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

February 2024

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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

February 2024