

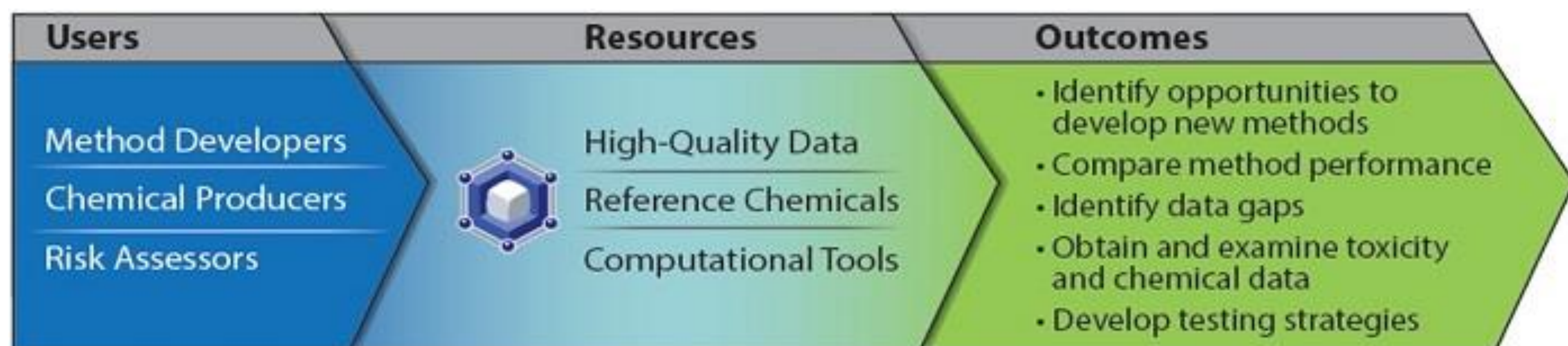
# Open, Accessible Toxicity Testing Data for Chemical Evaluation

Shannon Bell<sup>1</sup>, Patricia Ceger<sup>1</sup>, David Allen<sup>1</sup>, Nicole Kleinstreuer<sup>2</sup>

