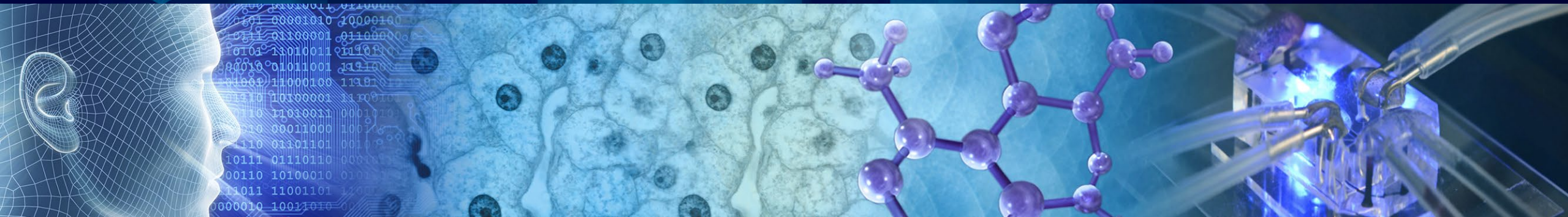




National Institute of  
Environmental Health Sciences  
Division of Translational Toxicology



# NICEATM's Integrated Chemical Environment (ICE): Updates, Enhancements, and Advances

**Brad Reisfeld, PhD, DABT, ATS**

**Inotiv, Inc., Contractor Supporting the NTP Interagency Center for the  
Evaluation of Alternative Toxicological Methods (NICEATM)**

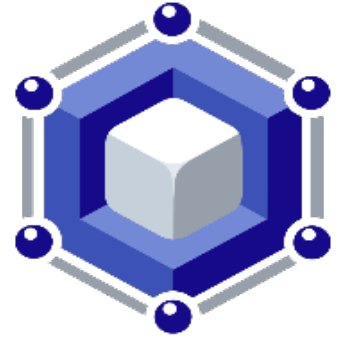
**SACATM 2024**

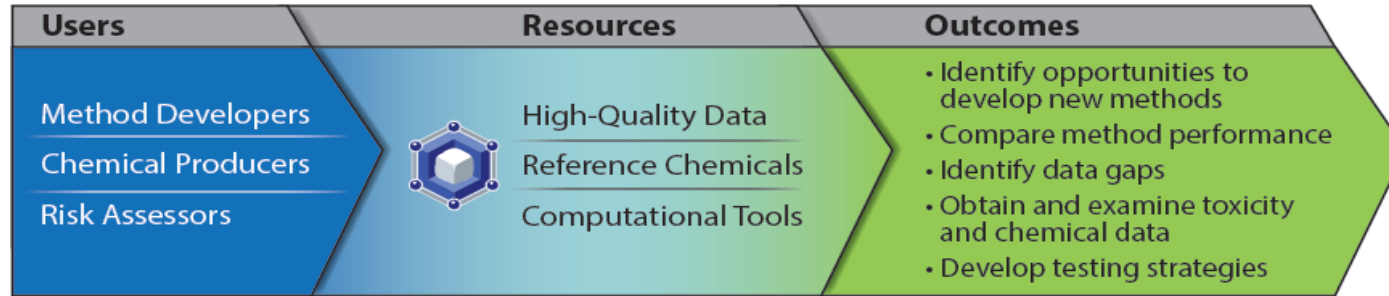
*Disclaimer: Inotiv staff provide technical support for NICEATM,  
but do not represent NIEHS, NTP, or the official positions of any federal agency.*

National Institutes of Health • U.S. Department of Health and Human Services




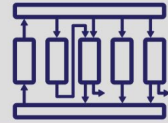
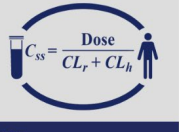



# Topics for today

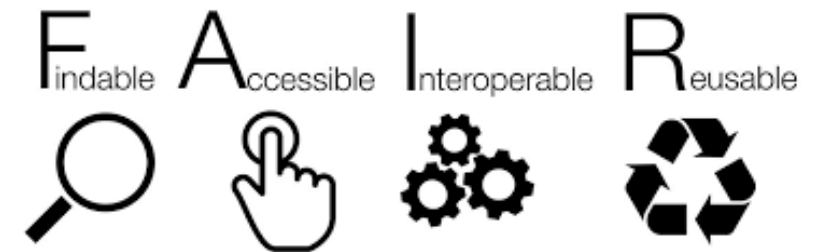
- What is the Integrated Chemical Environment (ICE)?
- Usage of the environment
- Data and updates
- Tools and updates
- Strategic activities to improve ICE
- Ongoing work and future enhancements





- Curated *in vivo* and *in vitro* test data
- In silico toxicity predictions and chemical property data
- Reference chemical lists
- Computational tools for chemical characterization and predicting toxicity

