pragmatic Tool for Industrial DILI Hazard Identification Armin Wolf, Friederike Wenz, Lola Fäs, Monika Tu, Natalie Zapiorkowska, Bruno Filippi InSphero AG, Schlieren, NA, Switzerland 12:40-1:00 Additional Q&A
1:00-2:30	Lunch + Poster Session II Poster Board Posters should be attended by presenters at a minimum between 1:30 pm - 2:15 pm.
2:30-3:00	Funding and Employment Opportunities Dr. Hao Zhu [OR-16] NIEHS Funding Opportunities for Cellular and Computational Toxicology Methods Development Lingamanaidu Ravichandran Division of Extramural Research and Training, NIEHS, NIH, Research Triangle Park, USA [OR-17] Employment Opportunities at US EPA Office of Pollution Prevention and Toxics Iris Camacho EPA, Washington, DC, USA

THURSDAY, OCTOBER 20th, 2022

3:00-4:00 4:00-5:00	Models supporting Next Gen Risk Assessment Ms. Amy Carpenter, Dr. Ruchir Shah 3:00-3:20 [OR-18] Integrating High-Throughput Toxicokinetics and Concentration-Dependent Toxicity Data Into Adverse Outcome Pathway Models of Hepatotoxicity Daniel Russo ¹ , Lauren Aleksunes ² , Hao Zhu ¹ ¹ Rutgers University, Camden, NJ, USA. ² Rutgers University, Piscataway, NJ, USA 3:20-3:40 [OR-19] OPERA Models to Support Regulatory Needs Kamel Mansouri ¹ , Todd Martin ² , Xiaoqing Chang ³ , Dave Allen ³ , Antony Williams ² , Nicole Kleinstreuer ¹ ¹ NIH/NIEHS/DNTP/NICEATM, RTP, NC, USA. ² CCTE/ORD/EPA, RTP, NC, USA. ³ Inotiv, RTP, NC, USA 3:40-4:00 [OR-20] Integration of Technological Interference into the Interpretation of Curated High-throughput Screening (cHTS) Data Victoria Hull ¹ , Alexandre Borrel ¹ , Agnes Karmaus ¹ , Kim To ¹ , David Allen ¹ , Nicole C. Kleinstreuer ² ¹ Inotiv, Research Triangle Park, NC, USA. ² NIH/NIEHS/DNTP/NICEATM, Research Triangle Park, NC, USA Sponsor Tools Showcase Ms. Jessica Conley, Dr. Jessica Ponder SABEU Dennis Benkmann InSphero Armin Wolf Scitovation Les Recio
5:00-5:30	Break
5:30-6:00	ASCCT Business Meeting Dr. Marie Fortin, Ms. Erin Hill, Ms. Kristie Sullivan Everyone is welcome!
6:00-6:30	Awards Ceremony Ms. Erin Hill, Dr. Sue Leary
6:30-8:30	Reception & Dinner

FRIDAY, OCTOBER 21tst, 2022

8:00-9:30	CE course: Weighing the evidence in safety evaluation and risk assessment: data considerations and the potential for NAM integration.
	Dr. Alysha Simmons
	Speakers:
	Anna Lowit, US Environmental Protection Agency Nikaeta Sadekar, Research Institute for Fragrance Materials
9:30-11:00	Envisioning decision-making with NAMs Dr. Kelly Carstens, Dr. Jack Fowle Oral Presentations
	9:30-10:00 [OR-24] An FDA/CDER Perspective on Nonclinical Testing Strategies Including New Approach Methodologies Paul Brown
	Food and Drug Administration/CDER, College Park, USA
	10:00-10:30 [OR-25] Integration of New Approach Methodologies for Prospective Selection of Chemicals for Additional Study Katie Paul Friedman
	Environmental Protection Agency, Research Triangle Park, USA
	10:30-10:45 [OR-26] Novel Non-Animal Preclinical Safety Testing Strategy for Recombinant Human Monoclonal Antibodies Directed Against Foreign Targets April Naab ¹ , Jeffrey Brown ¹ , Esther Wenzel ² , Stefan Dübel ² , Paul Stickings ³ , Michael Hust ² ¹ PETA Science Consortium International e.V., Stuttgart, Germany. ² Technische Universität Braunschweig, Braunschweig, Germany. ³ National Institute for Biological Standards and Control, Hertfordshire, United Kingdom
	10:45-11:00 [OR-27] Investigating the Impact of Cytochrome P450 Metabolism on Chemical-Mediated Transcription Factor Transactivation Agnes Karmaus ¹ , Amber Daniel ¹ , Victoria Hull ¹ , Emily Reinke ¹ , Alex Medvedev ² , David Allen ¹ , Nicole
	Kleinstreuer ³ , Warren Casey ³ ¹ Inotiv, RTP, NC, USA. ² Attagene, Inc., Morrisville, NC, USA. ³ NIH/NIEHS/DNTP/NICEATM, RTP, NC, USA
11:00-12:30	Building Confidence as a Community: Identifying and Overcoming Barriers to NAM use for Risk Assessment Dr. Shaun McCullough, Dr. Anax Oliveira
	Panelists:
	Annie Jarabek, US EPA Andrew Maier, TERA Gavin Maxwell, Unilever Octavio Presgrave, BRACVAM