<sup>1</sup>ILS, RTP, NC, USA; <sup>2</sup>NIH/NIEHS/DNTP/NICEATM, RTP, NC, USA

## What is ICE?

### Integrated Chemical Environment



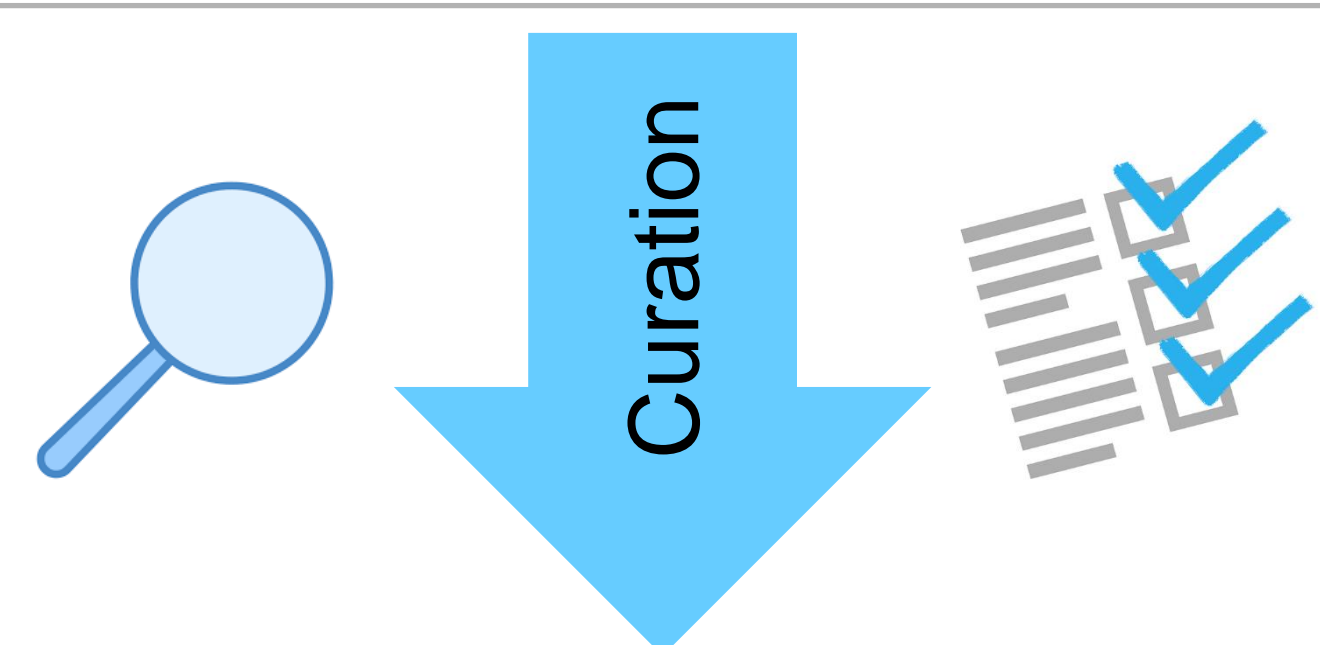
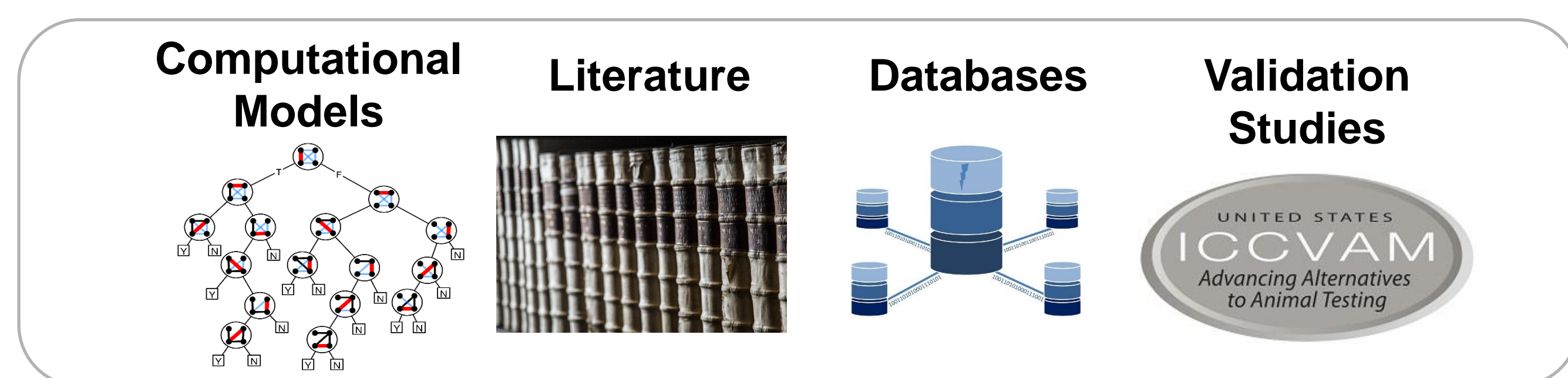
#### ICE provides free online access to:

- 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?

