Welcome to the New Approach Methods (NAMs) Tools Training Program

In-Person Workshop

April 24–25, 2024 (Public)
April 26 (EPA Only)
Research Triangle Park, NC

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EPA NAMs Overview

Reducing the use of vertebrate animals for toxicity testing is a priority for the U.S. Environmental Protection Agency (EPA), and, as such, the Agency is working on the development and application of New Approach Methods (NAMs). NAMs are defined as any technology, methodology, approach, or combination that can provide information on chemical hazard and risk assessment to avoid the use of vertebrate animal testing.

EPA is committed to providing transparent and publicly available tools and data on these NAMs. The www.epa.gov/comptox-tools website is a centralized hub that links to our commonly used tools and data. In addition, we have developed a NAMs Training portal that provides training materials and other learning resources for these tools and highlights upcoming training events.

Workshop Purpose

The purpose of this workshop is to provide an opportunity for large and small group training on the suite of NAMs online tools and to provide one-on-one guidance for tool users. This in-person workshop builds on the virtual trainings that have been offered via the NAMs Training Pilot Program since May 2022.

Agenda

Note: All times are in Eastern Daylight Time.

**Any sessions denoted with an asterisk below require pre-training materials, which can be accessed at www.scgcorp.com/EPANAMs2024/Workshop_Materials.*

Day One—Wednesday, April 24, 2024

Time	Session Title	Location
7:45 – 8:50 a.m.	**Entry to Campus, Registration**	
9:00 – 9:15 a.m.	**Welcome and Introductions** *Christina Baghdikian*	**Auditorium C111**
9:15 – 10:00 a.m.	**History of NAMs, Where Are We Now, the Way Ahead** *Rusty Thomas*, *Annette Guiseppi-Elie* and *Anna Lowit*	**Auditorium C111**
10:00 – 10:15 a.m.	**Break**	
10:15 – 11:35 a.m.	**Track Overview (25 minutes)** *Monica Linnenbrink* **Tool Introductions, Part 1 (10 minutes each)** 1. CompTox Chemicals Dashboard *Nisha Sipes* 2. GenRA *Esra Mutlu* 3. AOP-Wiki *Steve Edwards* 4. Cheminformatics and Proofs of Concept *Tony Williams* 5. TEST *Todd Martin*	**Auditorium C111**
11:35 a.m. – 12:50 p.m.	**Lunch**	
12:55 – 1:35 p.m.	**Tool Introductions, Part 2 (10 minutes each)** 6. httk *John Wambaugh* 7. ChemExpo *Kristin Isaacs* 8. ECOTOX *Jennifer Olker* 9. SeqAPASS *Carlie LaLone*	**Auditorium C111**

1:35 – 1:50 p.m.	**Overview of NAMs Training Resources and Online Tools** *Scarlett VanDyke*	**Auditorium C111**
1:50 – 2:05 p.m.	**Break**	
2:05 – 3:05 p.m.	**Choose Your Own Adventure!**	
	1. Introduction to R/R Studio *Celia Schacht* *Recommended for those who are new to R/R Studio and are interested in the httk or SHEDS-HT sessions.*	**Auditorium C111**
	2. New Tools Sneak Peek: Using the NTA WebApp and RapidTox, A tandem approach to emerging contaminant discovery and screening level assessment *Jason Lambert and Jon Sobus*	**Room C113**
3:05 – 3:30 p.m.	**Break/Flex Time** *Tool Owners will be available for informal chats. Stop by to ask quick questions to help map out your concurrent sessions.*	**C Hallway**
3:30 – 5:00 p.m.	**Concurrent Session #1 (4 Options)**	
	1. Bioactivity & Hazard—CompTox Chemicals Dashboard and Hazard Data *Nisha Sipes, Madison Feshuk and Risa Sayre*	**Auditorium C111**
	2. Exposure—httk R Package* *Marina Evans*	**Room C113**
	3. Chemistry—DSSTox/CompTox Chemicals Dashboard *Charles Lowe and Tony Williams*	**Room C114**
	4. Ecotoxicology—ECOTOX* *Jennifer Olker*	**Room C112**
5:00 – 5:15 p.m.	**Closing** *EPA Representative*	**Auditorium C111**
5:30 – 6:30 p.m.	**Optional Off-Site Networking Event**	**Boxyard RTP** 900 Park Offices Dr Research Triangle Park, NC 27709