ASCCT Awards

Edward Carney Predictive Toxicology Award

Dr. Edward Carney was an active and dedicated member of the ASCCT, and a partner, mentor and friend to many in our fields. His passion and leadership will continue to inspire investigators in *in vitro* and *in silico* toxicology through the Edward Carney Predictive Toxicology Award. This \$500 award is provided to an exemplary presenter at each ASCCT annual meeting.

Previous Ed Carney Predictive Toxicology Awardees:

2021: Dr. Kelly Carstens, US EPA ORISE

2020: Eva Vitucci, University of North Carolina, Chapel Hill

2019: Ignacio Tripodi, University of Colorado, Boulder

2018: Sudin Bhattacharya, Michigan State University

2017: Ellen Garcia, Virginia Tech

2016: Emma Bowers, University of North Carolina, Chapel Hill

2015: Nicole Kleinstreuer, NICEATM

Ray Tice Tox21 Student Award

Dr. Ray Tice, a leader in the development and use of high-throughput test methods and other alternatives, established the Tox21 Student Award. This \$500 award is provided to a graduate student first author of a poster or oral presentation at the ASCCT annual meeting.

Previous Ray Tice Tox21 Student Awardees:

2021: Anouck Thienpont, Vrije Universiteit Brussel

2020: Sherri Bloch, Université de Montréal

2019: Vy Tran, Johns Hopkins University

2018: Dan Russo, Rutgers University

2017: Wenyi Wang, Rutgers University

Suzanne Fitzpatrick Student Travel Award

Dr. Suzanne Fitzpatrick, Senior Science Advisor for Toxicology in FDA's Center for Food Safety and Applied Nutrition, is the principal FDA representative to ICCVAM and to the Tox 21 partnership with EPA, NCATS, and NIEHS. Dr. Fitzpatrick established this award to reimburse travel expenses for a student to present a poster at the 11th Annual Meeting.

ASCCT Poster Awards

Three \$200 awards will be selected from poster presenters who indicated interest at registration.

The William and Eleanor Cave Award



William and Eleanor Cave were devoted officers of The American Anti-Vivisection Society (AAVS) for decades. They recognized the opportunities in developing new technologies and alternative methods to address the problems of animal experimentation. They dedicated resources to fund research, eventually resulting in the establishment of the Alternatives Research & Development Foundation.

The William & Eleanor Cave Award is presented to honor achievements in advancing alternatives to the traditional use of animals in testing, research, or education. The award, presented biennially, is accompanied by an honorarium of \$10,000.

