

In silico toxicity predictions and chemical property data

Computational tools and workflows related to safety testing

Reference chemical lists

## Open, Accessible Toxicity Testing Data for Chemical Evaluation

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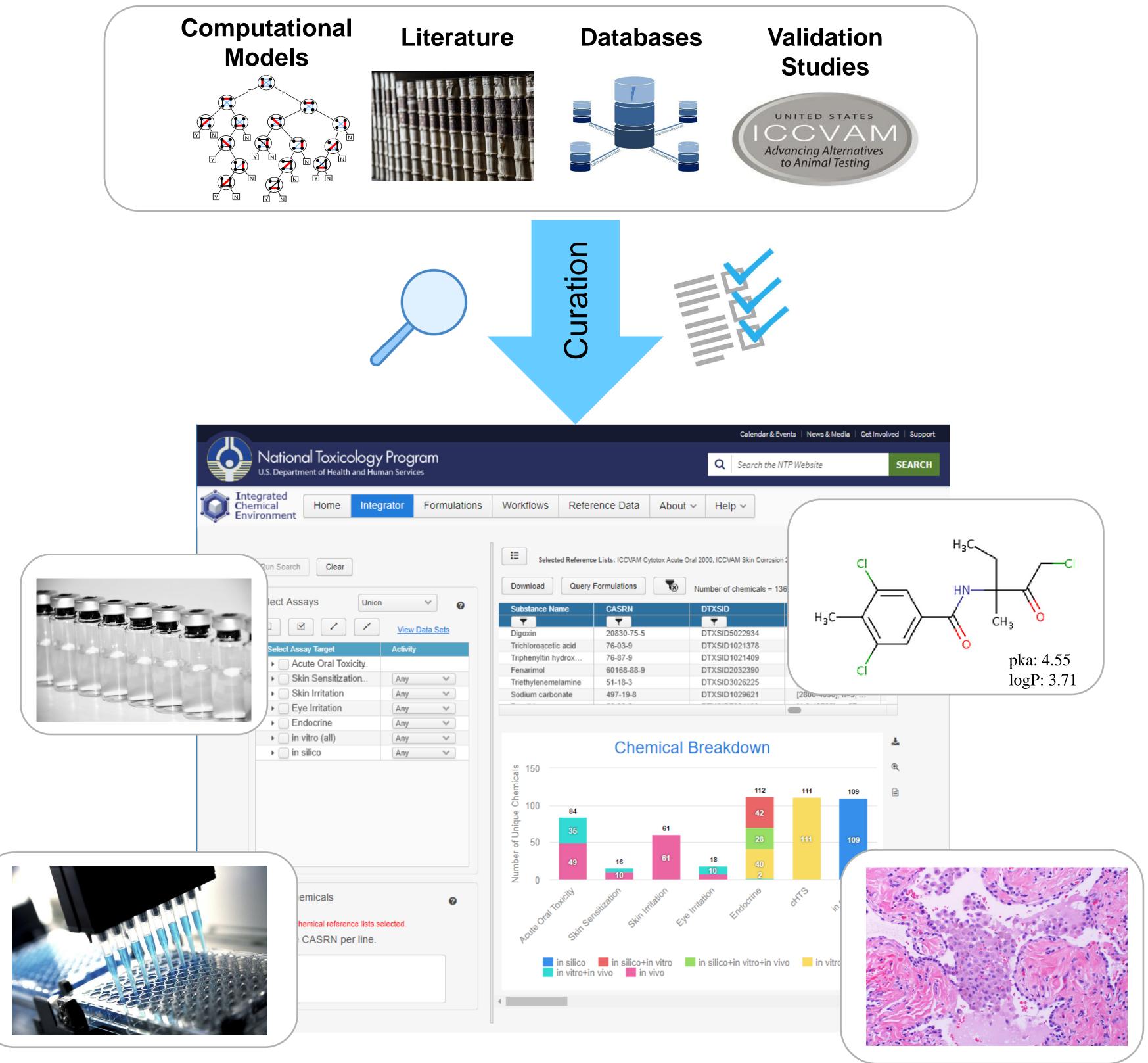
### What is ICE? Integrated Chemical Environment Users Outcomes Resources Identify opportunities to develop new methods Method Developers **High-Quality Data** Compare method performance Chemical Producers Reference Chemicals Identify data gaps Obtain and examine toxicity Risk Assessors Computational Tools and chemical data Develop testing strategies ICE provides free online access to: **ICE** supports: • Data integration: brings together available data, including data on formulations • Curated in vivo and in vitro chemical test data