Day Two—Thursday, April 25, 2024

Time	Session Title	Location
7:45 – 8:50 a.m.	**Entry to Campus**	
9:00 – 9:30 a.m.	**Open Discussion, Address Day 1 Questions** *EPA Representative*	**Auditorium C111**
9:30 – 11:00 a.m.	**Concurrent Session #2 (4 options)**	
	1. Bioactivity & Hazard—CompTox Chemical Dashboard and Bioactivity Data *Nisha Sipes*, *Logan Everett* and *Madison Feshuk*	**Rooms C111 A/B**
	2. Exposure—ChemExpo *Katherine Phillips* and *Sakshi Handa*	**Room C112**
	3. Chemistry—TEST *Todd Martin*	**Room C114**
	4. Ecotoxicology—SeqAPASS* *Carlie LaLone* and *Marissa Brickley*	**Room C111 C**
11:00 a.m. – 12:00 p.m.	**Lunch**	
12:00 – 1:30 p.m.	**Concurrent Session #3 (3 options)**	
	1. Bioactivity & Hazard, Ecotoxicology—AOP-Wiki* *Dan Villeneuve*	**Rooms C111 A/B**
	2. Exposure—SHEDS-HT* *Kristin Isaacs*	**Room C112**
	3. Chemistry—Cheminformatics Analysis Modules *Tony Williams* and *Todd Martin*	**Room C114**
1:30 – 1:45 p.m.	**Break**	
1:45 – 3:15 p.m.	**Concurrent Session #4 (3 options)**	
	1. Bioactivity & Hazard, Chemistry—GenRA* *Esra Mutlu*	**Rooms C111 A/B**
	2. Exposure—Bioactivity:Exposure Ratio and SEEM Case Study *John Wambaugh* and *Katie Paul Friedman*	**Room C112**
	3. Ecotoxicology—ToxCast/SeqAPASS/ECOTOX Case Study *Madison Feshuk*, *Carlie LaLone*, *Marissa Brickley* and *Jennifer Olker*	**Room C114**
3:15 – 4:15 p.m.	**Tool Mentoring: All Tools and Data** *Now that you know more about the tools and data, come talk 1-1 with tool and data experts to get input on questions you still have or use-specific needs.*	**Auditorium C111**
4:15 – 5:00 p.m.	**Open Discussion and Workshop Closing** *EPA Representative*	**Auditorium C111**

Day Three (EPA Only)—Friday, April 26, 2024

Time	Session Title	Location
9:00 – 9:15 a.m.	**Opening, Questions, Solicit Feedback from Group** *EPA Representative*	**Auditorium C111**
9:15 – 10:00 a.m.	**SeqAPASS** *Carlie LaLone and Marissa Brickley* *Offering a brief presentation that includes instances where SeqAPASS data has contributed to risk assessments. Opportunity to ask questions about specific challenges EPA partners face where SeqAPASS could potentially be applied.*	**Auditorium C111**
10:00 – 10:15 a.m.	**Break**	
10:15 – 11:00 a.m.	**AOP-Wiki** *Dan Villeneuve* *Offering a brief overview of Wiki features and solicit feedback from group. Opportunity for Q&A.*	**Auditorium C111**
11:00 – 11:45 a.m.	**ECOTOX Knowledgebase** *Jennifer Olker* *Presentation on new chemical information and new features that are soon to be released in ECOTOX. Opportunity to provide suggestions for new chemicals and new features that could be added.*	**Auditorium C111**
11:45 a.m. – 12:05 p.m.	**Break – Please feel free to bring lunch to the next session!**	
12:05 – 12:50 p.m.	**NTA WebApp: Lunch and Learn!** *Jon Sobus and Alex Chao* *Offering a brief overview of NTA WebApp features and solicit feedback from group. Opportunity for Q&A.*	**Auditorium C111**
12:50 – 1:00 p.m.	**Wrap Up, Release for Questions** *EPA Representative*	**Auditorium C111**

Session Descriptions

Using the NTA WebApp and RapidTox: A tandem approach to emerging contaminant discovery and screening level assessment

Non-targeted analysis (NTA) approaches often reveal a complex landscape of emerging contaminants including manufactured chemicals and associated transformation products in various environmental matrices. Ascertaining potential human health hazards associated with exposure(s) to such emerging contaminants has historically been resource and time intensive. This session will demonstrate a coordinated approach to NTA and hazard profiling using existent Office of Research and Development/Center for Computational Toxicology and Exposure tools and approaches. This tandem chemical evaluation concept may significantly advance the protection of human health and the environment through more timely knowledge delivery from chemical discovery to screening level assessment. [Includes: Demonstration; Q/A]

Concurrent Session Track Descriptions

Concurrent Session	Bioactivity & Hazard	Exposure	Chemistry	Ecotoxicology
1	CompTox Chemicals Dashboard & Hazard	httk R Package	DSSTox/CCD	ECOTOX
2	CompTox Chemicals Dashboard & Bioactivity	ChemExpo	TEST	SeqAPASS
3	AOP-Wiki	SHEDS-HT	Cheminformatics Analysis Modules	*(Attend AOP-Wiki)*
4	GenRA	Bioactivity:Exposure Ratio and SEEM Case Study	*(Attend GenRA)*	ToxCast/SeqAPASS/ ECOTOX Case Study

Track 1 – Bioactivity & Hazard: EPA researchers use rapid chemical screening to test thousands of chemicals quickly and efficiently for potential human and environmental effects. This track will focus on tools that allow you to access and use EPA's wealth of chemical bioactivity and hazard information to help fill gaps and inform decision-making.