Previous William & Eleanor Cave Award recipients:

- 2020 Suzanne Fitzpatrick, US Food and Drug Administration
- 2018 Robert Kavlock, Kavlock Consulting
- 2016 Raymond Tice, RTice Consulting
- 2014 Frank Gerberick, Procter & Gamble Company
- 2012 Mel Andersen. Hamner Institute for Health Sciences
- 2010 Alternatives to Laboratory Animals (Michael Balls, Editor), FRAME
- 2008 Rodger Curren, Institute for In Vitro Sciences
- 2006 Daniel Smeak, Ohio State University
- 2002 Leon Bruner, Gillette Company
- 2000 John Sheasgreen, MatTek Corporation
- 1998 George Russell, Adelphi University
- 1996 Ruy Tchao, Philadelphia College of Pharmacy & Science

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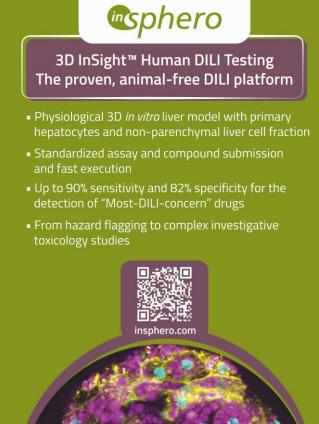
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Poster Session I

PW-01 Developing Metrics to Track Animal Use and the Impact of NAMs Sue Marty1, Amanda Andrus1, <u>Katherine Groff2</u> 1 Dow, Inc., Midland, MI, US. 2 People for the Ethical Treatment of Animals, Norfolk, VA, US

PW-02 Practical Pathways to Address Reagent Source as a Variable in Study Reproducibility

Katherine Groff1, Tilo Weber2 1 PETA Science Consortium International e.V., Stuttgart, Germany. 2 German Animal Welfare Federation, Bonn, Germany

PW-03 Engineering a Computable Epiblast for in silico Gastrulation and Predictive Modeling of Developmental Toxicity with in vitro Data from the ToxCast Stem Cell Assay

Kaitlyn Barham1,2, Richard Spencer3, Thomas Knudsen1

1 U.S. Environmental Protection Agency, Durham, NC, US. 2 Oak Ridge Associated Universities, Oak Ridge, TN, US. 3 General Dynamics Information Technology, Falls Church, VA, US

PW-04 Progress Towards the Replacement of In Vivo Leptospirosis Vaccine Potency Testing in the United States

Bridget Rogers1, Jeffrey Brown2, David Allen3, Warren Casey4, Amy Clippinger1

1 PETA, Norfolk, VA, US. 2 PETA, London, United Kingdom. 3 Inotiv, Durham, NC, US. 4 NIEHS NTP, Durham, NC, US

PW-05 Characterizing the Sub-Chronic Tissue Toxicity and Mutagenicity of Formaldehyde Fumes at Low Concentrations in an in Vitro Human Airway Model

Yuan Le1, Baiping Ren1, Levan Muskhelishvili2, Kelly Davis2, Yiying Wang1, Diego Rua3, Xuefei Cao1

1 National Center for Toxicological Research, Jefferson, AR, US. 2 Toxicologic Pathology Associates, Jefferson, AR, US. 3 Center for Devices and Radiological Heath, Sliver Spring, MD, US **PW-06** Metabolic Similarity in Read-Across Prediction: A Case Study in Using Graph Kernels and Predicted Metabolism Information

Brett Hagan1,2, Grace Patlewicz2, Imran Shah2 1 Oak Ridge Associated University, Oak Ridge, TN, US. 2 US EPA, RTP, NC, US

PW-07 Identification of Candidate Reference Chemicals Using Multidimensional Literature and Database Mining Using EPA's PubMed Abstract Sifter

Nancy Baker1, Thomas Knudsen2 1 Leidos, Research Triangle Park, NC, US. 2 EPA, Research Triangle Park, NC, US

PW-08 Benefits of a GIVIMP Certification Program

Amanda Ulrey, <u>Erin Hill</u>
Institute for In Vitro Sciences, Inc., Gaithersburg, MD, US

PW-09 Chemical Grouping Using an Automated KNIME Workflow: An Interpretable Machine Learning Approach

Jose Teofilo Moreira-Filho, Mike Conway, Charles Schmitt, Nicole Kleinstreuer, Kamel Mansouri DNTP/NIEHS/NIH, Durham, NC, US

