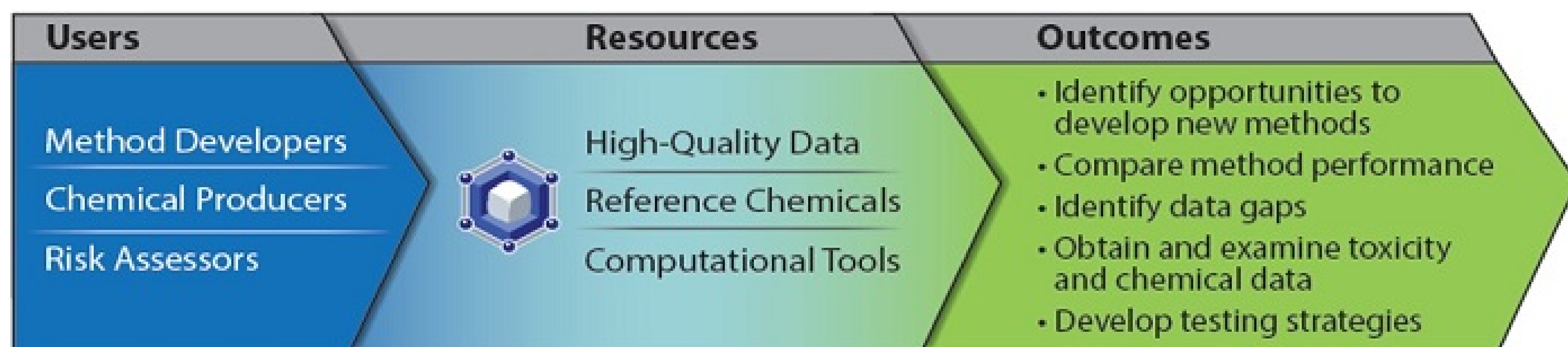# Open, Accessible Toxicity Testing Data for Chemical Evaluation

Shannon Bell[1], Patricia Ceger[1], David Allen[1], Nicole Kleinstreuer[2]

[1]ILS, RTP, NC, USA; [2]NIH/NIEHS/DNTP/NICEATM, RTP, NC, USA

What is ICE?

Integrated Chemical Environment

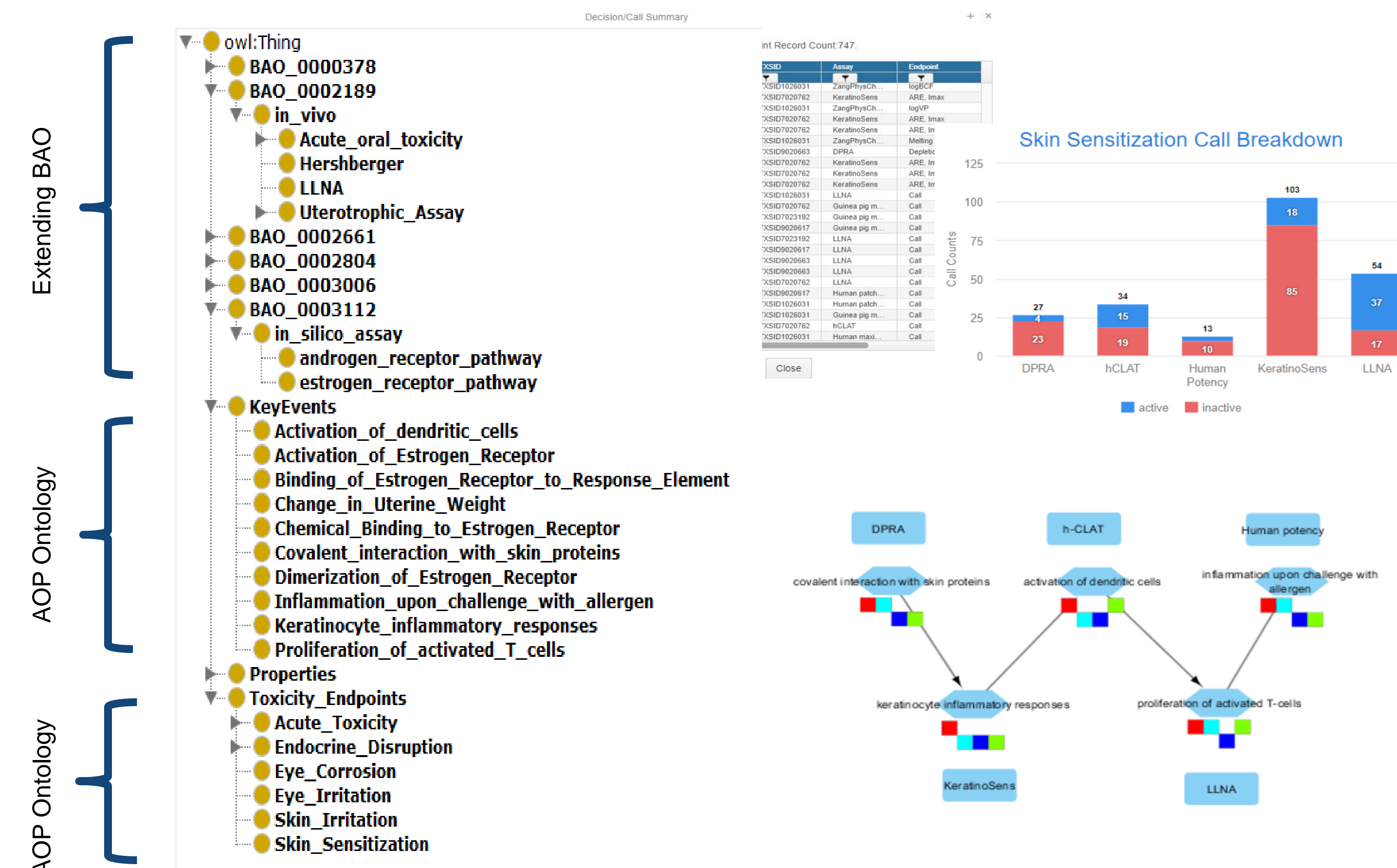| Users	Resources	Outcomes
Method Developers	High-Quality Data	• Identify opportunities to develop new methods
Chemical Producers	Reference Chemicals	• Compare method performance
Risk Assessors	Computational Tools	• Identify data gaps
		• Obtain and examine toxicity and chemical data
		• Develop testing strategies