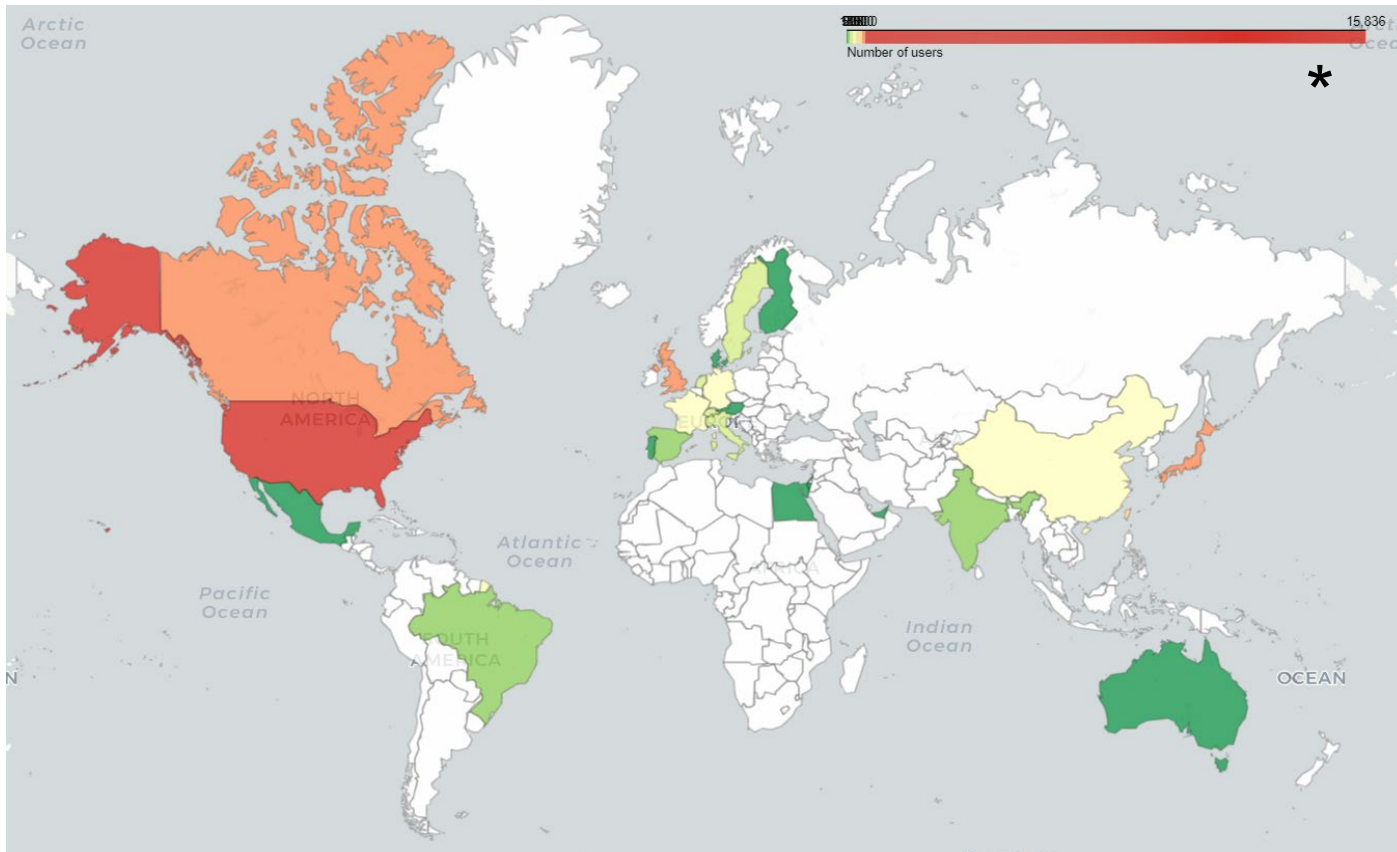
 Search >	 Chemical Quest >	 Curve Surfer >	 PBPK >
 IVIVE >	 Chemical Characterization >	 Data >	 Help Videos >



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

# ICE: Usage of the platform

## ICE user sessions based on website analytics



### July 2023 - August 2024

- 27 countries
- 19,043 user sessions

\*nonlinear color bar to show qualitative differences

## ICE: Usage of the platform (2)

### Some applications of ICE described in the recent scientific literature

Kvasnicka, et al. Two-Stage Machine Learning-Based Approach to Predict Points of Departure for Human Noncancer and Developmental/Reproductive Effects. *Environ Sci Technol*. 2024 Sep 3;58(35):15638-15649.

Luiz, et al. A novel approach to triazole fungicides risk characterization: Bridging human biomonitoring and computational toxicology, *Science of The Total Environment*, 2024, 953.

Kreutz, et al. Integrated Approach for Testing and Assessment for Developmental Neurotoxicity (DNT) to Prioritize Aromatic Organophosphorus Flame Retardants. *Toxics*. 2024 Jun 18;12(6):437.

Silva. Investigating open access new approach methods (NAM) to assess biological points of departure: A case study with 4 neurotoxic pesticides. *Curr Res Toxicol*. 2024 Feb 15;6:100156.

Silva and Kwok. Use of computational toxicology models to predict toxicological points of departure: A case study with triazine herbicides. *Birth Defects Res*. 2023 Mar 15;115(5):525-544.

Chang, et al. Quantitative in vitro to in vivo extrapolation for developmental toxicity potency of valproic acid analogues. *Birth Defects Res*. 2022 Oct 1;114(16):1037-1055.

Hines et al. Application of an Accessible Interface for Pharmacokinetic Modeling and In Vitro to In Vivo Extrapolation. *Front Pharmacol*. 2022 Apr 13;13:864742. doi: 10.3389/fphar.2022.864742.

