ACC Science and Research Highlights

American Chemistry Council

ACC Science & Research at the Society of Toxicology Meeting March 11-15, 2018

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Society of Toxicology (SOT) Annual Meeting March 11-15

Approximately 7,000 scientists from more than 50 countries will participate in the annual meeting of the Society of Toxicology (SOT) in San Antonio March 11-15. The SOT is the largest professional society of toxicologists in the world. For ACC, the annual SOT meeting, through both scientific sessions and poster presentations, provides a unique opportunity to communicate our latest research results and to interact with others engaged in related areas of research, testing and assessment. The SOT meeting also provides a great opportunity for networking with leaders in the field and for catalyzing collaborations within and across sectors.

ACC's LRI Research: Presentations by ScitoVation Scientists: Fifteen presentations by ScitoVation scientists leading LRI research investigations are slated for the SOT meeting (summarized below). LRI research actualizes ACC members' continuing commitment to advance scientific understanding of the potential impacts of chemicals on human health and the environment and is guided by ACC's LRI 2015-2019 Research Strategy. ACC's LRI research projects are oriented toward: 1) Further development and use of predictive exposure models; 2) Refinement of tools and approaches that can extrapolate results from in vitro high throughput assays to real-world human exposures; and 3) Development of fit-for-purpose assays that are envisioned to provide the means to conduct targeted cellular-based safety assessments. The selection of these LRI research projects for presentation at the SOT meeting reflects the importance and credibility of LRI research and the prominence of LRI researchers, and demonstrates LRI's commitment to scientific excellence and public dissemination of research results. LRI's Principles ensure that LRI funded research meets the highest standards for scientific excellence, transparency, and fair and unbiased conduct.

SOT Awards ACC Manuscript Best Scientific Publication in 2017: A research project initiated by ACC's Computational Profiling Work Group resulted in an article that the SOT's Risk Assessment Specialty Section selected as the Best Scientific Publication Demonstrating an Application of Risk Assessment for the year 2017. ACC's Rick Becker led this collaborative research project. The article *"How well can carcinogenicity be predicted by high throughput "characteristics of carcinogens"* is open access at Reg Tox Pharm 185-196. The investigation used extensive statistical analyses and machine learning prediction algorithms to evaluate how well ToxCast/Tox21 data for so-called key characteristics of carcinogens predict cancer hazard. The project was undertaken because IARC, without any explicit or transparent analysis, started using ToxCast/Tox21 data to infer carcinogenic potential (and EPA is poised to follow suit). In the study, ToxCast/Tox21 data (with and without adjusting for the cytotoxicity burst effect commonly observed in such assays) were analyzed for substances EPA has formally classified as having cancer hazard potential (designated as positives) and substances not posing a carcinogenic hazard (designated as negatives). Using the same assignments as IARC of ToxCast/Tox21 assays to the seven key characteristics of carcinogens, the Becker et al. analysis showed that the ability to predict cancer hazard for each key characteristic, alone or in combination, was no better than chance. Thus, a more rigorous mode-of-action pathway-based framework should be used, with knowledge of exposure, to evaluate potential carcinogenic hazards and risks to humans.
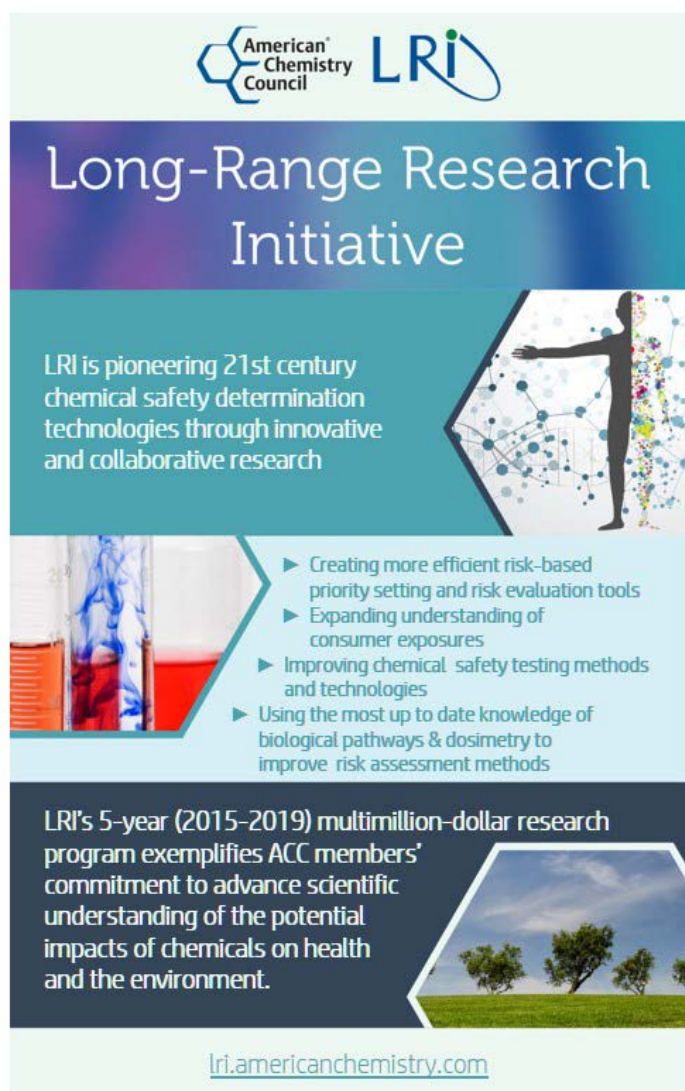
ACC Science and Research Highlights is a publication for ACC members and staff to communicate information on scientific research projects conducted or supported by ACC departments