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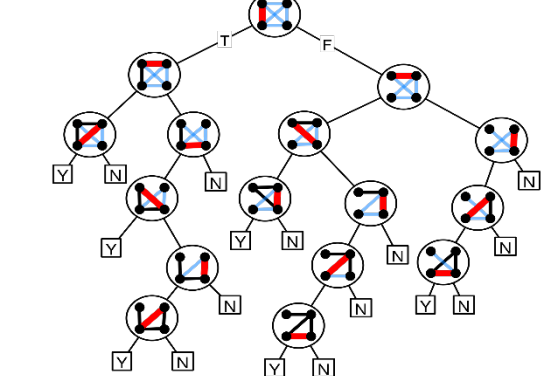
ICE supports:
- Data integration: brings together available data, including data on formulations
- Results exploration: dynamic, graphical exploration with publication-quality graphics
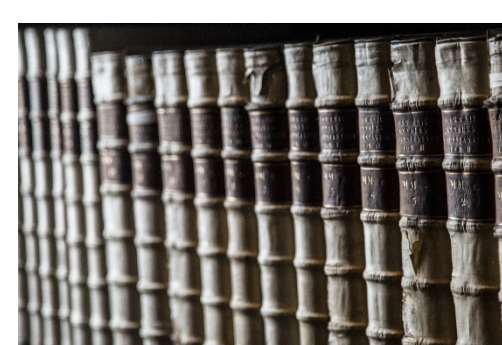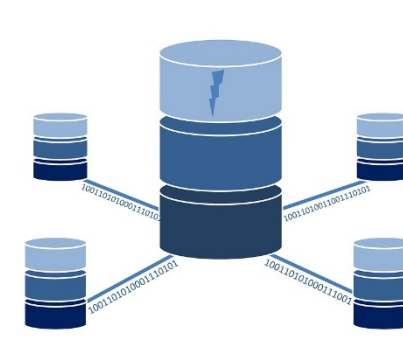- Data analysis: online workflows allowing characterization of data