# ICE Data

ICE Data Sets
Data Sets
Acute Lethality
Cancer
Cardiotoxicity
DART
Endocrine
Irritation-Corrosion
Sensitization
cHTS
Chemical Properties
Exposure Predictions
Chemical Use

## Size of Data Sets

Datasets	Data points
Acute Dermal	2757
Acute Inhalation	5590
Acute Oral	16839
ADME Parameters	3821
Cancer	10502
cHTS	3599802
DART	138480
Endocrine: in vitro	16629
Endocrine: in vivo	2270
Exposure Predictions	1439598
Eye Irritation	3028
Functional Use	266926
Functional Use Category	29784
Skin Irritation: in vitro	7058
Skin Irritation: in vivo	2079
Skin Sensitization: in vitro	9259
Skin Sensitization: in vivo	14997
<b>Total</b>	<b>5,569,419</b>

+ OPERA predictions for the DSSTox chemicals (50 M data points)

## ICE Data (*in vivo* and *in vitro*)

Toxicity endpoint	Assays	# of chemicals	
Chemical Parameters	Experimental physicochemical properties	~20000	New in release v4.1: Updated cHTS data to include annotations to OBO Foundry ontologies.
ADME Parameters	Fu, intrinsic clearance, Caco2 permeability	~3000	
Acute Toxicity	In vivo acute oral, dermal, and inhalation toxicity	~10000	
Cancer	In vivo and in vitro cancer, and Weight of Evidence	3038	
DART	In vivo and in vitro DART	628	
Skin Sensitization	In vivo and in vitro skin sensitization	1771	New in release v4.1: Versioning information to data sets. Links to the NTP CEBS database and EPA CompTox Chemicals Dashboard in data downloads.
Skin Irritation	In vivo and in vitro skin irritation/corrosion	595	
Eye Irritation	In vivo and in vitro eye irritation/corrosion	455	
Endocrine	In vivo and low throughput in vitro data on AR and ER agonist and antagonist activity	384	
cHTS	Curated US EPA's ToxCast and Federal Tox21 assays (In vitro)	~10000	

## ICE Data (In Silico Models/Integrated Approaches)

Endpoint	Model	# of chemicals	
Physicochemical Properties	OPEn (q)saR App (OPERA) Mansouri et al. J Cheminform 2018	1M+	New in release v4.1: Inclusion of applicability domain information for OPERA predictions in the ICE graphical user interface and REST API
Structural Properties	OPEn (q)saR App (OPERA) Mansouri et al. J Cheminform 2018	1M+	
Predicted ADME Properties	OPEn (q)saR App (OPERA) Mansouri et al. J Cheminform 2018	1M+	
Environmental Fate	OPEn (q)saR App (OPERA) Mansouri et al. J Cheminform 2018	1M+	
Acute Oral Toxicity	Collaborative Acute Toxicity Modeling Suite (CATMoS) - Rat acute oral toxicity. Mansouri et al. EHP 2021	1M+	
Endocrine	Estrogen Receptor pathway Model. Browne et al. ES&T 2015	1812	
	Androgen Receptor Pathway Model. Kleinstreuer et al. Chem Res Tox 2017	1855	
	Collaborative Estrogen Receptor Activity Prediction Project (CERAPP). Mansouri et al. EHP 2016	1M+	
	Collaborative Modeling Project for Androgen Receptor Activity (COMPARA). Mansouri et al. EHP 2020	1M+	
Exposure Predictions	Systematic Empirical Evaluation of Models (US EPA'S SEEM3). Ring et al. Environ Sci Technol 2019	475,000+	



## ICE Chemical Quick Lists

### Reference Chemical List

AR In Vitro Agonist

AR In Vitro Antagonist

ER In Vivo Agonist

ER In Vitro Agonist

Eye Irritation-Corrosion

Genotoxicity

OECD Defined Approach to Skin  
Sensitization: Human

OECD Defined Approach to Skin  
Sensitization: LLNA

Skin Corrosion

### Non-reference Chemical List

AR In Vivo Agonists

AR In Vivo Antagonists

EPA Pesticide Active Ingredients

EPA Pesticide Inert Ingredients, Food and  
Nonfood Use

EPA IRIS Cancer Assessment

EPA IRIS Non-Cancer Assessment

EPA PFAS Master List

IARC Classifications

Mixtures and Formulations in ICE

NTP Cancer Bioassay Chemicals

RoC Classifications

Steroidogenesis - Androgen

Steroidogenesis - Estrogen

Thyroid

Tox21

ToxCast Phase I, Phase II, and e1k

New in release v4.1:

- New PFAS Quick List.
- Updated RoC Classifications Quick List based on the 15th Report on Carcinogens.

# ICE Tools



**Search**

Query ICE data and visualize results



**Chemical Quest**

Identify similar chemicals



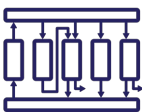
**Chemical  
Characterization**

Explore chemical properties and use categories



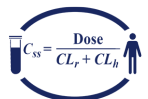
**Curve Surfer**

Explore concentration-response curves



**PBPK**

Predict tissue-specific chemical concentrations



**IVIVE**

Predict equivalent administered dose from in vitro data



Input

The Search tool allows you to query ICE data using chemical quick list selections (chemical names, CASRNs, or chemical identifiers) and a selection of data sets organized by toxicity endpoints of regulatory interest.