PW-10 Urban Particulate Matter Induces Cell Cycle Arrest and Senescence in a Human keratinocyte Cell Line (HaCaT). Juanita Alzate Ramirez, Natalia Rendón Serna, Jean Paul Delgado, Belfran Carbonell-M Universidad de Antioquia, Medellín, Antioquia, Colombia

PW-11 Methods for Selecting Analogs and Quantifying Suitability for SAR-Based Toxicological Safety Assessment Cathy Lester, Byrd ElLantae', Mahmoud Shobair, Gang Yan

The Procter & Gamble Co., Mason, OH, US

PW-12 Developing NAMs for Evaluating the Safety of Inhalation Exposure to Chemicals With Complex Physico-Chemical Properties

Nikaeta Sadekar1, Anne Marie Api2 1 Research Institute for Fragrance Materials, Woodcliff Lake, NJ, US. 2 RIFM, Woodcliff Lake, NJ, US

PW-13 Evaluation of the ToxCast Assay Suite for Detection of Neuroactivity Amy Carpenter1,2, Kelly Carstens1, Melissa Martin1, Timothy Shafer1, Katie Paul Friedman1 1 Center for Computational Toxicology and

Exposure, ORD, US EPA, RTP, NC, US. 2 Oak Ridge Institute for Science and Education, Oak Ridge, TN, US

PW-14 Next Generation Risk Assessment (NGRA) using NAMs for skin sensitization: Reproducibility and precision of the GARDskin Dose-Response assay for PoD determination.

Andy Forreryd1, Shashi Donthamsetty2, Paul Sterchele2, Xiao Huang2, Gregory Ladics2, Mihwa Na3, Isabelle Lee3, Anne Marie Api3, Robin Gradin1, Henrik Johansson1

1 SenzaGen AB, Lund, Sweden. 2 International Flavors & Fragrances, Hazlet, NJ, US. 3 Research Institute for Fragrance Materials, Woodcliff lake, NJ, US

PW-15 Application of the ToxProfiler Reporter Assay in Toxicological Case Study of Selected Sartans

Bas ter Braak, Liesanne Wolters, Giel Hendriks, Torben Osterlund Toxys B.V., Oegstgeest, Netherlands

PW-16 Integrating Population Enzyme Variability Into Physiologically-Based Kinetic Models of Parent Chemicals and Metabolites

David Hines1, Bethany Cook1, <u>Victoria Hull1</u>, Dave Allen1, Jean-Lou Dorne2, Jeremy Erikson3, Nicole Kleinstreuer3, Kamel Mansouri3

1 Inotiv, Morrisville, NC, US. 2 European Food Safety Authority, Parma, Italy. 3 NIH/NIEHS, RTP, NC, US

Poster Session I

PW-17 Assessing the Effects of Silver Nanoparticles on ARPE-19 Cells via Imaging-Based High Throughput Phenotypic Profiling

Gabrielle Byrd1,2, Alice Goldstein-Plesser3,2, Johanna Nyffeler1,4, Clinton M. Willis1, Anna Fisher3, William K. Boyes3, Joshua A. Harrill1 1 Center for Computational Toxicology and Exposure, ORD, US EPA, RTP, NC, US. 2 Oak Ridge Associated Universities, Oak Ridge, TN, US. 3 Center for Public Health & Environmental Assessment, ORD, US EPA, RTP, NC, US. 4 Oak Ridge Institute for Science and Education, Oak Ridge, TN, US

PW-18 Descriptor Free QSAR Modeling for Fraction Unbound in Human Plasma and Microsomal Clearance

Sayak Mukherjee, Michael Riedl, Mitchell Gauthier Battelle, Columbus, OH, US

PW-19 Assessing the Language We Use to Build the Bioactivity Narrative Shannon Bell1, Patricia Ceger1, Michelle Angrish2 1 RTI International, Research Triangle Park, NC, US. 2 US EPA/CPAD/CPHEA, Research Triangle Park, NC. US

PW-20 An in Vitro 3D Model of Human Renal Proximal Tubule for Nephrotoxicity Screening Studies Adam Pearson, Gregory Travlos, Stephen Ferguson NIEHS, Durham, NC, US

PW-21 Robust Phenotypic Profiling Assay for Predictive Toxicity on Human Hepatic Cells

