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

Open-Source Computational Tools
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.
- Chemical quick lists containing reference or non reference chemicals categorized by regulatory endpoint or data type.
- Computational tools for in vitro to in vivo extrapolation (IVIVE), physiologically based pharmacokinetic (PBPK) predictions, chemical characterization, chemical similarity searching, and exploring in vitro concentration response curves.

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/whatwestudy/niceatm/comptox

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Open-Source Computational Tools

Open Structure-activity/property Relationship App (OPERA)

https://github.com/NIEHS/OPERA

OPERA is a downloadable tool that provides quantitative structure-activity relationship (QSAR) model predictions for:

- Physicochemical properties
- Pharmacokinetic properties
- Environmental fate and toxicity endpoints

OPERA predictions include information about applicability domain and accuracy assessments.

OPERA is available in command line and user-friendly graphical interface versions for Windows and Linux. Model predictions are available through NICEATM s Integrated Chemical Environment (https://ice.ntp.niehs.nih.gov).

ChemMaps.com

https://sandbox.ntp.niehs.nih.gov/chemmaps

ChemMaps.com is a cheminformatics-powered web server that allows users to explore drug and environmental chemical properties by point and-click navigation. Overlaying chemical features, such as physico chemical properties (e.g., molecular weight, LogP), with bioactivity data from ToxCast/Tox21 assays facilitates interpretation and analysis.

DASS App

https://ntp.niehs.nih.gov/go/952311

The DASS App allows users to apply internationally harmonized defined approaches to predict skin sensitization hazard and potency of their chemicals. Results are provided in a user-friendly, color coded format and can be evaluated against reference data.

https://ntp.niehs.nih.gov/whatwestudy/niceatm/comptox

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