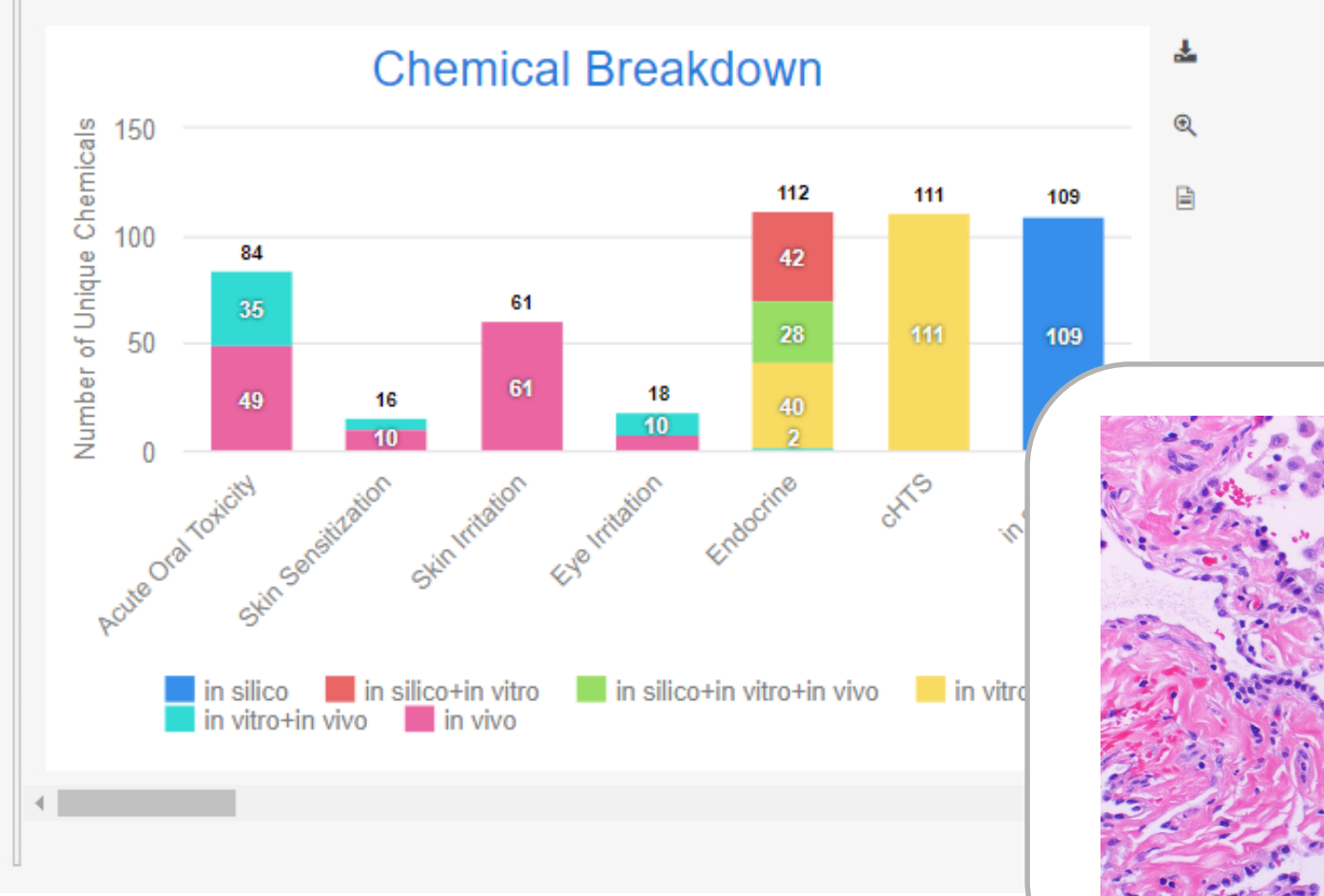## What Goes into ICE?

Computational Models

Literature

Databases

Validation Studies

ICCVAM — Advancing Alternatives to Animal Testing

Curation

National Toxicology Program
U.S. Department of Health and Human Services

pka: 4.55
logP: 3.71

Chemical Breakdown

ICE Ontology Aids Mapping to Outcomes

Skin Sensitization Call Breakdown

Extending BAO

AOP Ontology

AOP Ontology

- owl:Thing
  - BAO_0000378
  - BAO_0002189
    - in_vivo
      - Acute_oral_toxicity
      - Hershberger
      - LLNA
      - Uterotrophic_Assay
  - BAO_0002661
  - BAO_0002804
  - BAO_0003006
  - BAO_0003112
    - in_silico_assay
      - androgen_receptor_pathway
      - estrogen_receptor_pathway
  - KeyEvents
    - 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
    - Endocrine_Disruption
    - Eye_Corrosion
    - Eye_Irritation
    - Skin_Irritation
    - Skin_Sensitization

DPRA — covalent interaction with skin proteins

h-CLAT — activation of dendritic cells — keratinocyte inflammatory responses

Human potency — inflammation upon challenge with allergen — proliferation of activated T-cells

