User-friendly Toxicology Tools from ICE Workflows

S. Bell¹, J. Phillips², N. Cariello¹, P. Ceger¹, X. Chang¹, F. Hermes¹, K. Mansouri¹, R. Rai¹, D. Allen¹, W. Casey³, N. Kleinstreuer³

¹ILS, RTP, NC, USA; ²Sciome LLC, RTP, NC, USA; ³NIH/NIEHS/DNTP/NICEATM, RTP, NC, USA

The Integrated Chemical Environment

ICE provides free online access to:

- Curated in vivo and in vitro test data
- In silico toxicity predictions and chemical property data
- Reference chemical lists
- Computational tools and workflows related to chemical characterization and predicting toxicity

ICE supports:

- Data integration: brings together available data, including data on formulations
- Results exploration: enables dynamic, graphical exploration with publication-quality graphics
- Data analysis: allows characterization of data using online workflows
- FAIR data access
What Goes into ICE?
Making Data and Tools Available

In Vitro to In Vivo Extrapolation

\[ C_{ss} = \frac{Dose}{CL_r + CL_h} \]

Use high-throughput in vitro data available from ICE to estimate external dose via a one-compartment model

IVIVE tools planned for future releases:

- Three-compartment physiologically based pharmacokinetic model
- Glucuronidation and sulfation predictions
Reverse toxicokinetics predictions
Calculations with user-provided data on ICE platform

**Machine Learning**

Use the machine learning tool for hypothesis generation and to explore different machine learning approaches using ICE data. Selected endpoints (for classification and regression modeling) and algorithms are available through ICE to facilitate the ease of use by those with limited background in computational toxicology

Endpoints for prediction

- LLNA: call
- Uterotrophic: call, LEL
- Human Potency: call, NOEL/LOEL

Machine learning methods available

- rf: random forest
- rpart: recursive partitioning
- knn: k-nearest neighbor
- svmRadial: support vector machine with a radial kernel
• pls: partial least squares regression

Chemical Characterization

Leverage ICE models to characterize a chemical list, getting information on the chemical space covered (or not covered) based on different physchem properties.
In the pipeline:

- Generate physchem and other structure-based predictions from user-provided chemical lists
- Prediction of chemical parameters for use in modeling (example: fraction unbound, pKa)
- Chemical use category overview provided by EPA’s Consumer Products Database (cpDAT)
- Integration with ChemMaps (http://www.chemmaps.com/)

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/cgi-bin/wa.exe?SUBED1=niceatm-l&A=1 and click “Subscribe.”

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