

NICEATM Computational Tools and Resources Supporting Alternative Test Method Development and Evaluation

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Role of Computational Approaches in Chemical Safety Testing

The NTP Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) develops and evaluates alternatives to animal use for chemical safety testing. As part of these activities, NICEATM reviews large amounts of data from a wide variety of in vivo and in vitro test methods that inform on a chemical's potential bioactivity. Computational tools and resources play a critical role in data access and evaluations such as:

- Aggregating and tagging data relative to toxicity endpoints of regulatory interest.
- Predictive modeling of in vivo toxicities using biologically relevant in vitro assay data.
- Exploring how chemical properties influence bioactivity patterns or assay predictive performance.
- Relating in vitro assay activity concentrations to in vivo doses and potential human exposures.
- Mapping data to biological systems to provide context needed for interpretation.
- Predicting physicochemical property values where experimental data are not available.

The Integrated Chemical Environment (ICE)

ICE is an access point for NICEATM data and tools. ICE allows users with limited computational expertise to explore and utilize these data and tools in the development and application of new approach methodologies.

ICE provides free online access to:

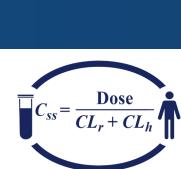
- Curated in vivo and in vitro data related to toxicity testing.
- In silico toxicity and parameter predictions and chemical property data
- Curated lists of chemicals with well-characterized
 Data analysis: allows characterization of data toxic effects (reference chemical lists).
- Computational tools for chemical characterization and predicting toxicity.

ICE supports:

- Data integration: brings together available data, including data on formulations.
- Data visualization: enables dynamic graphical exploration with publication-quality graphics
- using online workflows.
- FAIR (findable, accessible, interoperable and reusable) data principles.



- ICE includes quantitative structure-activity relationship (QSAR) predictions for >800,000 chemicals for toxicity endpoints and chemical parameters useful in modeling
- Chemical quick lists offer fast and easy searching options and can be useful in test method evaluation.







- Agency's (EPA) httk R package.

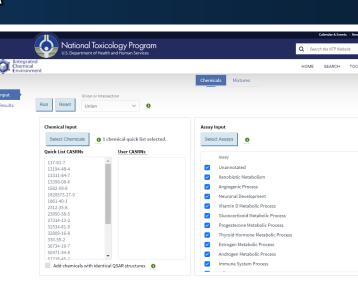
- See how EAD values differ for chemicals with similar in vitro bioactivity or chemical structure.
- Gain insight on the suitability of in vitro assays for



- Examine properties of ICE Chemical Quick Lists or user-provided CASRNs.

ICE Search and Data

- The ICE Search tool can query assay and chemical property data for over 10,000 chemicals
- ICE data are organized by toxicity endpoints of regulatory interest
- Data organization and annotation leverages expert curation and mapping to establish terminologies to support interoperability.



In Vitro to In Vivo Extrapolation (IVIVE)

The In Vitro to In Vivo Extrapolation (IVIVE) tool uses high-throughput in vitro data from the Tox21 program to estimate an in vivo equivalent administered dose (EAD) that would result in the plasma concentration of a chemical equal to the activity concentration in a given in vitro assay.

Modeling options include:

- One-compartment pharmacokinetic model including
- simulation of population diversity.
- Three-compartment physiologically based pharmacokinetic
- (PBPK) models using the U.S. Environmental Protection
- (http://dx.doi.org/10.18637/jss.v079.i04)
- Species-specific (rat/human) predictions.
- Multiple dosing routes (intravenous, oral, inhalation).

With the IVIVE tool users can:

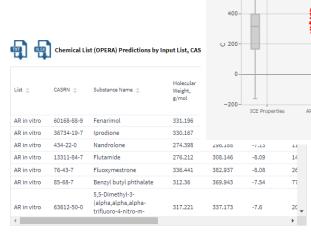
- Obtain estimates of in vivo exposure levels that could cause an adverse effect.
- predicting the effect level for in vivo endpoints.

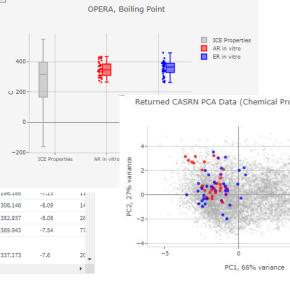


Stand-alone version available for use with custom datasets: https://github.com/NIEHS/ICE_IVIVEpipeline

Chemical Characterization

- The Chemical Characterization tool queries chemicals for available physiochemical properties and ADME properties predicted by the OPEn q(sar) App (OPERA) model. Users can:
- Compare the properties of two sets of chemicals.
- Results are returned as:
- Summary table of chemical properties.
- Interactive plots for visual comparisons of individual parameters.
- Principal component analysis (PCA) plots.







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

Contact Us

To get announcements of ICE updates and other NICEATM activities, visit the NIH mailing list page for NICEATM News at https://list.nih.gov/cgibin/wa.exe?SUBED1=niceatm-I&A=1 and click "Subscribe."





https://github.com/NIEHS/OPERA

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- Free, open-source and open-data
- Single chemical and batch mode
- Multiple platforms (Windows and Linux)
- Command line and GUI options
- Embeddable libraries (java, C, C++, Python)

https://github.com/NIEHS/OPERA https://ntp.niehs.nih.gov/go/opera https://doi.org/10.1186/s13321-018-0263-1

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