Scope of Search: Run Reset Union

**Chemical Input**

Select Chemicals

Quick List CASRNs

User Chemical Identifiers

133-06-2  
63-25-2  
DTXSID9020160  
BPA  
17alpha-Ethinylestradiol

**Data Selection**

Select Data Sets

Data Set	Description	Data Type
<div style="display: flex; justify-content: space-between; border-bottom: 1px solid #ccc;"> <span>Select Data Sets</span> <span>0</span> </div> <div style="display: flex; justify-content: space-between; border-bottom: 1px solid #ccc;"> <span>cHTS</span> <span>Acute Lethality</span> <span>Sensitization</span> <span>Irritation/Corrosion</span> <span>Endocrine</span> <span>Cancer</span> <span>Cardiotoxicity</span> <span>DART</span> <span>Chemical Properties</span> <span>Exposure</span> </div>		

**Click this button to view and select ICE Chemical Quick Lists.**

**Click "Select Data Sets" to select assays organized by toxicity endpoint.**

**Enter one chemical identifier per row. Identifiers can now include names and synonyms!**



Input

**Results**

Help

Help Video

Report an Issue

**Data Summary**    Query Summary (Beta)

**Search Results**

> Selected Chemical Quick Lists (1)

> Selected Assays (0)

> Chemical Identifiers Not Returned By Query (0)

Send filtered results to:

Download    Select tool...    Clear Filter    Long View    Number of chemicals = 96

Substance Name	Substance Type	CASRN (CEBS Link)	DTXSID (Dashboard Link)	QSAR Ready ID	Abnormal Growth and Differenti... Cell (# Assays=6)	Angiogenic Process Call (# Assays=28)	Cell Death Process Call (# Assays=12)	Cell Cycle Call (# Assays=68)	Cell Proliferat... Call (# Assays=6)	Cell Viability Process Call (# Assays=1...	Extra: Matrici: (# Assay
 17-Methyltestosterone	Chemical	58-18-4	DTXSID1033664	GCKMFJB... UHFFFAOY... N	Active,Not Tested(N=5)	Inactive(N... Tested(N=6)	Inactive(N... Tested(N=7)	Active(N=1... Omit(N=1... Tested(N=...	Inactive(N... Tested(N=...	Active(N=1... Tested(N=...	Activ Omit
 17alpha-Estradiol	Chemical	57-91-0	DTXSID8022377	VOXZDWN... UHFFFAOY... N	Active,Not Tested(N=5)	Active(N=3... Omit(N=2)... Tested(N=6)	Inactive(N... Tested(N=7)	Omit(N=1)... Tested(N=...	Inactive(N... Tested(N=...	e(N=3... Tested(N=...	Activ

<https://cebs.niehs.nih.gov/cebs/>

<https://comptox.epa.gov/dashboard/>

**Send filtered results to other ICE tools**

**CASRN links to NIEHS CEBS and DTXSID links to U.S. EPA's Comptox Dashboard**

**Click icons to view substance details**

**Click icons to filter results**



**Draw 2D structures or input chemical SMILES**

**Results show number of similar structures identified for each input chemical or structure**

**When specifying SMART strings, the substructure will be highlighted for easy identification**

**There are several filter options including filtering by specific substructures (SMARTS)**

The Chemical Quest tool uses fingerprints to calculate structure similarity. This tool uses fingerprints generated using Saagar features. Only 50 input chemical ids/structures are allowed.

Max hits per input: 10 | Tanimoto Coefficient: 0.7 or greater

Chemical ID input (one per line):  
63-25-2  
80-05-7  
133-06-2  
57-63-6  
82657-04-3

Smiles Structures for similarity search  
[Draw] [Enter]  
Chemical Structure: C(C)1=CC=C(C(C)C)=C1

Chemical Name: Captan  
CASRN: 133-06-2  
DTXSID: DTXSID9020243  
Tanimoto: top 10 hits and >0.7  
Hit Count: 10  
Passed Filter(s): 10/10  
Selected Item(s): 0/10

Similar Structures to: Captan  
Send filtered results to: [Select tool...]  
Select Filter to add to chain:  
CASRN  
Chemical Name  
DTXSID  
Name  
Tanimoto  
Has Bioactivity  
Select this item

SMARTs Filter  
Enter SMARTs: C-Br  
Add SMARTs Query  
Chemicals that match the entered SMARTs Query  
Select SMART Query

Search Text	Count	%
<input checked="" type="checkbox"/> C=C	10 (10)	100%
<input checked="" type="checkbox"/> C-F	1 (1)	100%

Items  
C=C  
C-F



Chemical Properties Summary

Values displayed are Open Structure-Activity/Property Relationship App (OPERA) predictions:

