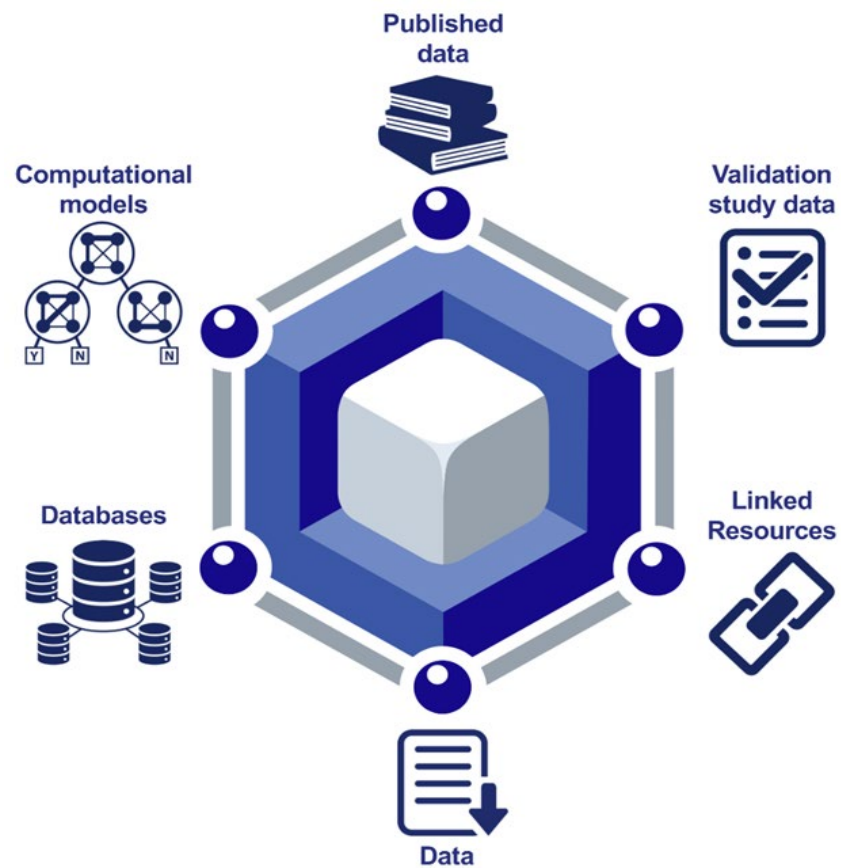


NICEATM tools: ICE and OPERA

Kamel Mansouri
Computational Chemist
NIH/NIEHS/DTT/NICEATM, RTP, NC, USA

The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of any federal agency.

Integrated Chemical Environment (ICE)



