

# **SoT Workshop**

# **New Approach Methodologies for Exposure: Advancing Chemical Risk Assessment**

Session Chairs: John Wambaugh and Angelika Zidek

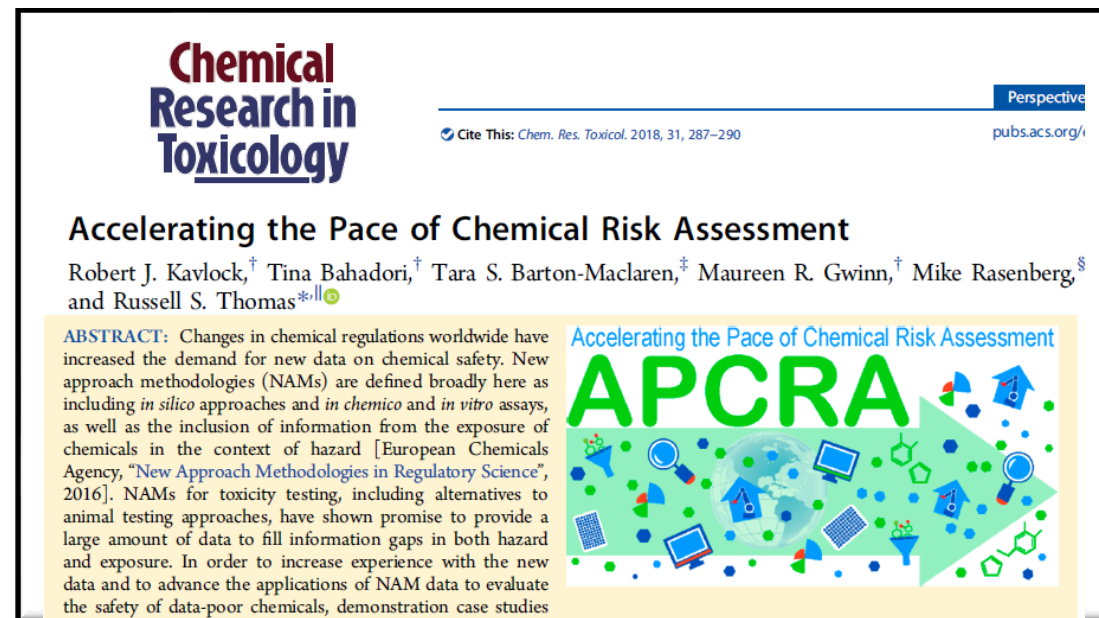
**Society of Toxicology Annual Meeting**

**March 16, 2021  
11:15 AM-2:00 PM**

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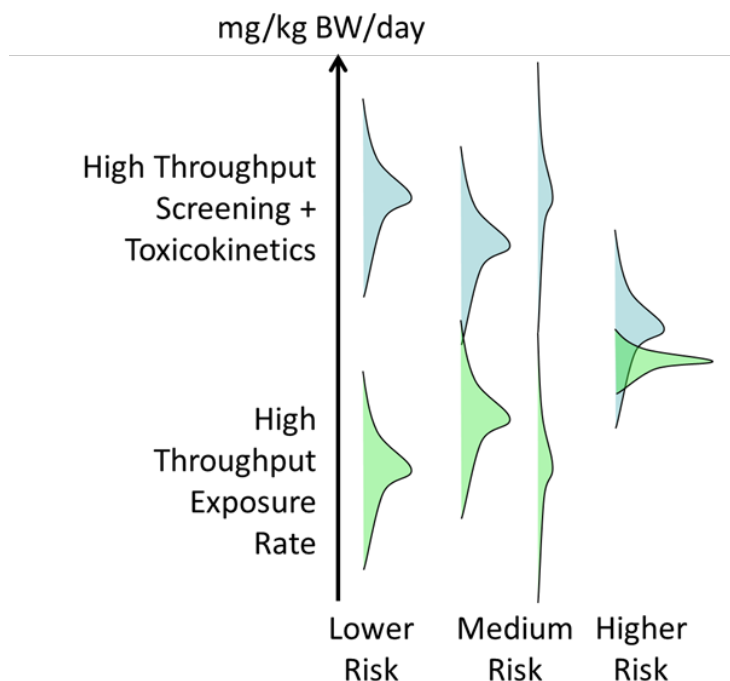
# New Approach Methodologies for Chemical Risk Identification

- In the United States the National Academies of Sciences, Engineering, and Medicine recommend (1983) that public health risk of chemicals be determined on the basis of hazard, exposure, and dose-response
- There are at least 10,000 chemicals produced, used in commerce, and potentially present in the environment
  - Traditional methods are too resource-intensive to address all of these
  - New Approach Methodologies (NAMs) have the potential to address these gaps
- NAMs might include:
  - **High throughput screening**
  - **High throughput exposure estimates)**
  - **High throughput toxicokinetics**

