An Integrated Chemical Environment to Support 21st Century Toxicology

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Integrated Chemical Environment

What is ICE?

ICE is the Integrated Chemical Environment, which houses:

- High quality, curated in vivo, in vitro and in silico data from the National Toxicology Program Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) and partners
- Reference chemical lists (chemicals that can be used as a reference for a given assay or endpoint) and associated data
- Computational tools and workflows (Summer 2017)

What need does ICE fill?

NICEATM developed ICE to:

- Provide a central location for computer-friendly versions of NICEATM data and computational models
- Facilitate data use by NICEATM stakeholders
What can ICE do?

Currently ICE supports:

- Data integration: bringing together data from different endpoints and experiments for comparison
- Results exploration: dynamic, graphical exploration of query results with capability to refine within query results
- Data accession: obtaining reference chemical lists and supporting data

Resources available soon (Summer 2017):

- Data analysis: downloadable computational tools and workflows to support test method development

Search by Chemical and Integrate Data from Multiple Assays

Querying ICE

ICE data are searchable by chemical and/or assay:

Select chemicals

- Input user-defined CASRNs
  or
- Select reference chemical lists to combine with your custom list or use on their own
  or
- Search selected datasets for all chemicals in ICE by leaving the input chemical field blank
- Chemicals not found in the results will be listed in a separate download file
Select assay data

- Data Integrator allows users to combine selected data streams of interest.
- Assay Selection field enables organization of data either by endpoints of regulatory interest or by data type (e.g., in vitro and in silico data)
- Queries are joined using “or” logic (e.g., ocular irritation or dermal irritation) by default
- Explore view allows users to dynamically refine queries
What Data Are in ICE?

Available data

- High quality, curated data from scientific literature sources
- Data used to support the reference chemical lists
- High-throughput screening Tox21/ToxCast data, curated by chemical QC results
- Computational predictions useful in developing models of health impacts or chemical characterization
- Other data useful in developing/evaluating new approaches or chemical safety

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AC50, concentration that increases activity by 50%; ACC, activity concentration at cut-off, a measure of the activity threshold for an assay response based on curve-fitting models; BCF, bioconcentration factor; DPRA,
direct peptide reactivity assay; EC3, in the LLNA, a test chemical concentration that produces a stimulation index of 3; hCLAT, human cell line activation test; HTS, high throughput screening; IC50, concentration that inhibits activity (in this context, decreases cell viability) by 50%; LC50, inhalation concentration expected to produce lethality in 50% of animals tested; LD50, dose expected to produce lethality in 50% of animals tested; LLNA, local lymph node assay; logP, octanol-water partition coefficient; logVP, vapor pressure, logBCF, bioconcentration factor; logS, water solubility

In vitro basal cytotoxicity assays proposed for setting starting doses for in vivo acute oral toxicity studies.

Explore Query Results

Interactive data exploration

- ICE displays results graphically with real-time updated exportable graphics
- User can filter search results to further refine results based on assay and/or chemicals
- User can dynamically explore results or export them to Excel or tab delimited files
Analyze and Export Your Query

Get data for your analysis

- Quick view of full query results prior to exporting
- Export data in Excel and tab delimited files
- See which chemicals were not found
- Query parameters are documented in export screen to ensure queries can be replicated, supporting reproducibility
Workflows (Launching July 2017)

- Physicochemical property predictions
- Physiologically based pharmacokinetic and toxicokinetic models

Current Timeline

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<th>Launch (v1.0)</th>
<th>March 2017, SOT Annual Meeting</th>
<th>• Launch of web resource highlighting the data integrator</th>
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<td>Update (v1.1)</td>
<td>July 2017</td>
<td>• Launch of tools/workflows section</td>
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<tr>
<td>Update (v1.4)</td>
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<td>• Interactive workflows</td>
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Quarterly updates will be conducted with notification and details of updates on the ICE webpage and announced through NICEATM News.

Contact Us

Access ICE

Want to explore the Integrated Chemical Environment? Scan the QR code to the below or go to the ICE landing page at [https://ice.ntp.niehs.nih.gov](https://ice.ntp.niehs.nih.gov)

Subscribe to the NICEATM News email list

To get announcements of ICE updates and other NICEATM activities, scan the QR code below or visit the NIH mailing list page for NICEATM News at [https://list.nih.gov/cgi-bin/wa.exe?SUBED1=niceatm-l&A=1](https://list.nih.gov/cgi-bin/wa.exe?SUBED1=niceatm-l&A=1) and click “Subscribe”
Read more about ICE!


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