Wei Chen1, Eric Sherer1, Zachary Sutake1, Clinton Willis2, Joshua A. Harrill2, Jessica LaRocca1

1 Corteva Agriscience, Crop Protection Research and Development, Indianapolis, IN, US. 2 Center for Computational Toxicology & Exposure, ORD, US EPA, Research Triangle Park, NC, US

PW-22 Application of BioPath Metabolism Tools within ChemTunes.ToxGPS for Next Generation Risk Assessment

Aleksandra Mostrag-Szlichtyng1, Oliver Sacher2, Bruno Bienfait2, Bryan Hobocienski1, James Rathman1,2, Jaoao Ribeiro1, Chihae Yang1,2 1 MN-AM, Columbus, OH, US. 2 MN-AM, Nurnberg, Germany **PW-23** The Use of the GARDskin Dose-Response Assay to Assess Skin Sensitizing Potency in Developing Novel Fragrance Ingredients

Tim Lindberg1, Christopher Choi2, Ulrika Mattson1, Satoshi Sasaki3

1 SenzaGen, Lund, Sweden. 2 Takasago International Corp, Rockleigh, NJ, US. 3 Takasago International Corp, Hiratsuka city, Kanagawa, Japan

PW-24 Applying Deep Learning Toxicity Models Across the Chemical Universe Sunggun Lee1, Ting Li2, Zhichao Liu2, Weida Tong2, Kamel Mansouri3, Nicole Kleinstreuer3 1 Duke University, Durham, NC, US. 2 National Center for Toxicological Research, FDA, Jefferson, AR, US. 3 NTP Interagency Center for the Evaluation of Alternative Toxicological Methods, NIEHS, Research Triangle Park, NC, US

PW-25 Evaluation of Skin Sensitization Classification Rules to Reflect Human Potency and Support Weight-of-Evidence Assessments

Judy Strickland1, Jaleh Abedini1, Dave Allen1, Anne Marie Api2, Dori Germolec3, John Gordon4, Victoria Hull1, Nicole Kleinstreuer3, Hon-Sum Ko5, Joanna Matheson4, Hermann-Josef Thierse6, Kim To1, Jim Truax1, Jens T. Vanselow6, Matthias Herzler6
1 Inotiv, Research Triangle Park, NC, US. 2 RIFM, Woodcliff Lake, NJ, US. 3
NIH/NIEHS/DNTP/NICEATM, Research Triangle

Park, NC, US. 4 U.S. Consumer Product Safety
Commission, Rockville, MD, US. 5 U.S. FDA, Silver
Spring, MD, US. 6 German Federal Institute for Risk
Assessment, Berlin, Germany

PW-26 Facilitating Global Connections through the Microphysiological Systems for COVID Research (MPSCoRe) Working Group

Amber Daniel1, Nicole Kleinstreuer2, Dave Allen1, Kyle Glover3, Tyler Goralski3, Bert Gough4, Mark Schurdak4, Catherine Sprankle1, Danilo Tagle5, Mark Williams6, Anthony Holmes7

1 Inotiv, Research Triangle Park, NC, US. 2
NIH/NIEHS/DNTP/NICEATM, Research Triangle Park, NC, US. 3 U.S. Army DEVCOM CBC, Aberdeen Proving Ground, MD, US. 4 University of Pittsburgh, Pittsburgh, PA, US. 5 NIH/NCATS, Bethesda, MD, US. 6 NIH/NIAID/DMID/OBRRTR, Rockville, MD, US. 7 NC3Rs, London, United Kingdom

PW-27 Effect of Inter-individual
Variability on a Phenotypic Endpoint
Assay Battery in an In Vitro Co-culture
Model of the Human Bronchus after
Exposure to Model Reactive Gas Acrolein
Alysha Simmons1, Emily Aungst2, Lisa Dailey2,
Nicholas Mallek1, Phillip Clapp1, Shaun
McCullough2
1 UNC-Chapel Hill, Chapel Hill, NC, US. 2 EPA,
Chapel Hill, NC, US