- **CompTox Chemicals Dashboard & Hazard Data (ToxValDB and ToxRefDB):** This session will provide an overview of the CompTox Chemicals Dashboard with an in-depth look at the Dashboard's *Hazard* Tab and its underlying EPA data resources, ToxValDB and ToxRefDB. The Toxicity Values Database (ToxValDB) is a compilation of various types of toxicity data from multiple public datasets, databases, and open literature, with an emphasis on quantitative estimates of relevant points-of-departure from *in vivo* toxicology studies such as those curated in the Toxicity Reference Database (ToxRefDB). [Includes: Demonstration; Q/A]

- **CompTox Chemicals Dashboard & Bioactivity Data (HTPP, HTTr, and ToxCast):** This session will provide an overview of the CompTox Chemicals Dashboard's *Bioactivity* Tab and enable users with an understanding of HTTr, HTPP, and ToxCast data generated by the EPA. High Throughput Transcriptomics (HTTr) examines gene expression changes following chemical exposure, whereas High Throughput Phenotypic Profiling (HTPP) uses cell painting technology to "profile" chemical effects on cell morphology. In addition to these high-content screens, heterogenous bioactivity assays from the Toxicity Forecaster (ToxCast) program is available for thousands of chemicals and targets. [Includes: Demonstration; Q/A]

- **GenRA:** This session will allow attendees to have an interactive experience with EPA's publicly available read-across tool, GenRA. GenRA is an automated approach to make reproducible read-across predictions of toxicity. Experts will lead a demonstration of GenRA features and functionality, including examples to generate objective and reproducible read-across predictions. [Includes: Demonstration; Q/A; Interactive Activity]

- **AOP-Wiki:** This session will allow attendees to gain familiarity with publicly accessible sources of computational toxicology data, like the CompTox Chemicals Dashboard, and associated translational knowledge frameworks, like the AOP-Wiki. Attendees will get the chance to apply data from new approach methods to address a toxicological question. [Includes: Demonstration; Q/A; Interactive Activity]

Track 2 – Exposure: EPA's rapid exposure and dosimetry research develops methods, data, tools, models, and approaches to rapidly generate exposure and dosimetry estimates for chemicals and mixtures found in commerce and in the environment. This track will explore the functions of EPA's exposure forecasting tools, allowing you to generate exposure and dose estimates and more.

- **Httk R package:** Toxicokinetics (TK) provides a bridge between toxicity and exposure assessment by predicting tissue concentrations due to exposure. The U.S. EPA's freely available httk R package (v2.3.0) uses data from in vitro high-throughput screening datasets, which can be used to fill data gaps in traditional TK methods. This session will be led by experts and will demonstrate EPA's generic and open-source models and data for toxicokinetics, including reverse dosimetry and physiologically based pharmacokinetic (PBPK) modeling for internal dose calculation. [Includes: Demonstration; Q/A; Interactive Activity] *New to R/R Studio? We recommend attending the Introduction to R/R Studio Session before attending this session.*

- **ChemExpo:** ChemExpo is an interactive web application for exploring chemical data curated from public documents relevant to exposure assessment. ChemExpo surfaces data collected by EPA about how chemicals occur in consumer and industrial products from the Chemicals and Products Database (CPDat). This session will cover the data and functionality of ChemExpo, including a live demonstration. [Includes: Demonstration; Q/A]

- **SHEDS-HT:** This session will cover the Stochastic Human Exposure and Dose Simulation (SHEDS) Models, which are probabilistic models that can estimate exposures people face from chemicals encountered in everyday activities, including the use of consumer products. SHEDS estimate of exposure via multiple scenarios and routes and has been used to inform state prioritization EPA human health risk assessments consensus exposure predictions used in chemical prioritization. SHEDS estimate of exposure via multiple scenarios and routes and has been used to inform state prioritization programs, EPA human health risk assessments, consensus exposure predictions used in chemical prioritization. [Includes: Demonstration; Q/A] *New to R/R Studio? We recommend attending the Introduction to R/R Studio Session before attending this session.*

- **Bioactivity:Exposure Ratio and SEEM Case Study:** The Systematic Empirical Evaluation of Models (SEEM) framework is used to develop consensus models. Using SEEM, predictors of exposure are combined according to calibrated weights reflecting estimates of their predictive ability based on monitoring data. This session will focus on a multi-tool case study for the use of SEEM, building on introductions to httk and ToxCast from previous sessions. [Includes: Demonstration; Q/A]

Track 3 – Chemistry: EPA's chemical characterization and informatics research includes models to predict physicochemical properties (e.g., molecular weight, melting point, boiling point, vapor point) and chemical transformation as well as approaches for read-across (a data gap filling technique) and cross-

species extrapolation of toxicity. This track will focus on EPA computational tools used for interpreting and predicting chemical and biological data.