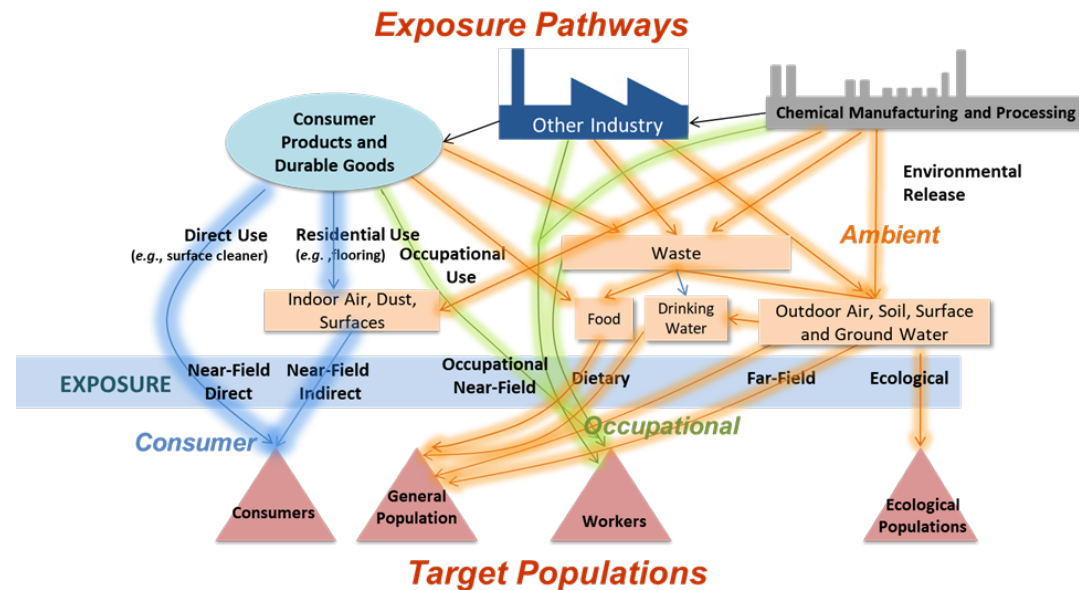


The tools to characterize both toxicity and exposure have evolved significantly in the past decade

NAMs for exposure science are being developed to enable risk assessors to more rapidly address public health challenges and chemical regulation



# NAMs for Exposure Science



Author's Personal Copy  
Available online at [www.sciencedirect.com](http://www.sciencedirect.com)

**ScienceDirect**

Current Opinion in  
**Toxicology**

**New approach methodologies for exposure science**  
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Xiaoyu Liu<sup>7</sup>, David E. Meyer<sup>2</sup>, Seth R. Newton<sup>4</sup>,  
Katherine A. Phillips<sup>4</sup>, Paul S. Price<sup>4</sup>, Caroline L. Ring<sup>8</sup>,  
Hyeong-Moo Shin<sup>9</sup>, Jon R. Sobus<sup>4</sup>, Tamara Tal<sup>10</sup>,  
Elin M. Ulrich<sup>4</sup>, Daniel A. Vallero<sup>4</sup>, Barbara A. Wetmore<sup>4</sup> and  
Kristin K. Isaacs<sup>4</sup>

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# NAMs for Exposure Science

Exposure NAM Class	Description	Traditional Approach	Makes Use of					
			Measurement	Toxicokinetics	Models	Descriptors	Evaluation	Machine Learning
Measurements	New techniques including screening analyses capable of detecting hundreds of chemicals present in a sample	Targeted (chemical-specific) analyses	-	●	●	●		●
Toxicokinetics	High throughput methods using in vitro data to generate chemical-specific models	Analyses based on in vivo animal studies	●	-		●		●
HTE Models	Models capable of making predictions for thousands of chemicals	Models requiring detailed, chemical- and scenario-specific information	●	●	-	●		
Chemical Descriptors	Informatic approaches for organizing chemical information in a machine-readable format	Tools targeted at single chemical analyses by humans				-		●
Evaluation	Statistical approaches that use the data from many chemicals to estimate the uncertainty in a prediction for a new chemical	Comparison of model predictions to data on a per chemical basis	●	●	●	●	-	●
Machine Learning	Computer algorithms to identify patterns	Manual Inspection of the Data	●	●		●		-
Prioritization	Integration of exposure and other NAMs to identify chemicals for follow-up study	Expert decision making	●	●	●	●	●	●

# Today's Speakers



**1) Heather Pangburn, Ph.D.:**  
“New Approach Methodologies Informing  
Operational Air Force Mission”



**2) Kristin Isaacs, Ph.D.:**  
“Filling Gaps in Exposure Data from Chemical Descriptors with  
Machine Learning”



**3) Jon Arnot, Ph.D.:**  
“High Throughput  
Exposure Models”



**5) Tatsiana Dudzina, Ph.D.:**  
“Making use of exposure  
NAMs to support chemical  
safety assessments”



**4) John Wambaugh, Ph.D.:**  
“High Throughput  
Toxicokinetics Enables  
Risk-based Prioritization”

# Today's Schedule

	Duration	Start time
Introduction by John Wambaugh	5	11:15:00 AM
Heather Pangburn	25	11:20:00 AM
Kristin Isaacs	25	11:45:00 AM
Jon Arnot	25	12:10:00 PM
John Wambaugh	25	12:35:00 PM
Tatsiana Dudzina	25	1:00:00 PM
Panel Discussion Moderated by Angelika Zidek	35	1:25:00 PM