Lists: Both Chemical Lists

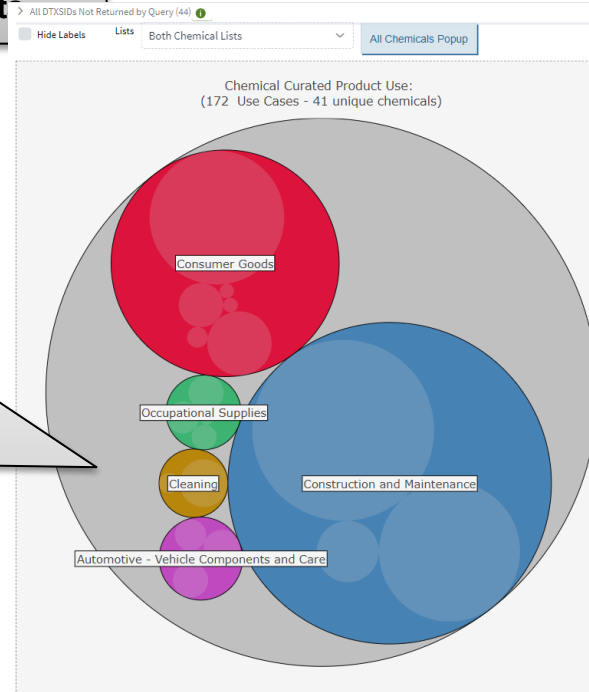
Send filtered results to: Select tool...

Chemical List (OPERA) Predictions by Input List, CASRN

Users can input one or two lists of chemicals and toggle results to show one or both list

List	Substance Name	CASRN (CEBS Link)	DTXSID (Dashboard Link)	Molecular Weight, g/mol	OPERA, Boiling Point, C	OPERA, Henry's Law Constant, atm-m <sup>3</sup> /mol
Custom Chemical List 1	Carbaryl	63-25-2	DTXSID9020247	201.221	314.943	-7.86
Custom Chemical List 1	Captan	133-06-2	DTXSID9020243	300.589	302.104	-5.43
Custom Chemical List 1	(+)-cis-Permethrin	54774-45-7	DTXSID5052208	391.288	401.446	-7.62

Summary details show product use details by category and by chemical



Nested bubble graphs show curated product use categories derived from EPA's Chemicals and Products Database (CPDat)

Chemical Curated Product Use Details (172 Use Cases - 41 unique chemicals)

Sub Category	Count
Construction and Maintenance	104
Consumer Goods	36
Automotive - Vehicle Components a...	12
Occupational Supplies	12
Cleaning	8

Curated Product Use Categories by DTXSID, CASRN

DTXSID (Dashboard)	Substance Name	CASRN (CEBS Link)	Sub Categories	Count
DTXSID8021482	Acetone	67-64-1	[Construction and Maintenance, Consumer Goods, Automotive - Vehicle Components and Care, Occupational Supplies, Cleaning]	57
DTXSID3020205	Benzyl butyl phthalate	85-68-7	[Construction and Maintenance, Consumer Goods, Automotive - Vehicle Components and Care, Occupational Supplies, Cleaning]	10
DTXSID8022292	Permethrin	52645-53-1	[Construction and Maintenance, Consumer Goods, Automotive - Vehicle Components and Care, Occupational Supplies, Cleaning]	9
DTXSID2021781	Dibutyl 1,2-benzenedi...	84-74-2	[Construction and Maintenance, Consumer Goods, Automotive - Vehicle Components and Care, Occupational Supplies, Cleaning]	8

Assay Call Results (DTXSIDs) (40 Chemicals)

Chemical List Statistical Summary of (OPERA) Predictions

Endpoint	Min	25th	Median	Mean	75th	Max
OPERA, Water Solubility, log <sub>10</sub> , moles/L	-10.4	-4.35	-2.33	-2.81	-0.869	1.355
Molecular Weight, g/mol	30.026	120.17	197.446	214.652	268.352	1202.611
OPERA, Octanol-Air Partition Coefficient, KOA log <sub>10</sub>	0.969	3.854	7.843	6.883	9.383	11.757



**Filter chain allows users to filter based on call, mechanistic target, assay, assay target, AC50, etc.**

**View data breakdown by filter terms and see selection highlighted**

**New in release v4.1: Additional information regarding data flags on results cards.**

**Plots have key features highlighted and details for assay and chemical information are provided below plots**

The screenshot displays the Curve Surfer interface. At the top, a filter chain shows 'Call' (3 selected, 626/1149), 'Mechanistic Target' (2 selected, 310/213/523), and 'AC50' (1 selected, 213). Below this, two assay plots are shown. The first plot is for 'ACEA\_AR\_agonist\_AUC\_viability' (82657-04-3) with a Hill fit. The second plot is for 'ACEA\_AR\_antagonist\_80hr' (82657-04-3) with a Hill fit. Below each plot is a results card with key features highlighted in blue. The AC50 filter window is also visible, showing 'Enter Values' (0.00001 to 194.900227) and 'Inverse Mode'.


Assay	Chemical Name	AC50 (uM)	Top of Curve	Mechanistic Target	Call
ACEA_AR_agonist_AUC_viability	Bifenhrin	27.14	48.66	Cell Viability Process	Active
ACEA_AR_antagonist_80hr	Bifenhrin	22.02	0.95	Androgen Metabolic Proc. Regulation, Steroid Hormone Nuclear Recept	Active

Close



**Input**

Results

 PBPK tool allows you to generate predictions of tissue-specific chemical concentration profiles following a dosing event

Run Reset

Species: human, ADME Source: Default, Model: Solve\_fetal\_pbtk, Exposure Route: iv, Exposure Interval: 24 Hours, Exposure Length: 0.25, Simulation Length: 3 Days, Body Weight: 70.0, Gestation Days: 91.0

Species	human	Exposure Route	iv
Body Weight	70	Exposure Interval, Hours	24
ADME Source	Default	Exposure Length, Hours	0.25
Exposure Dose	1.0	Simulation Length, Days	3
Gestational Day when Exposure Starts	91	Output Conc. Units	uM
Model	Solve_fetal_pbtk	Inhalation Dosing Method	Concentration
	Solve_pbtk	Inhalation Dosing Units	ppmv
	Solve_gas_pbtk		
	Solve_fetal_pbtk		

Model from the US  
external and fetal compartments  
shared by mother and fetus.

