



Informatics, Synthesis & Integration Research Area

Research conducted by CSS scientists, coupled with continually expanding amounts of traditional toxicological and exposure data, enables more informed chemical safety decisions, provided data are available. EPA's Chemical Safety for Sustainability Research Program supports the development of online tools and platforms to integrate chemical information to facilitate better access to information.

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 Informatics, Synthesis & Integration Research

The **Informatics, Synthesis, and Integration** research area provides integrated chemical information from multiple sources of data, models, and tools needed to efficiently evaluate the safety of chemicals. This research area integrates the output from other research areas and develops approaches to present, manage, and utilize the large data streams from EPA research and relevant external data sources.

The data, tools, and products developed by EPA researchers are often spread across online databases and websites. The ISI research area aims to increase efficiency in product development and deployment.

Why Is Informatics, Synthesis & Integration Research Important?

Chemical Safety for Sustainability conducts large amounts of research, generating extensive chemical information. In order to make this research available to interested parties, Informatics, Synthesis, and Integration research develops novel, efficient approaches to present, manage, and use large data streams in support of chemical safety assessments.

Interested In Learning More?

EPA's Chemical Safety Research Program: epa.gov/chemical-research

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The Question

How can we better integrate and use data from new scientific approaches?

Our Informatics, Synthesis & Integration Tools



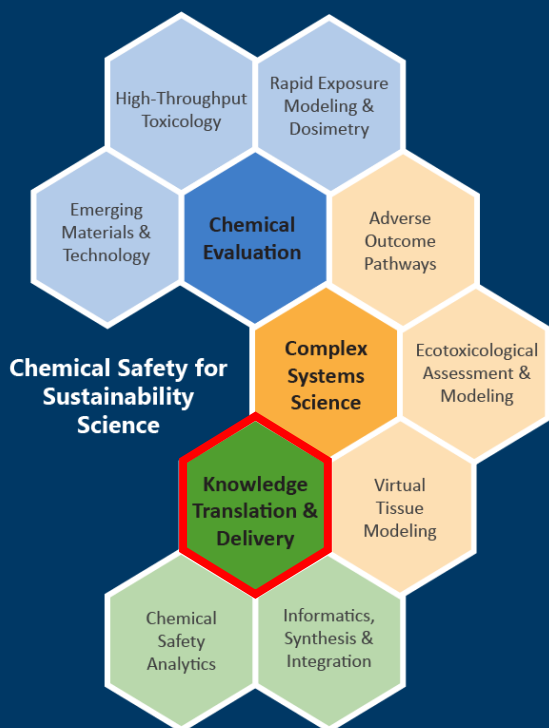
CompTox Chemicals Dashboard:

dashboard that provides chemistry data for thousands of chemicals across EPA's computational research databases including:

- ⇒ **CPDat:** database containing information on chemicals in consumer products
- ⇒ **ToxCast:** high-throughput screening data
- ⇒ **GenRA:** algorithmic, automated read-across information
- ⇒ **AcTOR:** Aggregated Computation Toxicology Online Resource
- ⇒ **ECOTOX:** application providing information on adverse effects of single chemicals on ecologically relevant aquatic and terrestrial species

Informatics, Synthesis & Integration Research Area Up Close

Visualizing the CSS Program



Our **Informatics, Synthesis & Integration** research is categorized under the **Knowledge Translation & Delivery** research topic. This topic is dedicated to delivering data and information resources relevant to chemical safety, providing risk assessors and decision-makers with scientifically sound toxicity testing methods, data, and tools.

How Informatics, Synthesis & Integration 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 & Delivery* research topic, our **Informatics, Synthesis & Integration** research is focused on developing efficient approaches to present, manage, and utilize large data streams and making data, tools, and modes more easily accessible for risk assessors and decision-makers.

Examples of Research and Products

CompTox Chemicals Dashboard v3.0

- ⇒ **Description:** A dashboard for chemistry, toxicity, and exposure information for over 760,000 chemicals, including recent updates such as a GenRA (Generalized Read Across) module, which lets users find chemicals similar to their target chemical, based on chemical structural similarity. Additional features include the display of sets of chemicals based on product or use categories, and more accessibility improvements.
- ⇒ **Impact:** Data and models within the Dashboard help with efforts to identify chemicals in most need of further testing and reduce the use of animals in chemical testing.
- ⇒ **Who Can Use It?:** CompTox is publicly available.
- ⇒ **Learn More:** comptox.epa.gov/dashboard

Computational models predicting impact of chemical exposures on androgen receptor activity and steroidogenesis

- ⇒ **Description:** In support of the Endocrine Disruptor Screening Program (EDSP), EPA demonstrates and evaluates the use of new high-throughput screening methodologies, models, and data to more rapidly prioritize and identify chemicals for potential endocrine system activity. EPA scientists have prioritized chemicals for EDSP Tier 1 testing based on predictive models for androgen receptor (AR) activity and steroidogenesis.
- ⇒ **Impact:** The AR and steroidogenesis models provide high-throughput strategies for screening and prioritizing chemicals for endocrine-disrupting potential.
- ⇒ **Who Can Use It?:** Everyone, including researchers and risk assessors
- ⇒ **Learn More:** epa.gov/endocrine-disruption/use-high-throughput-assays-and-computational-tools-endocrine-disruptor

Learn more

EPA's Chemical Safety Research Program: epa.gov/chemical-research