- **CompTox Chemicals Dashboard with DSSTox Intro:** This session will cover DSSTox which contains foundational chemistry data for all of EPA's Center for Computational Toxicology and Exposure tools. Following DSSTox, experts will demonstrate the CompTox Chemicals Dashboard, and how to access various types of data with a brief discussion at the end. [Includes: Demonstration; Q/A]

- **TEST:** This session will contain an overview of the downloadable version of TEST and a live demonstration of TEST's functionality in the browser-based WebTEST. The Prediction 1 and Prediction 2 modules from the Cheminformatics Analysis Modules will be included in the live demonstration. [Includes: Demonstration; Q/A]

- **Cheminformatics Analysis Modules:** Building on the modules covered in the TEST session, this session will include a deep dive of the Hazard Comparison Module and Structure/Substructure search available within the Cheminformatics online modules. The session will also cover a quick introduction of the proof-of-concept modules that are in development. [Includes: Demonstration; Q/A]

- **GenRA:** This session will allow attendees to have an interactive experience with EPA's publicly available read-across tool, GenRA. GenRA is an automated approach to make reproducible read-across predictions of toxicity. Experts will lead a demonstration of GenRA features and functionality, including examples to generate objective and reproducible read-across predictions. [Includes: Demonstration; Q/A; Interactive Activity]

Track 4 – Ecotoxicology: EPA's ecotoxicological assessment models span the sequence of events typical of ecological toxicity, including environmental release, fate and transport, exposure, internal dosimetry, metabolism, and toxicological responses. This track will explore EPA's ecotoxicology and computational toxicology tools, as well as conceptual frameworks that assemble existing knowledge about biological events that lead to adverse health effects in human populations and ecosystems.

- **ECOTOX Knowledgebase:** This session will allow attendees to deepen their knowledge of how the ECOTOX knowledgebase can be used with other EPA online tools like the CompTox Chemicals Dashboard. The session will begin with an example and then open up for users to ask questions about how to apply ECOTOX to their own work. [Includes: Demonstration; Q/A; Interactive Activity]

- **SeqAPASS:** This session will demonstrate how SeqAPASS can be used to help determine chemical susceptibility for animals with little toxicity data. Participants will see how SeqAPASS draws from other tools like the ECOTOX knowledgebase and the CompTox Chemicals Dashboard. [Includes: Demonstration; Q/A]

- **AOP-Wiki:** This session will allow attendees to gain familiarity with publicly accessible sources of computational toxicology data, like the CompTox Chemicals Dashboard, and associated translational knowledge frameworks, like the AOP-Wiki. You will get the chance to apply data from new approach methods to address a toxicological question. [Includes: Demonstration; Q/A; Interactive Activity]

- **ToxCast / SeqAPASS / ECOTOX Case Study:** This case study will explore how users may consider potency values derived from ToxCast bioactivity assays in combination with cross-species applicability information from SeqAPASS and curated records in ECOTOX. [Includes: Demonstration; Q/A]

PI Biographies

Christina Baghdikian

Christina Baghdikian is the Communications Director of the Center for Computational Toxicology and Exposure (CCTE) in EPA's Office of Research and Development (ORD). Christina coordinates strategic science translation and communication by facilitating two-way engagement with the agency's diverse stakeholders. Her goal is to increase the awareness, accessibility, and impact of agency environmental health research. Christina joined EPA as an American Schools and Programs of Public Health (ASPPH) fellow in 2013 and served as a Presidential Management Fellow from 2015 to 2017. Christina received her M.P.H. in Environmental Health Sciences from the University of Michigan, School of Public Health and a B.S. in Public Health Sciences from UC Irvine.

Marissa Brickley

Marissa Brickley received her master's degree in integrated biosciences from the University of Minnesota Duluth, where she was advised by Dr. Carlie LaLone (U.S. EPA/CCTE). Her master's research focused on broadening the definition of the taxonomic domain of applicability of adverse outcome pathways through bioinformatics approaches. Currently, Marissa is pursuing a PhD at the University of Minnesota-Duluth continuing under the direction of Dr. LaLone. Her research focus includes furthering adverse outcome pathway application and studying effects of pesticides across multiple species.

Alex Chao

Alex Chao's primary research focus is the development of tools that support processing and interpretation of high-res mass spectrometry (HRMS)-based non-targeted analysis (NTA) study data. This includes coding development and support on the EPA NTA WebApp as a standardized tool for processing NTA data. Other research areas include application of both the NTA WebApp and other new methods (i.e. metadata retrieval, machine learning, interactive visualizations) to support on-going exposomic studies. Alex received his Bachelor's in chemistry and Master's in analytical chemistry from the University of North Carolina at Chapel Hill.