**Chemical Input**

Select Chemicals

Quick List CASRNs	User Chemical Identifiers
	133-06-2
	63-25-2
	54774-45-7

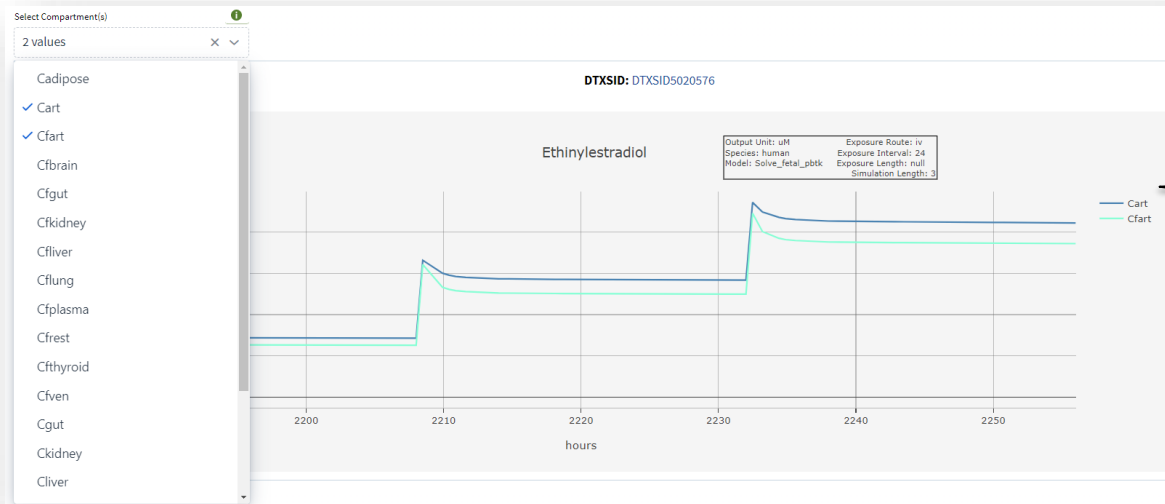
Choose human or rat (fetal model only allows human)

Choose from 3 PBPK models sourced from US EPA's httk package

Customize model parameters such as Exposure Route, Exposure Length, and Simulation Length

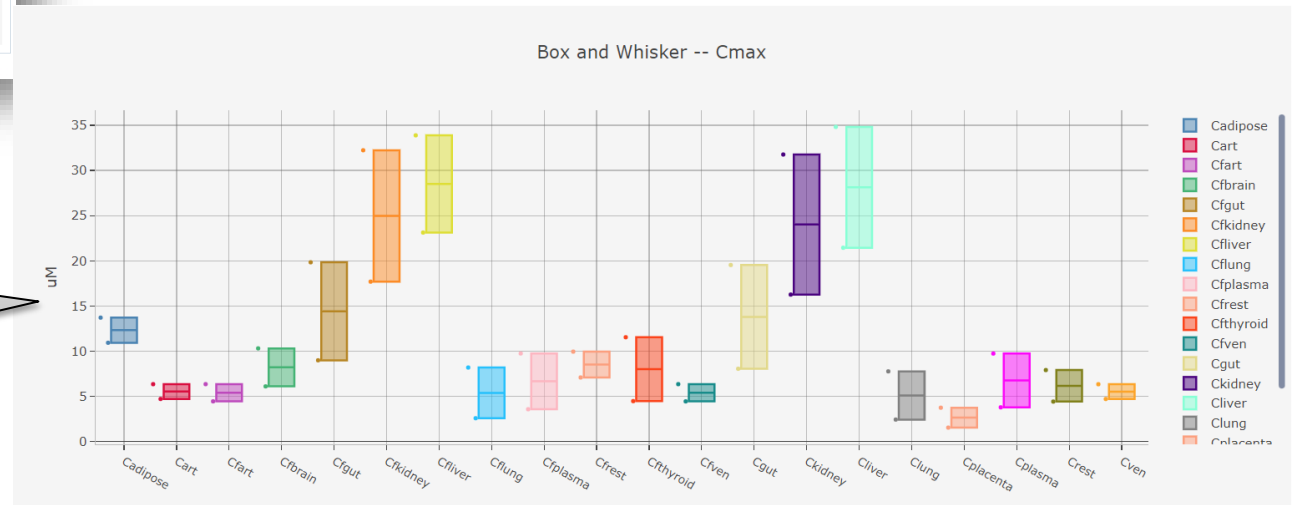






For each input chemical, the results show the concentration of the chemical over time in plasma and each tissue compartment

Boxplots show the Cmax distribution across all returned chemicals for each compartment





**Input**

Results

The IVIVE tool uses pharmacokinetic models to predict the equivalent administered dose (EAD) from the activity concentration of selected assays.

