

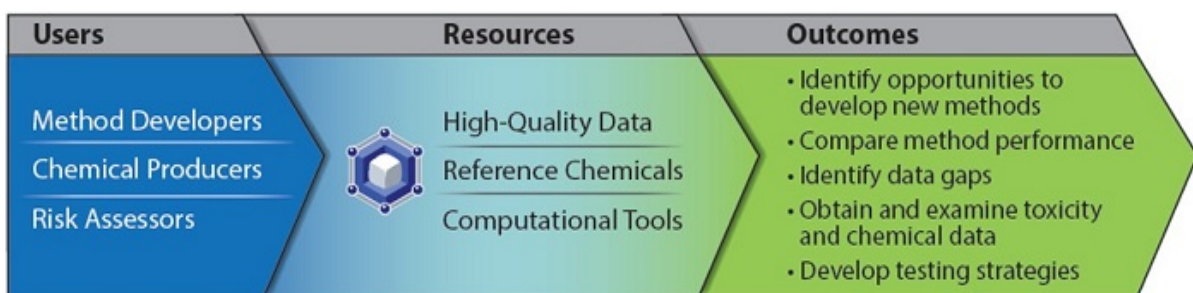
Open, Accessible Toxicity Testing Data for Chemical Evaluation

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What is ICE?

Integrated Chemical Environment



ICE provides free online access to:

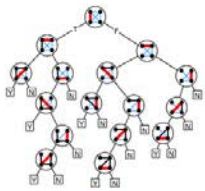
- Curated in vivo and in vitro chemical test data
- In silico toxicity predictions and chemical property data
- Reference chemical lists
- Computational tools and workflows related to safety testing

ICE supports:


- Data integration: brings together available data, including data on formulations
- Results exploration: dynamic, graphical exploration with publication-quality graphics
- Data analysis: online workflows allowing characterization of data

What Goes into ICE?