PW-28 Differences in Neurotoxic Outcomes of Organophosphorus Pesticides Revealed via Multi-Dimensional Screening in Adult and Regenerating Planarians Danielle Ireland1, Siqi Zhang2, Jui-Hua Hsieh3, Christina Rabeler1, Zane Meyer1, Eva-Maria S. Collins1,2,4

1 Swarthmore College, Swarthmore, PA, US. 2 University of California San Diego, La Jolla, CA, US. 3 National Institute of Environmental Health Sciences, Research Triangle Park, NC, US. 4 University of Pennsylvania, Philadelphia, PA, US

PW-29 Evaluation of Per- and Poly Fluoroalkyl Substances (PFAS) in Vitro Toxicity Testing for Developmental Neurotoxicity

Kelly Carstens1, Amy Carpenter1,2, Theresa Freudenrich1, Kathleen Wallace1, Seline Choo1,2, Grace Patlewicz1, Barbara Wetmore1, Katie Paul Friedman1, Tim Shafer1

1 US EPA, RTP, NC, US. 2 Oak Ridge Institute for Science and Education (ORISE), Oak Ridge, TN, US

Poster Session II

PTh-01 Improving the Efficiency of Literature Identification for the ECOTOXicology Knowledgebase Using Deep Learning

Brian Howard1, Christopher Norman1, Arpit Tandon1, Ruchir Shah1, Jennifer Olker2, Dale Hoff2 1 Sciome LLC, RTP, NC, US. 2 US EPA, Duluth, MN, US

PTh-02 A Modern Framework to

Establish Scientific Confidence in NAMs Anna J van der Zalm1, João Barroso2, Patience Browne3, Warren Casey4, Tala R Henry5, Nicole C Kleinstreuer6, Anna B Lowit7, Monique Perron8, Amy J Clippinger1

1 PETA Science Consortium International e.V., Stuttgart, Germany. 2 European Commission, JRC, Ispra, Italy. 3 OECD, Hazard Assessment and Pesticides Programmes, Environmental Directorate, Paris, France. 4 NIH, Division of the NTP, NIEHS, RTP, NC, US. 5 U.S. EPA, OPPT, Washington D.C, US. 6 National Toxicology Program Interagency Center for the Evaluation of Alternative Toxicological Methods, RTP, NC, US. 7 U.S. EPA, OPPT, Washington D.C., US. 8 U.S. Environmental Protection Agency, OPP, Washington D.C., US

PTh-03 Policy Initiatives for Integrating New Approach Methodologies for Pharmaceutical Testing

Emily Anderson, Elizabeth Baker Physicians Committee for Responsible Medicine, Washington, DC, US

PTh-04 Bringing NAMs Into Regulatory Decision-Making: Replacing the Use of Animals in Personal Lubricant Biocompatibility Testing via FDA's MDDT Program

Andrew Nguyen1, Jeffrey Brown1, Gertrude-Emilia Costin2

1 PETA Science Consortium International e.V. (PSCI), Stuttgart, Germany. 2 Institute for In Vitro Sciences Inc. (IIVS), Gaithersburg, Maryland, US

PTh-05 Strength in Teams: Al-Human Hybrid Intelligence, Defined Approaches, and Improved Risk Assessment Lyle Burgoon Raptor Pharm & Tox, Ltd, Apex, NC, US the Reconstructed Human Epidermis Model for Skin Irritation and Corrosion Jessica Ponder1, Hans Raabe2, Kristie Sullivan1 1 Physicians Committee for Responsible Medicine, Washington, DC, US. 2 Institute for In Vitro Sciences, Gaithersburg, MD, US

PTh-06 Advantages and Applications of

PTh-07 Liquid Application Dosing Alters Air-Liquid Interface Bronchial Epithelial Culture Physiology and Toxicity Testing Relevant Endpoints

Nicholas Mallek1, Elizabeth Martin2, Shaun McCullough3

1 University of North Carolina, Chapel Hill, NC, US. 2 National Institute of Environmental Health Sciences, Durham, NC, US. 3 US EPA, Chapel Hill, NC, US

PTh-08 In Vitro to In Vivo Extrapolation to Facilitate the Animal-free Risk Assessment of Potential Developmental Toxicants