Run Reset

Endpoint: AC50, Species: human, ADME Source: Default, Model: Solve\_fetal\_pbtk, Exposure Route: Iv, Exposure Interval: 24.0 Hours, Exposure Length: null, Simulation Length: 3.0 Days, Gestational Days: 91.0, Body Weight: 70.0

In Vitro Endpoint: AC50

Species: human

Body Weight: 70

ADME Source: Default

Gestational Day when Exposure Starts: 91

Model: Solve\_fetal\_pbtk

Exposure Route: Iv

Exposure Interval, Hours: 24

Exposure Length, Hours:

Simulation Length, Days: 3

Inhalation Dosing Method: Concentration

Inhalation Dosing Units: ppmv

Model from the US EPA httk package that includes both maternal and fetal... the joint organ shared by mother and fetus. For details see User Guide [?].

1C

Solve\_pbtk

Solve\_3comp

Solve\_gas\_pbtk

✓ Solve\_fetal\_pbtk

Chemical Input

Select Chemicals

Quick List CASRNs

User Chemical Identifiers

Data Input

Select Assays

Assay	Description	Assay Type

Upload Custom In Vivo or Exposure Data to Overlay on Charts

Upload Drop file here

Uploaded Files

File Name	MIME Type

Type of activity concentration (AC50 or ACC)

Choose from in house ICE models and models sourced from US EPA's httk Package

Customize model parameters such as Exposure Route, Exposure Length, and Simulation Length

Upload custom in vivo or exposure data to overlay on charts or upload custom in vitro data to run through IVIVE





**Box and whisker plots show Equivalent Administered Dose (EAD) based on in vitro inputs**

IVIVE Results Visualizations

Select EAD to visualize: EAD 50th

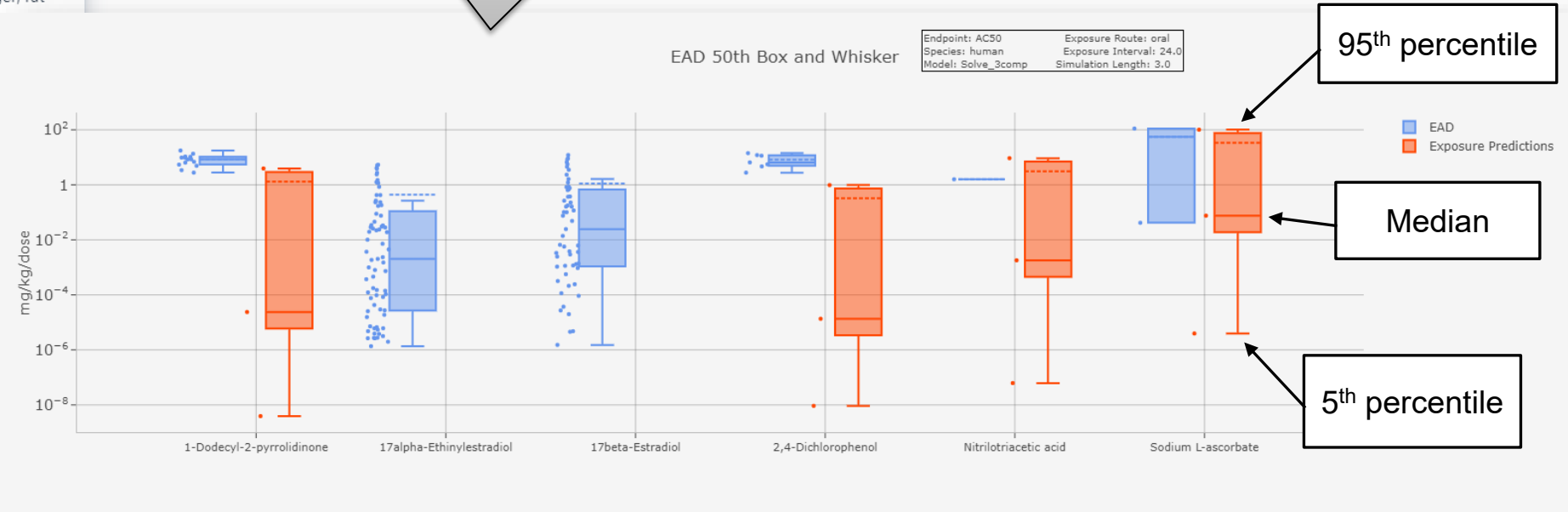
Select in vivo data or exposure data to display: Exposure Predictions

Log Axis

Select Page: 1 of 1

- Estrogen Modulation (Uterotrophic LEL)
- Acute Lethality (Acute Oral Toxicity Assay LD50)
- Androgen Modulation (Hershberger, rat agonist LEL)
- Androgen Modulation (Hershberger, antagonist LEL)
- Exposure Predictions

**Users can now overlay Exposure Predictions from EPA's SEEM3 model**



# Summary of changes and enhancements in ICE v4.1



## Data updates

- Added links to the NTP CEBS database and EPA CompTox Chemicals Dashboard in data downloads
- Updated cHTS data: Inclusion of annotations to OBO Foundry ontologies

## Tool updates

- Additional information regarding data flags on Curve Surfer results cards.
- Chemical Quick Lists: New PFAS Quick List, Updated RoC Classifications Quick List

