National Toxicology Program
U.S. Department of Health and Human Services

Free public resource

Integrated Chemical Environment (ICE)

https://ice.ntp.niehs.nih.gov

ICE provides data and tools for the development and evaluation of new chemical safety testing methods.

Gain free online access to:

- Curated in vitro and in vivo experimental data with toxicologically relevant assay annotations.
- In silico toxicity predictions and chemical property data.
- Reference chemical quick lists.
- Computational tools for in vitro to in vivo extrapolation (IVIVE), physiologically based pharmacokinetic (PBPK) modeling, chemical characterization, and chemical similarity searching.

Use ICE resources to:

- Retrieve and examine toxicity and chemical data anchored to relevant regulatory endpoints.
- Interactively explore and visualize results to generate publication-quality figures.
- Merge and compare data from different test methods and endpoints across chemicals.
- Perform IVIVE and PBPK analyses via a simple user interface.

For more information, contact ICE-support@niehs.nih.gov.

https://ntp.niehs.nih.gov/go/niceatm

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Free public resource

Open Structure-activity/property Relationship App (OPERA)

https://github.com/NIEHS/OPERA

OPERA is a free and open-source quantitative structure-activity relationship (QSAR) tool.

Use OPERA to predict:

- Physicochemical properties (logP, logD, pKa, melting point).
- Environmental fate endpoints (bioconcentration, biodegradability).
- Pharmacokinetic properties (Fub, CLint, Caco2).
- Toxicity-using consensus models.
  - CERAPP: Collaborative Estrogen Receptor Activity Prediction Project.
  - CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity.
  - CATMoS: Collaborative Acute Toxicity Modeling Suite.

OPERA can be used through:

- Executables and source code (https://github.com/NIEHS/OPERA):
  - Stand-alone application (GUI and command line).
  - Embeddable libraries (java, C, C++, Python).
  - Multiple platforms (Windows and Linux).
- EPA's Chemistry Dashboard (https://comptox.epa.gov/dashboard).
- NTP's Integrated Chemical Environment (https://ice.ntp.niehs.nih.gov).

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