Xiaoqing Chang1, Jessica Palmer2, Elizabeth Donley2, Emily Reinke1, David Allen1, Nicole Kleinstreuer3

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PTh-09 In Vitro Modeling of Human Hepatic Responses to Chemical Exposures With 3D Spheroid Transcriptomics

Stephen Ferguson1, Sreenivasa Ramaiahgari1, Katelyn Lavrich1, Scott Auerback1, Dhiral Phadke2, Ruchir Shah2, Georgia Roberts1, Jenni Gorospe3, Barney Sparrow3, Michael DeVito4, Alex Merrick1 1 NIEHS, RTP, NC, US. 2 Sciome, Durham, NC, US. 3 Battelle, West Jefferson, OH, US. 4 EPA, RTP, NC, US

PTh-10 NURA Program Trains Scientists in New Approach Methodologies to Advance Human Relevant Science Eryn Slankster-Schmierer, Phoebe Woodruff, Kristie Sullivan

Physicians Committee for Responsible Medicine, Washington, DC, US

PTh-11 Panel of Bacterial Mutagenicity in Silico Models for Substructure-Based Analysis

Vijay Gombar1, Alex Sedykh1, Ruchir Shah1, Kristine Witt2, Warren Casey2 1 Sciome LLC, RTP, NC, US. 2 National Institute of Environmental Health Sciences, Division of the National Toxicology Program, RTP, NC, US

PTh-12 Characterizing the Impacts of Assay Design on Cytotoxic Concentration Range

Kimberly To1, Agnes Karmaus1, Victoria Hull1, Dave Allen1, Nicole Kleinstreuer2 1 Inotiv, Research Triangle Park, NC, US. 2 NIH/NIEHS/DNTP/NICEATM, Research Triangle Park, NC, US

PTh-13 Application of in Vitro and Aquatic Models to Predict Developmental Toxicity and Endocrine Disruptors in New Product Development

Enrica Bianchi, Jessica LaRocca Corteva Agriscience, Indianapolis, Indiana, US

PTh-14 Collective Cellular Dynamics for Nano Safety Assessment

Karmveer Yadav

ICAR-National Dairy Research Institute, Karnal, Haryana, India

PTh-15 Synthetic Cooling Agents in US-marketed E-cigarette Refill Liquids and Popular Disposable E-cigarettes:

Chemical Analysis and Risk Assessment Sairam Jabba1, Hanno Erythropel2, Deyri Torres2, Lauren Delgado2, Jackson Woodrow2, Paul Anastas2, Julie Zimmerman2, Sven-Eric Jordt1 1 Duke University School of Medicine, Durham, NC, US. 2 Yale University, New Haven, CT, US

PTh-16 Prediction of Endocrine
Disruption Potential of Chemicals Using
QSAR Modeling of In vitro and In vivo
Assays

Mounika Girireddy, Suman Chakravarti, Roustem Saiakhov

MultiCASE Inc., Beachwood, OH, US

PTh-17 ICE Tools to Facilitate PBPK Modeling and IVIVE for Various Exposure Scenarios

Aswani Unnikrishnan Inotiv, Research Triangle Park, NC, US

Poster Session II

PTh-18 A Potential Novel Integrative
Strategy for Read-Across to Evaluate
Large Numbers of Nitro-Polycyclic
Aromatic Hydrocarbons (NPAHs) for
Cancer Hazard Evaluation
William Bisson1, Kamel Mansouri2, Sanford
Garner1, Whitney Arroyave1, Andrew Ewens1, Amy
Wang2, Gloria Jahnke3, Ruth Lunn2
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NIH/NIEHS/DTNP, Research Triangle Park, NC, US.
3 AGOVx, Research Triangle Park, NC, US

PTh-19 Multi-Scale Regression Modeling on Acute Toxicity using Data Augmentation, Feature Engineering and Perturbation Theory Machine Learning Approaches.