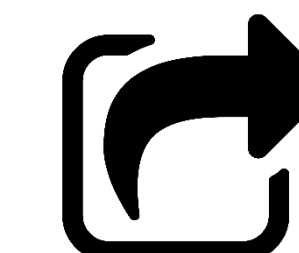KeratinoSens

LLNA

Making Data and Tools Available
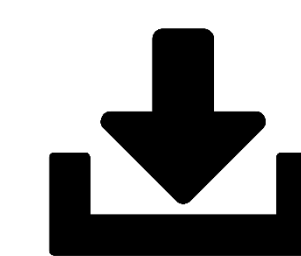
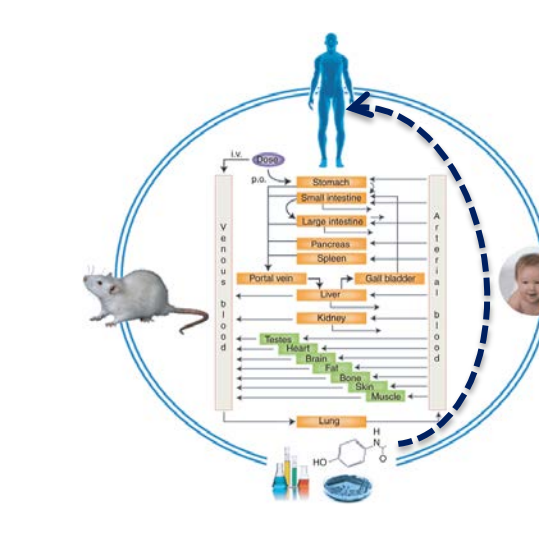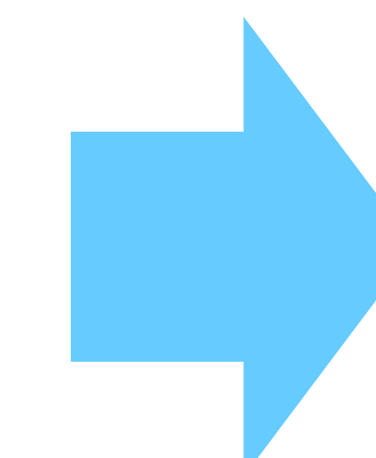**Download reference lists**
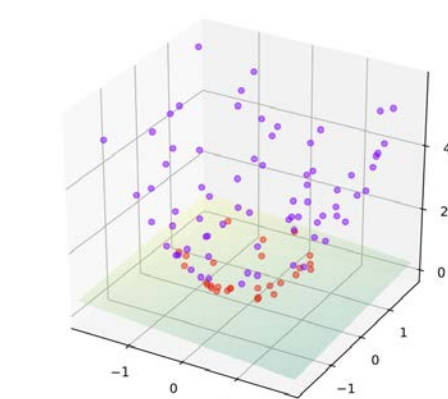
Export queries
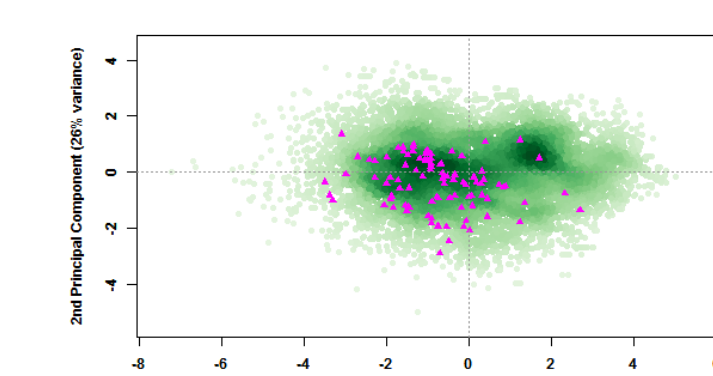
Link to other resources

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

Abstract

New testing approaches that leverage advances in science and technology promise to more efficiently evaluate substances and better protect human health and the environment than traditional laboratory animal methods. A key component to the development and implementation of such non-animal approaches is the availability of curated data, as well as the tools and infrastructure to allow users to utilize the data. This poster will provide an overview of NICEATM's Integrated Chemical Environment (ICE), focusing on the diversity of available data. Examples include curated in vivo data generated using guideline regulatory methods and in silico parameters for modeling. Highlights of the ICE ontology and tools to allow users to explore the data will be included. *This project was funded in whole or in part with Federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.*

Meeting program URL
http://www.opentox.net/events/opentox-usa-2018/program