ACC's Science and Research Division, Regulatory & Technical Affairs Department

ACC's Chemical Products & Technology Division	Investigators
Research supported by the ACC Olefins Panel • In Vitro Approaches to Grouping of Complex Substances and UVCBs: A Case Study of Olefin Streams (Thursday Mar 15 8:30 AM - 11:30 AM) Abstract # 3325: Poster Board - P106	W. D. Klaren, F. A. Grimm, H. Shen and I. Rusyn
Research supported by the ACC Diisocyanates Panel • Critical Evaluation of Thresholds for Respiratory Effects of Toluene Diisocyanate (Monday March 12 9:15 AM to 4:30 PM) Abstract # 3325: Poster Board - P248	H.N. Lynch, R.L. Prueitt, I. Mohar, and J.E. Goodman

ACC LRI Research (presented by ScitoVation researchers)	Investigators
Case Studies on the Use of In Vitro Data for Quantitative Evaluation of Dose-Response and Margin of Exposure (Sun, Mar 11 7:00-7:45) (Continuing Education SR02)	R. Clewell
Examples of the Use of Physiologically-Based Pharmacokinetic Models in Support of In Vitro Based Safety Assessment: Hands-On Demonstration of a Work Flow (Sun, Mar 11 8:15-12:00) (Continuing Education AM07)	M. Yoon
A Novel Approach to Rapidly Identify Chemical Metabolites by Combining In Silico Prediction, In Vitro Generation, and Non-Targeted Analytical Detection (Mon, Mar 12 1:30-3:00 CC Exhibit Hall) Abstract #1304/P402	J. R. Enders, M. B. Phillips, R. Norini, M. Smeltz, P. Balbuena-Venancio, M. Strynar, E. Ulrich, J. Sobus, R. Karsten, H. Clewell, M. Yoon
Can Pharmacokinetic Modelling Keep Up with Risk Assessment in the 21st Century? (Mon, Mar 12 1:30-2:30 Room 217C) (Exhibitor-Hosted Session)	H. Clewell, H. Barton, M. Embry, J. Gearhart, P. Hinderliter, J. Wambaugh, M. Whelan
Hepatocytes as a Metabolic-Activating System for Genotoxicity Testing: A Case Study with Octadiene (Mon, Mar 12 3:00-4:30 CC Exhibit Hall) Abstract #1508/P726	M. Phillips, K. Dunnick, M. Smeltz, P. Balbuena-Venancio, J.R. Enders, R. Norini, S. Rowley, R. Clewell, M. Yoon
A Machine Learning Model for Prediction of Compound Mode-of-Action from Toxicogenomics (Tues, Mar 13 10:45-12:15 CC Exhibit Hall) Abstract #2492/P851	P. D. McMullen, K. Mansouri, S. N. Pendse, S. Haider, M. B. Black, M. E. Andersen, R. Clewell
Pathway Analysis and Mode-of-Action Prediction Based on Computational Modeling of High-Throughput Toxicogenomics (Tues, Mar 13 10:45-12:15 CC Exhibit Hall) Abs. #2494/P853	S. Haider, K. Mansouri, M. B. Black, P D. McMullen, S. Pendse
Applying a Tiered Risk-Based Approach to Prioritizing Thousands of Chemicals for Further Evaluation: A Comparison of Current High-Throughput Computational Approaches (Tues, Mar 13 10:45-12:15 CC Exhibit Hall) Abstract #2487/P846	C. I. Nicolas, K. Mansouri, P. D. McMullen, R. Clewell, M. Yoon, M. Phillips, G. Patlewicz, H. J. Clewell
Designed-for-purpose complex liver cell cultures for improving in vitro hepatotoxicity testing (Wed, Mar 14 10:30-11:30 Room 217A) (Exhibitor-Hosted Session)	J. Hartman, M. Phillips
Towards Incorporation of the Metabolite Exposure in High-Throughput In Vitro to In Vivo Extrapolation (HT-IVIVE) (Wed, Mar 14 1:30-3:00 CC Exhibit Hall) Abstract #3188/P827	M. Moreau, M. Phillips, S. Haider, C. Nicolas, K. Mansouri, P. Mallick, S. Pendse, R. Clewell, H. Clewell, M. Yoon
Development of a Multi-Functional Fit-for-Purpose Rat Liver Co-Culture Assay for Hepatotoxicity Testing (Wed, Mar 14 1:30-3:00 CC Exhibit Hall) Abstract #3155/P788	J. Hartman, A. Stefanowicz, T. Beames, M. Phillips, M. Yoon, R. Clewell