Gerardo Casanola-Martin1, Karel Dieguez-Santana2, Humbert Gonzalez-Diaz2, Bakhtiyor Rasulev1

1 North Dakota State University, Fargo, North Dakota, US. 2 University of Basque Country, Leioa, Spain

PTh-20 Utilizing 3D Chemical Featurs to Determine Potential Interactions For Early Risk Assessment Bethany Cook1, Lyle Burgoon2 1 RTI International, Research Triangle Park, North Carolina, US. 2 Raptor Pharm & Tox, Ltd, Apex, North Carolina, US

PTh-21 Integration of Machine Learning and Cheminformatics Approaches Towards Nanomaterials Toxicity Assessment

Bakhtiyor Rasulev North Dakota state University, Fargo, ND, US

PTh-22 Simulated Gastric Leachate of 3D Printer Metal-Containing Filaments Induces Cytotoxic Effects in Rat and Human Intestinal Models Haley Clapper1, Getachew Tedla1, Kim Rogers2, Michael Hughes2
1 ORISE, Research Triangle Park, NC, US. 2 US EPA, Research Triangle Park, NC, US

PTh-23 Data-Driven Derivation of an Adverse Outcome Pathway Linking VEGF and Cardiotoxicity

Daniel Ehrlich1, Shagun Krishna2, Nicole Kleinstreuer2

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PTh-24 Integrating High Throughput Transcriptomics into a Tiered Framework to Prioritize Chemicals for Toxicity Testing

Jesse Rogers1,2, Katie Paul-Friedman1, Logan Everett1

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PTh-25 Use of Chemical Structure and Bioactivity to Map Mechanistic Pathways for Acute Oral Systemic Toxicity Mark D. Nelms1, Virginia K. Hench1, Jessica Ponder2, Bethany Cook1, David Williams1, Stephen W. Edwards1, Kristie Sullivan2 1 GenOmics, Bioinformatics, and Translational Research Center, RTI International, Research

PTh-26 Use of Two Simple Techniques for Spheroids Production With Toxicity in Vitro Assessment

Triangle Park, NC, US. 2 Physicians Committee for

Responsible Medicine, Washington, DC, US

Angie Castro, Dayan Guerra, Andrés Pareja Universidad CES, Medellín, Colombia

PTh-27 In-Vitro Toxicity Assessments of Air Pollutants Using Two Co-Culture Strategies for Skin and Ocular Models Dayan Guerra, Angie Castro, Andres Pareja Universidad CES, Medellín, Antioquia, Colombia PTh-28 In Silico Approach That Supports Neurotoxicity Assessment of Chemical Substances by IATA: Refining Categories by Using Substructures and Physicochemical and Biochemical Parameters Related to Neurotoxicity Takashi Yamada, Shinji Tsujii, Minoru Miura, Akiko Saito, Tomoko Kawamura, Taeko Maruyama, Naruo Katsutani, Akihiko Hirose National Institute of Health Sciences, Kawasaki, Japan

PTh-29 Potency Classifications for Contact Dermal Sensitization as Determined by the h-CLAT Assay George DeGeorge MB Research Laboratories, Spinnerstown, PA, US

PTh-30 Intralaboratory Validation of a Non-Animal Integrated Testing Strategy (ITS) to Identify GHS Categories NC, 1, 2 Irritants via the BCOP-EIT Assays Rachael Koch, Christopher Kalimtzis, George DeGeorge

MB Research Laboratories, Spinnerstown, PA, US

PTh-31 Aerosolized fluorescent tracers provide insight into particle deposition and cellular uptake at the air-liquid interface

Jessica Murray1, Elise Carlsten2,1, Wyatt Zander2, Jason Weinstein1, Q. Todd Krantz1, Adam Speen3,1, Mark Higuchi1

1 US EPA, Research Triangle Park, NC, US. 2 ORAU, Oak Ridge, TN, US. 3 ORISE, Oak Ridge, TN, US

PTh-32 Towards systematic read-across using Generalised Read-Across (GenRA) Grace Patlewicz, Imran Shah US EPA, RTP, NC, US

PTh-33 Towards Reproducible Structure-Based Chemical Categories for PFAS to Inform and Evaluate Toxicity and Toxicokinetic Testing Grace Patlewicz, Ann Richard, Antony Williams, Richard Judson, Russell Thomas US EPA, RTP, NC, US

Notes





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