Jessica Daniel

Jessica Daniel supports EPA ORD's National Research Programs with outreach and stakeholder engagement, including the Chemical Safety for Sustainability Research Program. She also helps lead the NAMs Training Program. Jessica has been with EPA ORD for the past 13 years working to increase access to EPA's research through advancing outreach and engagement strategies. Jessica received her Bachelor's degree in environmental communications from Oglethorpe University and her Master of Environmental Management from Duke University.

Stephen Edwards

Dr. Steve Edwards is the Director for the Scientific Computing and Data Curation Division in CCTE. Dr. Edwards previously worked as a Bioinformatics Senior Scientist within the GenOmics, Bioinformatics, and Translational Research Center at RTI International. His research examined the combined impact of genetic and environmental factors on disease manifestation to better support both precision medicine and public health protection. Prior to joining RTI, Steve worked for EPA where he used computational approaches to describe the mechanisms by which chemicals cause disease and thereby aid the interpretation of high-throughput toxicity test results. Steve received his Bachelor of Science in chemistry from the University of North Carolina at Chapel Hill and his Doctorate in Pharmacology from Vanderbilt University Medical Center.

Jennifer Ehlinger

Jennifer Ehlinger is a graduate of the NC State Technical Writing program with a focus in STEM popularization and science communications. They have previously assisted in communications for NC State's CALS International Programs department by developing journalistic articles about ongoing faculty and student environmental and agricultural research. Jennifer began their work with the EPA as a Student Services Contractor through ORAU's National Student Services Contract in 2021. They currently serve as part of the Outreach Stakeholder Engagement and Training Section (OSETS) as a Research Outreach and Communications Specialist.

Marina Evans

Dr. Marina V. Evans is a biomedical engineer in CCTE. Her Ph.D. focused on the development and evaluation of pulmonary models used for clinical measurements. She joined EPA with the goal of generating experimental data used to calibrate inhalation physiologically based pharmacokinetic (PBPK) models. An engineer and systems physiologist by training, Dr. Evans has focused her research on the modeling of multiple organs systems and evaluation using experimental data. At EPA, she has focused on the development of PBPK models and their application in risk assessment.

Logan Everett

Dr. Logan Everett is an experienced scientist with a wealth of expertise in bioinformatics, computer science, genomics, statistics, genetics and molecular biology. His research in CCTE is focused on advancing the application of high-throughput transcriptomics in chemical screening. He received a B.S. in computer science and Ph.D. in genomics and computational biology, followed by extensive postdoctoral training in various applications of next-generation sequencing data analysis.

Madison Feshuk

Madison Feshuk is a biologist in CCTE multidisciplinary scientific research efforts by developing and applying innovative data science solutions. These efforts are crucial to promote the adoption of NAMs and increase data interoperability to ultimately achieve reductions in animal testing and improve environmental risk assessment and regulatory decision-making. Her expertise includes database development and maintenance, data wrangling and analysis, project management, user acceptance testing, and quality evaluation efforts, specifically supporting *in vitro* chemical screening data in the Toxicity Forecaster (ToxCast)'s invitroDB and legacy *in vivo* toxicity study curations in the Toxicity Reference Database (ToxRefDB).

Annette Guiseppi-Elie

Dr. Annette Guiseppi-Elie is the Director of the Chemical Safety for Sustainability National Research Program in EPA's Office of Research and Development. Dr. Guiseppi-Elie first joined EPA in 2015 as the Associate Director for Exposure Science at the agency's National Exposure Research Laboratory. Dr. Guiseppi-Elie is also a Fellow of the American Institute of Medical and Biological Engineering.

Sakshi Handa

Sakshi Handa currently serves as a Biologist/Data Lead within the Scientific Computing and Data Curation Division (SCDCD) of EPA's CCTE. She has been with EPA since 2017, beginning as an Oak Ridge Institute for Science and Education (ORISE) participant in toxicokinetic modeling. She graduated from North Carolina State University with a Bachelor of Science in biological engineering. She currently acts as the data lead for Factotum, an internal data curation tool, as well as the related public-facing ChemExpo tool for surfacing consumer product and exposure relevant data.

Claire Holesovsky

Claire Holesovsky is a science communication professional interested in linking research with practice to support the community of those interested in science. She works for EPA as a Public Affairs Specialist within ORD. Much of her work focuses on communicating about research within the Center for Public Health and Environmental Assessment. Claire holds a Master's degree in Life Sciences Communication from the University of Wisconsin-Madison, where she researched public attitudes and policies surrounding controversial science and public engagement with science. Her experiences, working in both academic and non-academic settings, have enabled her to develop a commitment to building productive collaborations and partnerships with diverse groups of people and perspectives.

