

EPA Tools and Resources Webinar:

Chemical Safety Research Online Tools & Resources

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Presentation Outline

- Chemical Safety Research Overview
- Examples of Online Tools and Resources
- Complete List of Online Tools and Resources
- How to Learn More
- Contact Information



Chemical Safety Research

What we do:

- Provide research to rapidly evaluate potential human health and environmental risks due to exposure to environmental chemicals
- Expand understanding of quantitative human and ecological exposures to thousands of chemicals

How we do it:

- Perform rapid screening and evaluation on thousands of chemicals to evaluate for potential risk
- Develop information systems containing data with software tools to use to inform a range of human health and environmental decisions
- Actively engage a wide-range of stakeholders to help make new chemical information more understandable and usable

Why we do it:

- Help Region and Program Offices, states, tribes, and communities use information to make decisions to sustain a healthy society and environment
- Research and data used to support Toxic Substance Control Act, Endocrine Disrupting Screening Program and Contaminants of Emerging Concern



EPA's Safer Chemicals program produces a variety of computational tools to assist users in decision-making, researching, and evaluating chemical information. These tools offer a wealth of chemistry, toxicity, and exposure data that is publicly accessible.



ChemExpo Knowledgebase

The Chemical Exposure Knowledgebase (ChemExpo) is an interactive tool for exploring and searching information on how chemicals are used in commerce and in consumer products.

[ChemExpo Resource Hub](#)



Cheminformatics Modules

Cheminformatics analysis modules provide high-quality chemical structures, experimental and predicted physicochemical properties, environmental fate and transport information, and linked toxicity data.

[Cheminformatics Resource Hub](#)



CompTox Chemicals Dashboard

The CompTox Chemicals Dashboard provides publicly-accessible chemistry, toxicity, and exposure information for over one million chemicals. This information includes physicochemical data, hazard data, and much more.

[CompTox Chemicals Dashboard Resource Hub](#)



GenRA Tool

The Generalized Read-Across (GenRA) tool is an algorithmic approach to permit objective and reproducible read-across.



ECOTOX Knowledgebase

The Ecotoxicology (ECOTOX) Knowledgebase is a comprehensive database providing information on



SeqAPASS Tool

The Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS) tool is a web, online screening tool that allows

Where to start?

comptox.epa.gov

CompTox Chemicals Dashboard

- Contains information for over one million chemicals
- Includes chemistry, toxicity, and exposure data
- For example: chemical structures, experimental and predicted physicochemical and toxicity data, hazard and bioassay data, and additional links to relevant websites and applications.

State Use Examples: **California, Minnesota and Washington**



ChemExpo Knowledgebase

- Publicly accessible data search and visualization tool for exploring chemical data relevant to exposure assessment that has been curated from public documents.
- Focuses on data collected about how chemicals are used in commerce and how they occur in consumer and industrial products.

State Use Example: **California, Minnesota and Washington**



EcoTox Knowledgebase

- Comprehensive, publicly available application that provides information on adverse effects of single chemical stressors to ecologically relevant aquatic and terrestrial species.
- Data are curated from scientific literature after an exhaustive search protocol.
- Compiled from over 53,000 references, ECOTOX currently includes over one million test records covering more than 13,000 aquatic and terrestrial species and 12,000 chemicals.

State Use Example: **New York, New Hampshire, Wisconsin and Pennsylvania**



epa.gov/ecotox

APIs and Data

- EPA APIs enable users to extract specific data from various databases and integrate them into their applications.
 - Searching for chemicals, files for chemical structure and chemical details
 - Human and ecological hazard data
 - Chemical bioactivity data
- Data
 - Animal toxicity
 - High-throughput screening
 - Chemicals and chemistry
 - Exposure and Dose

Computational Toxicology and Exposure Data

What are they used for?

