



## Chemical Safety Analytics Research Area

*Curated data and scientifically defensible models are required for chemical safety decisions, yet many chemicals lack sufficient information on hazard, exposure, dosimetry, or susceptible populations. EPA's Chemical Safety for Sustainability Research Program develops predictive models and tools to address data gaps in chemical safety decisions.*

### EPA's Chemical Safety for Sustainability Research Program

The goal of EPA's Chemical Safety for Sustainability (CSS) National Research Program is to provide information and methods to make better-informed, more timely decisions about the safety of chemicals, many of which have not been thoroughly evaluated for potential risks to human health and the environment.

### About Chemical Safety Analytics Research

The **Chemical Safety Analytics** research area provides inherent information on chemicals and develops models and tools that facilitate more integrated and efficient safety evaluations. This research improves the understanding of chemical fate and activity in both organisms (humans and wildlife) and the environment to support chemical safety decision making.

Research includes:

- Efforts to efficiently assemble data from an array of sources to inform chemical safety decisions
- The extrapolation of the effects of certain chemicals across species to predict responses in other groups
- The development of web tools for high-throughput prediction of toxicity and physical properties and features to visualize toxicity data for multiple chemicals and toxicity categories

### Why Is Chemical Safety Analytics Research Important?

Research conducted by Chemical Safety Analytics provides curated chemical information and develops predictive models and tools to establish common principles linking biological and chemical properties to potentials for toxicity, exposure, environmental persistence, and transformations in environmental and biological systems.

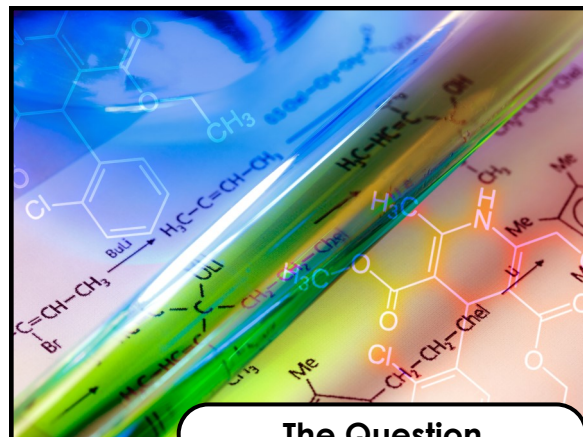
### Interested In Learning More?

EPA's Chemical Safety Research Program: [epa.gov/chemical-research](http://epa.gov/chemical-research)

#### Contact Us:

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### The Question

How can we collect and disseminate information on chemicals to help with safety evaluation?

### Our Chemical Safety Analytics Tools



**CompTox Chemicals Dashboard:** dashboard providing access to chemistry data for thousands of chemicals across EPA's computational research databases including:

⇒ **EDSP21 Dashboard:** high-throughput screening and exposure estimates for evaluating chemicals for potential endocrine activity



**SeqAPASS:** tool allowing researchers and regulators to extrapolate toxicity information across species



**AOP-Wiki:** interactive, crowd-sourced tool for AOP development, organizing available knowledge and evidence into written descriptions of individual pathways. The platform allows users to capture, review, browse, and comment on AOPs.

## Chemical Safety Analytics Research Area Up Close



### How Chemical Safety Analytics Fits In

CSS is organized around three research topics that address specific science challenges in assessing the safety of chemicals: Chemical Evaluation, Complex Systems Science, and Knowledge Translation & Delivery.

Included in our *Knowledge Translation & Knowledge Delivery*, our **Chemical Safety Analytics** research is delivering predictive computer models and tools to address data gaps in chemical safety decisions, particularly for chemicals lacking information on hazard or impacts on susceptible populations (including the very young and elderly).

### Examples of Research and Products

#### A Web-enabled version of Toxicity Estimation Software Tool (T.E.S.T)

- ⇒ **What is it?:** A tool that allows users to easily estimate the toxicity of chemicals using Quantitative Structure Activity Relationships (QSARs), mathematical models used to predict measures of toxicity from the physical characteristics of the structure of chemicals.
- ⇒ **Impact:** A web-based version of T.E.S.T. enables users to estimate human health hazard, ecotoxicity, and physicochemical properties directly within a web browser and from EPA tools such as the Chemical Transformation Simulator
- ⇒ **Who Can Use It?:** Everyone, particularly US EPA partners responsible for chemical safety, chemical companies performing alternatives assessments, and the general scientific community.
- ⇒ **Learn More:** [epa.gov/chemical-research/toxicity-estimation-software-tool-test](http://epa.gov/chemical-research/toxicity-estimation-software-tool-test)

#### Incorporation of Generalized Read-Across (GenRA) with CompTox Chemicals Dashboard

- ⇒ **What is it?:** An automated approach to make reproducible read-across predictions of toxicity outcomes from *in vivo* studies, called Generalized Read-across (GenRA), that has been incorporated into the CompTox Chemicals Dashboard
- ⇒ **Impact:** GenRA provides an easily accessible, more objective approach to read-across, or the process of using data on one chemical to predict the behavior of similar chemical with less data. GenRA combines as many expert considerations used within current read-across approaches as possible with data-driven approaches to transition read-across towards a more systematic and data-based method of making predictions.
- ⇒ **Who Can Use It?:** Anyone looking for chemical data, particularly about chemicals with little information
- ⇒ **Learn More:** [comptox.epa.gov/dashboard](http://comptox.epa.gov/dashboard)

#### Learn more

EPA's Chemical Safety Research Program: [epa.gov/chemical-research](http://epa.gov/chemical-research)