Computational Models




Literature




Databases




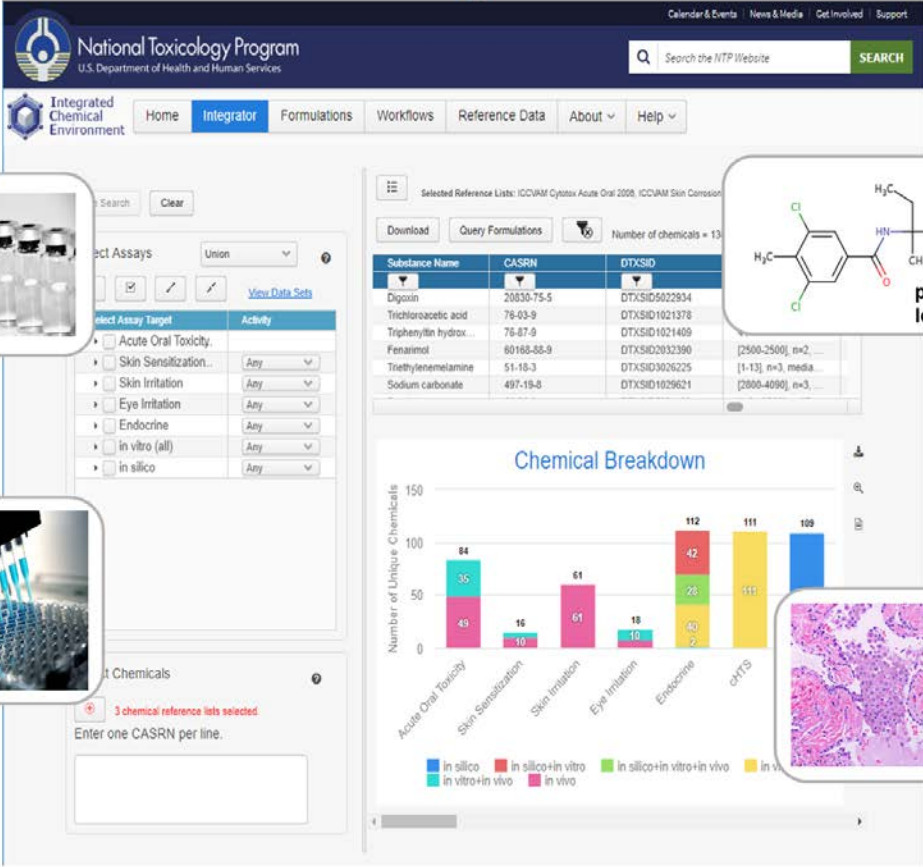
Validation Studies






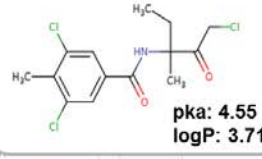
↓
Curation





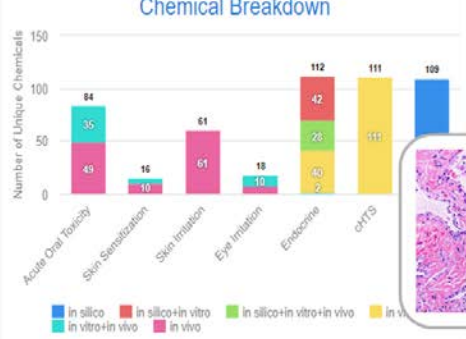



Substance Name	CASRN	DTXSID
Digoxin	20830-75-5	DTXSID5022934
Trichloroacetic acid	76-03-9	DTXSID1021378
Triphenyltin hydroxide	76-67-9	DTXSID1021409
Fenafamil	80168-88-9	DTXSID2032390
Triethylenemelamine	51-18-3	DTXSID3026225
Sodium carbonate	497-19-8	DTXSID1029621

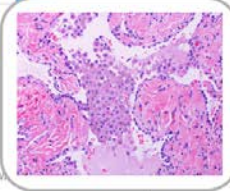


pKa: 4.55
logP: 3.71

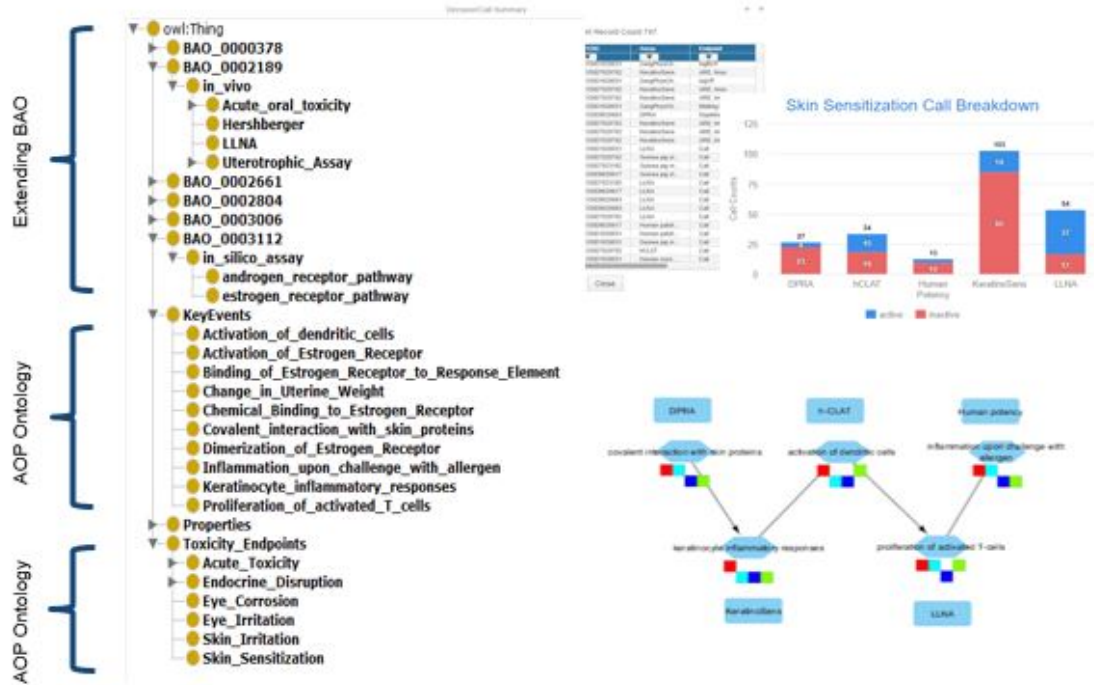
Chemical Breakdown



Assay Type	In silico	In silico+in vitro	In silico+in vitro+in vivo	In vitro+in vivo	In vivo	Total
Acute Oral Toxicity	35	49	0	0	0	84
Skin Sensitization	10	16	0	0	0	26
Skin Irritation	10	51	0	0	0	61
Eye Irritation	2	18	0	0	0	20
Endocrine	42	26	0	0	0	68
oHTS	111	0	0	0	0	111



ICE Ontology Aids Mapping to Outcomes



Making Data and Tools Available



Download reference lists



Export queries



Link to other resources

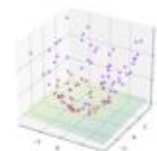
Coming this fall....



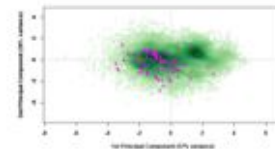
Run workflows



In vitro to in vivo extrapolation



Machine learning



Chemical space characterization



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<https://ice.ntp.niehs.nih.gov/>



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