Kristin Isaacs

Dr. Kristin Isaacs is a Research Physical Scientist in the CCTE at EPA. Since 2014, she has been a co-lead of the Exposure Forecasting (ExpoCast) project under the Office of Research and Development (ORD) and its Chemical Safety for Sustainability National Research Program. Her research focuses on characterizing chemical exposure pathways for human and ecological receptors and developing high-throughput computational approaches for quantifying exposures for use in chemical safety decision-making. She is currently a Government Councilor the Board of Directors of the International Society for Exposure Science and serves on a variety of national and international workgroups related to advancing exposure science.

Carlie LaLone

Dr. Carlie LaLone's primary research interest is developing tools for researchers and decision makers to extrapolate biological knowledge from one species to the diversity of species and predict chemical susceptibility to species that could never be tested in the laboratory. Her research uses complex bioinformatics approaches and translates them into user-friendly pipelines and web-based tools useful for making predictions of chemical susceptibly across hundreds to thousands of species. Therefore, Dr. LaLone's research interests span understanding adverse effects of chemical and non-chemical stressors across species, with an emphasis on aquatic organisms. She leads a research team that integrates computational and laboratory studies to evaluate pharmaceuticals, veterinary drugs, pesticides, endocrine disrupting chemicals, and current chemicals of concern to the Agency. Specifically, the focus of her research is on applied science relative to developing methodology and computer applications to be used in ecological risk assessment, based on sound scientific supporting evidence.

Jason Lambert

Dr. Jason Lambert is a board-certified toxicologist and human health risk assessor in the CCTE within EPA, who spent 14 years serving as Chemical manager for more than 30 Integrated Risk Information System (IRIS) or Provisional Peer-Reviewed Toxicity Value (PPRTV) human health assessments. In 2007, Dr. Lambert founded an Alternative Methods team, which led the integration of read-across into PPRTVs for data-poor chemicals. He has also led or co-authored multiple EPA methods and approaches documents pertaining to chemical mixtures risk assessment. Dr. Lambert earned a Ph.D. (2003) and M.S. (2001) in pharmacology and toxicology and a B.S. (1998) in biology with a double-major in recombinant genetics and chemistry. His research expertise includes mechanisms of hepatic and gastrointestinal injury and repair, molecular and cellular signal transduction, and the development of cellular therapeutics, such as recombinant probiotics.

Monica Linnenbrink

Monica Linnenbrink leads CCTE's Research Planning and Implementation team, where she directs high level scientific and administrative staff responsible for planning, coordinating and evaluating research.

Monica also coordinates external stakeholder engagement strategies aimed at encouraging use of NAMs through outreach and training activities such as workshops, demonstrations, webinars, presentations and training videos. Monica received her Bachelor's in public relations from the University of Florida and her Master's in public administration from Florida State University.

Charlie Lowe

Dr. Charles (Charlie) Lowe is a computational chemist in EPA's ORD, CCTE, Chemical Characterization and Exposure Division (CCED), Computational Chemistry and Cheminformatics Branch (CCCB). He received his Bachelor's degrees in chemistry and applied mathematics from Marshall University and his doctorate in physical (computational) chemistry from Clemson University. During his postdoctoral research, he gained expertise in the analysis of environmental exposure data generated through nontargeted and suspect screening analyses, constructed machine learning models to predict the amenability of chemicals to liquid chromatography–mass spectrometry (LC-MS) and developed cheminformatics tools to rapidly acquire, curate and model environmentally-relevant chemical data. As a principal investigator, his interests involve the continued addition and curation of chemical data for DSSTox, the development of new models for physicochemical properties to support other research within the Agency, and the development of a new database, VSSTox, to capture virtual chemicals not necessarily identified in existing scientific literature. In his free time, he enjoys hiking, cooking, and managing a large collection of plastic models.

Anna Lowit

Dr. Anna B. Lowit received her Ph.D. in Environmental Toxicology from the University of Tennessee in 1998 where she was a Graduate Fellow in Sustainable Waste Management. Dr. Lowit began her career with EPA in 1998. She is currently the Senior Science Advisor in the Office of Pollution Prevention and Toxics. She advises senior managers and leads multidisciplinary teams on a variety of cross-cutting topics related to human health and ecological risk assessment. Some of these topics include new approach methods, PBPK models, mode of action/adverse outcome pathways, and cumulative risk assessment. She served as the one of the Co-Chairs of the Interagency Coordinating Committee on the Validation of Alternative Methods (ICCVAM) from 2013 to 2024. She is the US lead for the OECD Working Party on Hazard Assessment.

Todd Martin

Dr. Todd Martin is an expert in computational toxicology with more than 20 years of experience. He is the lead developer of TEST (Toxicity Estimation Software Tool) which allows users to easily estimate toxicity and physical property endpoints from molecular structure.