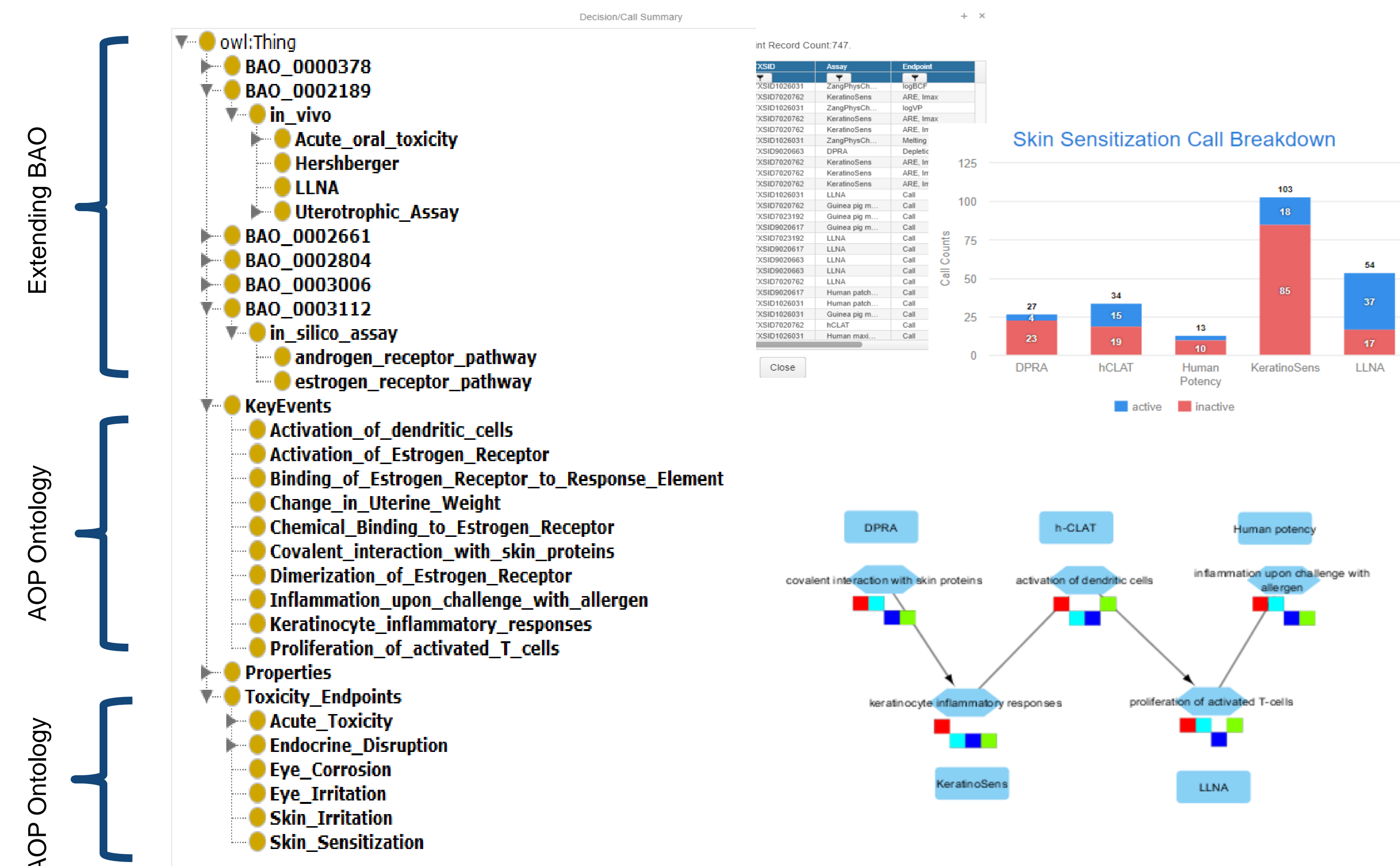


**Chemical Breakdown**

Assay	In silico	In silico+in vitro	In silico+in vitro+in vivo	In vitro	In vitro+in vivo	In vivo
Acute Oral Toxicity	84	35	49	16	61	18
Skin Sensitization	16	10	18	2	111	109
Skin Irritation	61	18	10	2	111	109
Eye Irritation	112	42	23	2	111	109
Endocrine	111	111	111	111	111	109
DTTS	109	109	109	109	109	109

**Chemical Structure:** CC(C)C(=O)Nc1ccc(Cl)c(Cl)c1  
pKa: 4.55  
logP: 3.71

## 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**

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

## Acknowledgements

ICE has been funded in whole or in part with federal funds from the National Institute of Environmental Health Sciences, National Institutes of Health, Department of Health and Human Services, under Contract No. HHSN273201500010C. The views expressed above do not necessarily represent the official positions of any federal agency. Since the poster was written as part of the official duties of the authors, it can be freely copied.