Results exploration: dynamic, graphical exploration with publication-quality

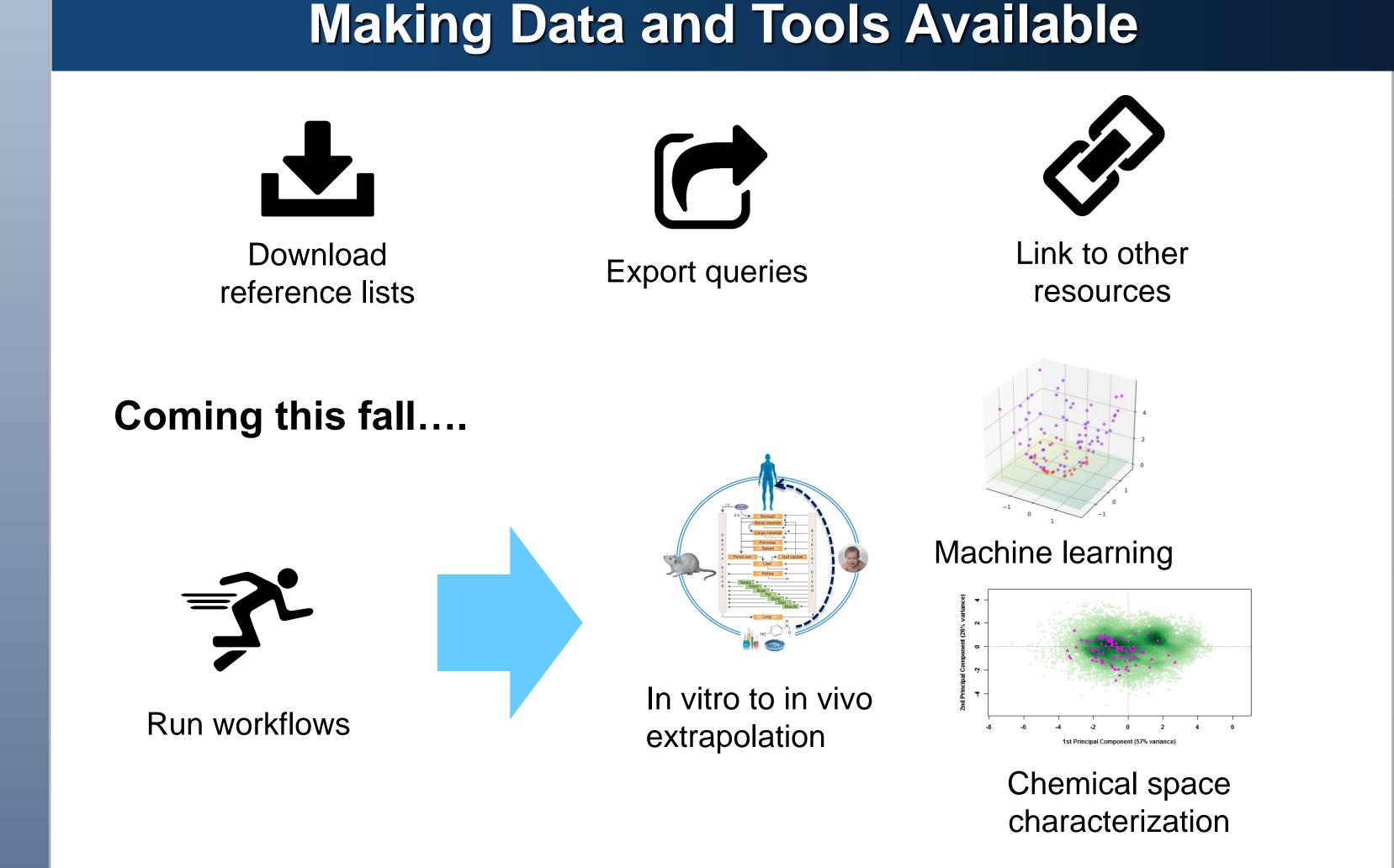
• Data analysis: online workflows allowing characterization of data

# What Goes into ICE?

graphics



#### ICE Ontology Aids Mapping to Outcomes Decision/Call Summary ▶ ■ BAO 0000378 ▼ BAO\_0002189 ▼ oin vivo ► Acute oral toxicity Skin Sensitization Call Breakdow Hershberger Uterotrophic Assay --- BAO 0002661 ► BAO 0002804 ► BAO 0003006 ▼ BAO 0003112 ▼ in silico assay androgen receptor pathway -- estrogen receptor pathway Activation of dendritic cells Activation\_of\_Estrogen\_Receptor Binding\_of\_Estrogen\_Receptor\_to\_Response\_Element Change\_in\_Uterine\_Weight Chemical\_Binding\_to\_Estrogen\_Receptor Covalent interaction with skin proteins Dimerization\_of\_Estrogen\_Receptor Inflammation\_upon\_challenge\_with\_allergen Keratinocyte\_inflammatory\_responses Proliferation\_of\_activated\_T\_cells Properties ▼ ● Toxicity\_Endpoints ► Acute\_Toxicity • F G Endocrine\_Disruption Eye\_Corrosion Eye\_Irritation Skin\_Irritation Skin\_Sensitization



### Acknowledgements

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