Interfaces (APIs) enable users to extract specific data from various databases and computational toxicology and exposure data APIs are a suite of REST APIs that provide information. These APIs are hosted on cloud.gov, a secure cloud environment managed by the General Services Administration specifically for US Federal Government applications.

What is available?

There are three microservices: Chemical, Hazard, and Bioactivity:

The Chemical microservice offers APIs for searching chemicals, retrieving chemical structure files in various formats (e.g., mol and svg), mol, and mrv, accessing both experimental and predictive chemical properties, and other chemical-related information.

The Hazard microservice provides APIs for retrieving hazard data linked to a requested chemical, using the chemical's dtxsid. This microservice has three endpoints for retrieving all hazard data or specific data for human health, ecological, and chemical safety.

The Bioactivity microservice offers APIs for retrieving data using either the dtxsid or aeid.

For more information, visit the Computational Toxicology and Exposure Data APIs page, which is located at <https://www.epa.gov/ccte/ccte.epa.gov/docs/> and the QR code above. To ensure efficient usability, the APIs are designed for authorized users with an API key. Please send an email to ccte_api@epa.gov to request an API key.

Want to Learn More ?

New Approach Methods (NAMs) Training

EPA's New Approach Methodologies (NAMs) Training website makes training materials and opportunities related to EPA-developed risk assessment tools freely available and easily accessible to all stakeholders.

The NAMs Training website contains more than 90 resources, including:



Featured tools cover include the CompTox Chemicals Dashboard, ECOTOX, SeqAPASS, G and more!



- EPA Training Program
 - Durham, NC In Person Training April 4-6, 2024
<https://www.epa.gov/chemical-research/new-approach-methods-nams-training>
- Demonstrations and presentations at conferences
- Regular webinars
- Provide in-depth customized trainings for states, tribes, EPA regions, EPA regulatory offices and other stakeholder groups

Demonstrations

- Could these online tools help inform decisions you make at work about chemicals?
- Which of these online tools most interest you?
- Quickly show demonstrations of online tools with most interest

More Online Tools and Resources

- [Adverse Outcome Pathway \(AOP\)-Wiki](#): The primary repository of qualitative information for the international AOP development effort coordinated by the Organisation for Economic Co-operation and Development (OECD).
- [Chemical Exposure \(ChemExpo\) Knowledgebase](#): An interactive tool for exploring and searching information on how chemicals are used in commerce and in consumer products.
- [Cheminformatics Modules](#): Provides high-quality chemical structures, experimental and predicted physicochemical properties, environmental fate and transport information, and linked toxicity data.
- [CompTox Chemicals Dashboard](#): Provides publicly-accessible chemistry, toxicity, and exposure information for over one million chemicals. This information includes physicochemical data, hazard data, and much more.
- [Ecotoxicology \(ECOTOX\) Knowledgebase](#): A comprehensive database providing information on adverse effects of single chemical stressors to ecologically relevant aquatic and terrestrial species.
- [Generalized Read-Across \(GenRA\) Tool](#): An algorithmic approach to permit objective and reproducible read-across predictions of *in vivo* toxicity and *in vitro* bioactivity.
- [High-Throughput Toxicokinetics \(httk\) R Package](#): Uses human *in vitro* data to make predictions about the fate of chemicals in humans, rats, mice, dogs, and rabbits.
- [Non-Targeted Analysis Web Application](#): A tool for making NTA studies more efficient, affordable, reproducible, harmonized, and actionable.
- [Sequence Alignment to Predict Across-Species Susceptibility \(SeqAPASS\) Tool](#): A fast, online screening tool that allows researchers and regulators to extrapolate toxicity information across species.
- [Toxicity Estimation Software Tool \(TEST\)](#): Easily estimate the toxicity of chemicals using Quantitative Structure Activity Relationships (QSARs) methodologies.
- [Toxicity Forecasting \(ToxCast\)](#): Makes *in vitro* medium- and high-throughput screening assay data publicly available for prioritization and hazard characterization of thousands of chemicals.

Contact

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