Integrated Chemical Environment to Support 21st Century Toxicology
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What is ICE?
ICE is an 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 in endpoint and associated data)
• Computational tools and workflows (Summer 2017)

Available data
• High quality, curated data from scientific literature sources
• Data supports the reference chemical lists
• High-throughput screening Tox21/ToxCast data, curated by chemical QC results
• Data used to support the reference chemical lists
• High quality, curated data from scientific literature sources

March 2017 in vivo Skin irritation/corrosion classification categories
Dermal irritation
March 2017 in vitro Assay ACC, AC50
March 2017 in silico Androgen receptor pathway model scores
Androgenic activity
July 2017 (tentative) in vivo Lowest effect level in the rodent Hershberger assay
Androgenic activity

March 2017 in vivo Lowest effect level in the rodent uterotrophic assay
Estrogenic activity

Data Types Availability Type Endpoint Examples
Acute oral toxicity
October 2017
Rat LD50
Acute inhalation toxicity
October 2017
Rat LD50
Dermal sensitization
Dermal sensitization
Dermal sensitization
Dermal sensitization
March 2017 in vitro Basal cytotoxicity assays proposed for setting starting doses for in vivo acute oral toxicity studies.

Partition coefficient; logVP, vapor pressure; logBCF, bioconcentration factor; logS, water solubility.

Assay Selection
Acute Oral Toxicity
Acute Inhalation Toxicity
Dermal Sensitization
Dermal Irritation
Dermal Corrosion
In vitro
In vivo
In silico

What can ICE do?
• CIDE 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 access: obtaining reference chemical lists and supporting data
Resource available soon (Summer 2017)
• Data analysis, downloadable computational tools and workflows to supported method development

Filtering

Explore Query Results
• Interactive data exploration
  • ICE displays results graphically with real-time updated superscripted graphics
  • User can filter search output to further refine results based on assay and/or chemicals
  • User can dynamically explore results or export them to Excel or tab delimited files

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Current Timeline
Launch (v1.0) January 2018
Update (v1.2) July 2017
Update (v1.2) October 2017
Update (v1.3) January 2018
Update (v1.4) April 2019

The Integrated Chemical Environment (ICE) is a web-based platform that supports the evaluation of alternative toxicological methods. ICE integrates high-quality, curated data from various sources, including scientific literature and high-throughput screening assays, to provide a comprehensive database for toxicology research. The platform offers tools for computing physicochemical properties and supports data integration, allowing users to search for and analyze chemical data. ICE is designed to facilitate data use by NICEATM stakeholders and to provide a central location for toxicological methods development information. The project is funded by the National Institutes of Health through the Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM).

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