Quantitative Bias Analysis of the Association of 2,2',4,4',5,5'-Hexachlorobiphenyl (PCB 153) and Type 2 Diabetes Mellitus (Wed, Mar 14 1:30-3:00 CC Exhibit Hall) Abstract #3190/P829	M. W. Dzierlenga, M. Yoon, F. Wania, P. L. Ward, J. M. Armitage, S. A. Wood, H. J. Clewell, M. P. Longnecker
Unification of Exposure and Pharmacokinetic Tools under the PLETHEM Framework (Wed, Mar 14 1:30-3:00 CC Exhibit Hall) Abstract #3168/P807	S. N. Pendse, I. Diallo, C. I. Nicolas, A. Y. Efremenko, C. Housand, P. D. McMullen, M. Yoon, H. J. Clewell
A Tiered Approach to Evaluating Xenoestrogens: Incorporating Bioactivation into Chemical Prioritization Using In Silico Modeling and Defining a Region of Safety Using Fit-for-Purpose Cell-Based Assays and IVIVE (Wed, Mar 14 3:00-4:30 CC Exhibit Hall) Abstract #2894/P419	R. Clewell, K. Mansouri, J. Hartman, T. Beames, A. Roberts, D. Doheny, M. M. Miller, M. Yoon, P. D. McMullen
Measuring the Emissivity of Semi-volatile Organic Compounds from Articles of Commerce (Thurs, Mar 15 8:30-11:30 CC Hall 1) Abstract #3527/P317	C. Nicolas, M.S. Minto, X. Liu, K.K. Issacs, K.A. Phillips, C. Addington, A. Sumner, J.F. Wambaugh

https://lri.americanchemistry.com/

ACC'S LONG-RANGE RESEARCH INITIATIVE
AT A GLANCE

ACC's Long-Range Research Initiative (LRI) addresses the challenges facing the industry in chemical safety assessment by pioneering 21st century tools and technologies through innovative and collaborative research, and linking that research to practice and policy.

American Chemistry Council

LRI Long-Range Research Initiative

4 GUIDING PRINCIPLES:

1. SCIENTIFIC EXCELLENCE
2. TRANSPARENCY
3. FAIR & UNBIASED CONDUCT
4. RELEVANCE TO CHEMICAL INDUSTRY

300 PUBLICATIONS IN TOP-20 RANKED JOURNALS IN TOXICOLOGY, ENVIRONMENTAL SCIENCNES AND EPIDEMIOLOGY

10 INTERNATIONAL CHEMICAL SAFETY WORKSHOPS WITH GLOBAL PARTNERS AND STAKEHOLDERS INCLUDING EUROPEAN CHEMICAL INDUSTRY COUNCIL (CEFIC) AND JAPAN CHEMICAL INDUSTRY ASSOCIATION (JCIA)

LRI RESEARCH FOCUSES ON DEVELOPING **TOOLS AND TECHNOLOGIES TO HELP PAVE THE WAY FOR** 21ST CENTURY SCIENCE TO BE USED IN THE REVISED **TOXIC SUBSTANCES CONTROL ACT**

LRI MISSION - IDENTIFY AND FILL GAPS IN UNDERSTANDING ABOUT HAZARDS POSED BY CHEMICALS AND IMPROVE METHODS AVAILABLE FOR ASSESSING RISKS. LRI'S INNOVATIVE RESEARCH PROGRAM IS DESIGNED TO IMPROVE THE WAY WE ADDRESS THE SAFETY OF OUR CHEMICALS.

3 RESEARCH AREAS FOR SUCCESS:

1. ADVANCE UNDERSTANDING OF CONSUMER EXPOSURES: PREDICTIVE MODELS FOR GENERATING EXPOSURE ESTIMATES
2. INTEGRATE HAZARD AND EXPOSURE TO ASSESS RISKS FROM CHEMICALS: NEW TOOLS FOR LINKING DATA IN A RISK CONTEXT
3. IMPROVE CHEMICAL SAFETY TESTING TECHNOLOGIES: DESIGN FIT-FOR-PURPOSE ASSAYS AND ADVANCE DATA INTERPRETATION

OVER 18 YEARS OF SUCCESSFUL COLLABORATIONS WITH GOVERNMENT AND ACADEMIC SCIENTISTS