Esra Mutlu

Dr. Esra Mutlu, DABT, is currently a program manager for one of EPA's human health assessment products and research outreach and communication specialist in the CCTE. She serves as technical point of contact for communicating CCTE research and translating complex scientific topics for a range of audiences. As a part of her role, Dr. Mutlu is co-leading the NAMs Training Pilot Program at and managing several extramural vehicles to support CCTE programs to organize activities, such as ensuring coordination of chemistry activities in support of short-term *in vivo* and transcriptomic studies across various teams. Prior to that, Dr. Mutlu worked as a chemist at the National Institute of Environmental Health Sciences (NIEHS) in the Division of the National Toxicology Program (NTP). In her position, she provided NTP with expertise in organic chemistry, analytical chemistry, and interpretation and application of mass spectrometry and served on NTP study design teams to provide technical assistance in these areas of chemistry.

Jennifer Olker

Dr. Jennifer Olker is the Coordinator for the ECOTOX Knowledgebase in the CCTE within EPA. Through the ECOTOX project, Dr. Olker works to support criteria development, assessments and research in EPA Program Offices, Regions and ORD using systematic methods to identify and curate ecotoxicity data. In addition, she is involved in research at the Duluth lab on endocrine disruption utilizing *in vivo* and *in vitro* assays and the development of adverse outcome pathways (AOPs). Prior to joining EPA in 2015, Dr. Olker received her Ph.D. in integrated biosciences and was at the University of Minnesota's Natural Resources Research Institute for more than 10 years conducting research in aquatic and landscape ecology.

Grace Patlewicz

Dr. Grace Patlewicz is a chemist and toxicologist by training, bringing industrial and regulatory experience from both Europe and the United States. Her research focuses on the development and application of quantitative structure-activity relationships ((Q)SARs), a technique that predicts properties of unknown molecules, and read-across for regulatory purposes, a way to use similar substances to predict the toxicity of other similar chemicals. She has authored journal publications and book chapters on numerous topics related to toxicology, chaired various industry groups, and has contributed to the development of technical guidance for (Q)SARs, chemical categories and AOPs under Organization for Economic Co-operation and Development (OECD) work programs.

Katie Paul Friedman

Dr. Katie Paul Friedman is a toxicologist in the CCTE within EPA. She works with predictive assay and systems biology models to prioritize chemicals and mixtures for further evaluation, with particular expertise in developmental and endocrine toxicities. One of her goals is to modernize and improve prioritization and risk assessment of environmentally-relevant chemicals. As part of her work, Dr. Paul Friedman coordinates and leads endocrine-related computational toxicology research, analyzes high-throughput screening assay datasets, integrates multiple data sources into systems biology models of toxicological relevance for endocrine function, and develops case studies that illustrate the utility of high-throughput screening data for prioritization and risk assessment tasks.

Katherine Phillips

Dr. Katherine Phillips' research focuses on collecting and curating data relevant to chemical exposure and using machine learning techniques to fill gaps in this data landscape. These techniques have been useful for investigating the proposal of chemical alternatives, as well as plausibility of chemicals identified in nontargeted analysis.

Risa Sayre

Dr. Risa Sayre is researching spatiotemporal statistics for exposure modeling in the CCTE at EPA. An as ORISE research participant, Dr. Sayre contributed to several projects within EPA's ExpoCast project involving machine learning (or machine training, as she thinks it should be called) and evaluation of models used to predict toxicology, toxicokinetics and exposure.

Celia Schacht

Dr. Celia Schacht is an ORISE Postdoctoral Fellow in the Center for Computational Toxicology & Exposure at EPA. She earned her M.S. in applied mathematics and Ph.D. in biomathematics, where she focused on characterizing uncertainty and variability in aggregate mathematical models and PBPK models. Her work at EPA focuses on developing PBTK models in the utilization of high-throughput

toxicokinetics, including inhalation and mixtures modeling. Other research interests include code development and programming, uncertainty quantification and dynamical systems.

Nisha Sipes

Dr. Nisha Sipes brings a multidisciplinary background in engineering, cell and molecular biology, and computational toxicology, as well as a driven passion to increase translation of our research for adoption and ultimate use. Her postdoctoral training at EPA involved analyzing the ToxCast high-throughput screening assays, developing predictive models of developmental toxicity, and evaluating the ToxCast assays with respect to their ability to predict broader *in vivo* outcomes utilizing the high-throughput toxicokinetic modeling (HTTK) approaches. In her professional role in the National Toxicology Program Division at NIEHS, Dr. Sipes focused on leveraging *in silico* methods in HTTK modeling approaches to allow for broader applicability of these approaches to Tox21 chemicals, flame retardants, and potential developmental neurotoxicants. Now back at EPA, Dr. Sipes aims to facilitate the translation of CCTE's research for use in decisions and provide scientific and technical expertise to EPA Program Offices, EPA Regions and outside stakeholder groups with an interest in using CCTE research to inform public health and environmental decisions.