## REST API

- Inclusion of applicability domain information for OPERA predictions
- Inclusion of Curve Surfer raw data

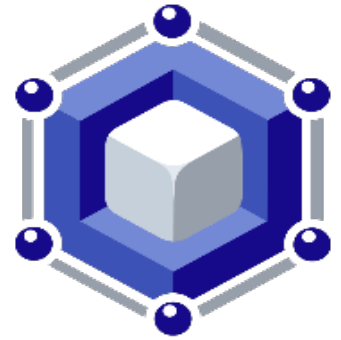
## Documentation

- Updated manuals, html pages, and help videos

# Strategic activities to improve ICE

## External review

- A team from ICF (a toxicologist, environmental scientist, computational chemist, and experienced software developer) recently conducted a review of ICE
- They assessed the usability of the front-end user interface and categorizing their findings in terms of (i) Functionality & Usability, (ii) Intuitiveness & Familiarity, (iii) Regulatory Utility, and (iv) Wishlist Functions
- They also conducted a full audit of the backend database schema and software stack



Their findings were provided in written reports and during an all-hands ICE Review and Planning Meeting on August 23, 2024

## Functionality & Usability

- Having web-based brief user guides, tutorial videos, and more detailed PDFs each serve useful purposes depending on how well versed the user is in each Tool or topic.
- Info bubbles are well written and prevent users from needing to search help pages, thus saving time.
- Sometimes links to [cebs.niehs.nih.gov](https://cebs.niehs.nih.gov) are broken or land on an empty page. For example, [Test Article Not Found \(nih.gov\)](#). If the CEBS website is the source of the issue, then a notice to the user would be helpful.

## Regulatory Utility

- Widespread use would likely require an increase in data coverage, especially for chemicals in classes of regulatory interest and for representative chemicals in data poor classes.
- More backend transparency is required for regulatory use, especially for EPA. For example, model coefficient values and statistical metrics are missing in the outputs. This is also important for non-regulatory purposes.

## Intuitiveness & Familiarity

- Overall interface is user friendly. Users can get from input to result in seconds.
- The time or root cause of expiring sessions is unknown and when it happens, work is unsaved and the tool is refreshed.
- Refreshing browser pages always brings the user back to the Quest tool instead of whichever tool they were working in.
- For many of the tools, the “Select Chemicals” button seems like an option to upload a list.
- Results download options are labeled inconsistently and differences in outputs could use descriptions.

## Wishlist Functions

- Increase in data coverage, especially for chemicals in classes of regulatory interest.
  - Tox based assays only had data for 4/14 test chemicals (data available in other platforms for chemicals not covered in ICE).
- Interoperability between all the tools. For example, selecting from output in IVIVE to carry to PBPK.
- A tool for QSAR or read across that includes tox outcomes for comparing chemicals. A "next step" to chemical quest.
- Adding a pause or cancel once a run starts.
- Listing the maximum number of input chemicals on each page.

## Strategic activities to improve ICE (2)

### All-Hands ICE Review and Planning Meeting: August 23, 2024

**Objective:** Characterize the current state of ICE, identify challenges and opportunities, and discuss potential future directions

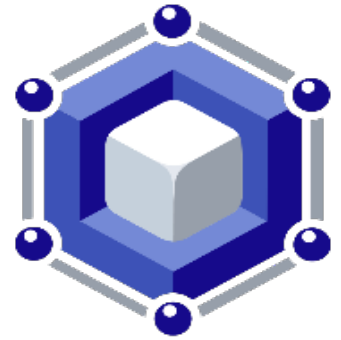
**Participants from** NIEHS, Inotiv, Sciome, ICF

### Agenda

- Reports from Inotiv tool leads and ICF consultants about what elements are working well, as well as challenges and opportunities related to the ICE front end
- Report from the Sciome leads and an ICF consultant about the overall backend architecture, code base quality, and state of the databases and servers
- Discussion about future directions for ICE

### Output

- A unified list of items related to ICE improvement, growth, and sustainability for future focused discussions and prioritization.

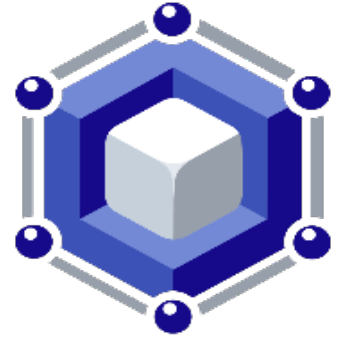


## Ongoing work and future enhancements

### Items in progress and planned for ICE v4.2

Based on feedback/requests from stakeholders, and informed by discussions at the recent ICE Review and Planning Meeting...

- Update cHTS data to align with invitrodb v4.1
- Update Tox21 quick list
- Integrate chemical quick lists into data pipeline
- IVIVE tool: Add feature to allow user-provided data
- PBPK tool: Add feature to allow user-provided data
- Chemical Characterization tool: update PCA plots





## The NICEATM Group



Integrated  
Chemical  
Environment

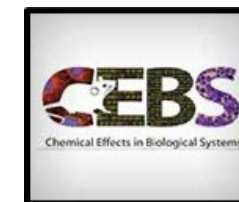


[https://github.com/  
NIHS/OPERA](https://github.com/NIHS/OPERA)



Sciome

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