Jon Sobus

Dr. Jon Sobus is a physical scientist in EPA's ORD, CCTE. He earned a Ph.D. in environmental sciences and engineering from The University of North Carolina at Chapel Hill in 2008, and then completed a 2-year postdoctoral traineeship at EPA in Research Triangle Park, North Carolina. Dr. Sobus was hired as a permanent EPA employee in 2011 and co-led ORD's biomarkers research program for 5 years. Beginning in 2016, Dr. Sobus helped launch EPA's nontargeted analysis (NTA) research program. As a leader of ORD's NTA research activities, Dr. Sobus oversees the coordination of EPA's NTA WebApp, which is being designed to facilitate production-level NTA by EPA and partner labs.

Rusty Thomas

Dr. Rusty Thomas is the Director of the CCTE within EPA. His area of expertise is in the application of high-throughput and high data content approaches to chemical toxicity testing. He has a broad, multidisciplinary background and experience, but his formal academic training was in chemistry, radiation health physics and toxicology. He received postdoctoral training in molecular biology and genomics. Following his academic training, Dr. Thomas performed bioinformatics and genomics research in the biotechnology sector and gained experience in high-throughput screening and *in vitro* assay development in the biopharma sector. Prior to coming to EPA, Dr. Thomas worked as an investigator and the Director of the Institute for Chemical Safety Sciences at The Hamner Institutes for Health Sciences.

Scarlett VanDyke

Scarlett VanDyke works with the Outreach Stakeholder Engagement and Training team in the CCTE within EPA. She helps communicate CCTE's research to EPA's Program Office partners, Regional representatives, industry professionals, academia and the general public. She assists with NAMs training opportunities, such as virtual trainings for the CompTox Chemicals Dashboard and the ECOTOX Knowledgebase.

Dan Villeneuve

Dr. Dan Villeneuve is an aquatic ecotoxicologist in the CCTE within EPA. He conducts research with a focus on use of alternatives to traditional *in vivo* guideline toxicity tests to assess the ecological safety of chemicals. Dr. Villeneuve is heavily engaged in the development and use of the AOP framework as a tool for facilitating the use of new approach methodologies in chemical safety assessments and risk-based

decision-making. He conducts both laboratory and field research aimed at the development and practical use of biological effects assays for assessing potential adverse effects of organic chemicals. Dr. Villeneuve is also engaged in development and evaluation of high throughput, transcriptomics-based aquatic toxicity assays for chemical screening and prioritization.

Taylor Wall

Taylor Wall collaborates on various data curation projects within the Data Extraction & Quality Evaluation Branch. Areas of focus include chemical exposure and toxicology, with notable projects including development of the Multimedia Monitoring Database (MMDB) under Dr. Kristin Isaacs and development of automated workflows for the Concentration versus Time Database (CvTdb) under Dr. John Wambaugh. He is also the product lead for the development of the Data Accuracy Tool (DAT), which is designed to be a browser-based application for standardizing dataset quality control and managing data provenance of any dataset. His graduate research focused on the experiences of lay counselors providing a novel family therapy to improve child mental health in Eldoret, Kenya.

John Wambaugh

Dr. John Wambaugh finds solutions that capture the essence of complex problems. He co-leads the EPA's ExpoCast project (Exposure Forecasting), the aim of which is to identify the chemicals to which people are the most exposed. Working with the ToxCast team, ExpoCast develops high-throughput tools to prioritize among commercial chemicals based on risk posed to public health. These tools include exposure assessment, toxicokinetics and toxicity testing. They use math modeling, machine learning and statistics to better understand existing data. They also design new experiments to fill data gaps. ExpoCast research helps identify chemical public health risks while reducing animal testing.

Tony Williams

As a Title 42 Principal Investigator, Dr. Tony Williams is focused on the application of cheminformatics to support multiple projects in the center. These include the development of the DSSTox database that underpins the CompTox Chemicals Dashboard, structure standardization approaches to support QSAR modeling, and the development of informatics systems to support nontargeted analysis mass spectrometry. Dr Williams conceived the Comptox Chemicals Dashboard (https://comptox.epa.gov) and was the product owner for 6 years and 11 releases. He is responsible for managing the development of a number of informatics prototypes to support the EPA mission. Dr. Williams applies his analytical science skills in developing informatics approaches to support mass spectrometry based nontargeted analysis.) and was the product owner for 6 years and 11 releases. He is responsible for managing the development of a number of informatics prototypes to support the EPA mission. Dr. Williams applies his analytical science skills in developing informatics approaches to support mass spectrometry based nontargeted analysis.