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



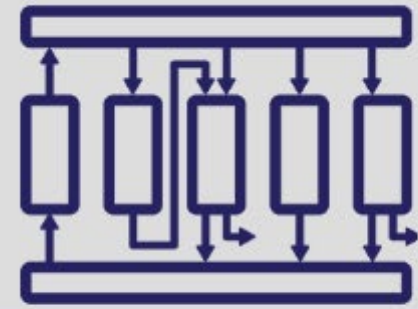
Search ▶



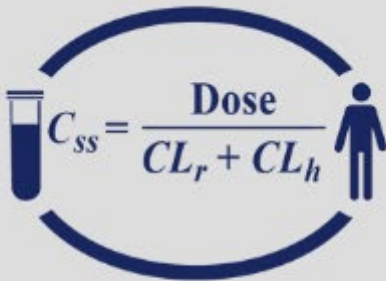
Chemical Quest ▶



Curve Surfer ▶



PBPK ▶



IVIVE ▶



Chemical Characterization ▶



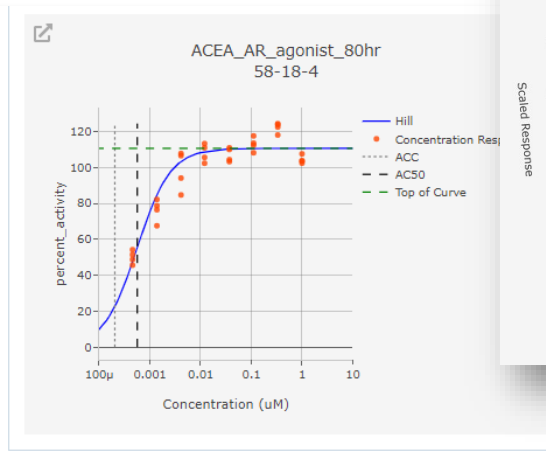
Data ▶



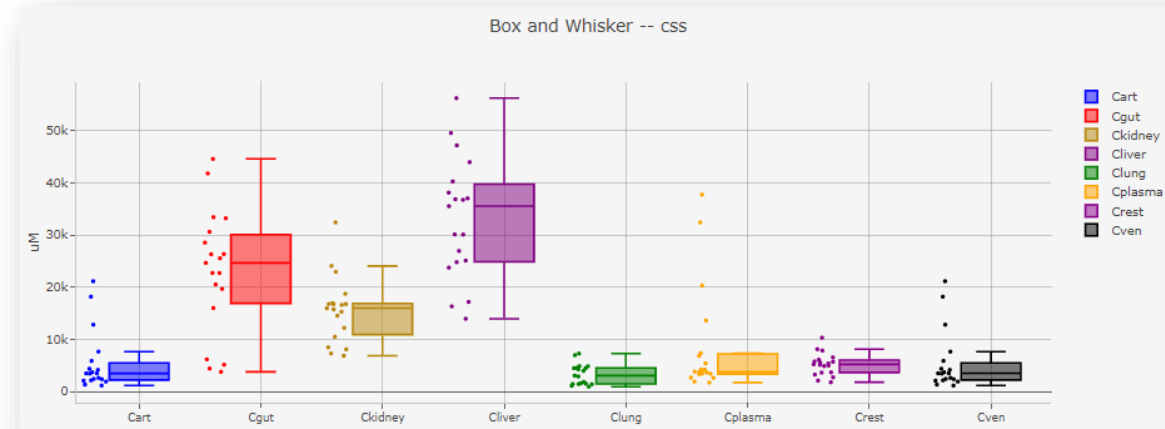
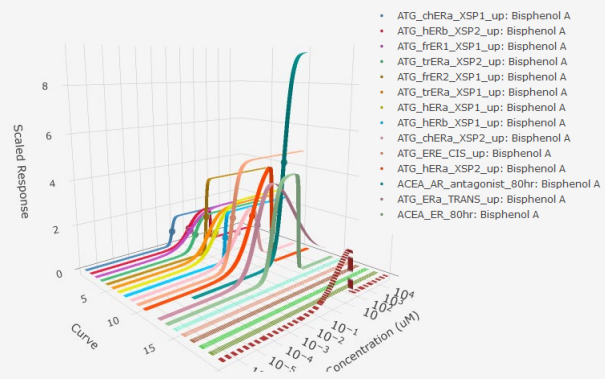
Help Videos ▶



cHTS Data Exploration



Concentration Response Curve Overlay: Scaled Response



Predicting Tissue Concentration

Chemical Similarity

Select Filter to add to chain:

Filtered Curves by Filter Type - Filtered (5) - Unfiltered

- Unfiltered: 50%
- Clustri: 40%
- Tanimoto: 13%
- Smarts: 0%
- Has Bioactivity: 1%

Smarts: 2 selected (10/10) | Has Bioactivity: 0 selected (10/10) | Tanimoto: 1 selected (9/10) | CASRN: 3 selected (5/9)

Select Page: 1 of 1 | Showing 1-5 of 5 hits | Sort Results By: Tanimoto

Select All Filtered | Clear Selected | Only show selected items

Select this item

CASRN: 20056-66-0
DTXSID: DTXSID3066552
Name: Phenol, 3-phenyl-
Tanimoto Value: 0.979167
Has Bioactivity: false

Oc1ccc(cc1)Cc2ccc(O)cc2

Select this item

CASRN: 29665-57-4
DTXSID: DTXSID0065967
Name: 3-Dodecylphenol
Tanimoto Value: 0.94
Has Bioactivity: false

Oc1ccc(cc1)CCCCCCCCCCCC

Select this item

CASRN: 139-84-4
DTXSID: DTXSID00864306
Name: 3-Nonylphenol
Tanimoto Value: 0.94
Has Bioactivity: false

Oc1ccc(cc1)CCCCCCCC

Enter Values: 0.000029 | 38.530482 | 100482

Mean: 19.52 | Std. Dev: 26.37 | Selected: 187

Chemical Consumer Use (1875 Chemicals - 203 unique): Cleaning Products and Household Care

Chemical Consumer Use Details: Cleaning Products and Household Care (270 Chemicals - 56 unique)

Sub Category	Count
General Household Cleaning	57
Laundry and Fabric Treatment	40
Carpet and Floor	38
Air Freshener	20
Dishwasher and Dishes	20

Send filtered results to:

Select tool...

Consumer Use Categories by DTXSID, CASRN

DTXSID (Dashboard)	Substance Name	CASRN (CEBS Link)	Sub Categories	Count
DTXSID7020762	Isopropanol	67-63-0	[Icons]	27
DTXSID9020584	Ethanol	64-17-5	[Icons]	27
DTXSID1024097	2-Butoxyethanol	111-76-2	[Icons]	24
DTXSID1020778	D-Limonene	5989-27-5	[Icons]	21

Assay Call Results (DTXSIDs) (50 Chemicals)

Legend: Active, Inactive, QC Omit

Chemical Exposure and Consumer Use

PBPK and IVIVE Tools Feature Enhancements:

- ICE PBPK and IVIVE tools now incorporate a gestational model from the U.S. Environmental Protection Agency (EPA)'s htk package (v2.2.2; released February 2023).
- Users modeling inhalation exposure now have the option of selecting a dose unit of ppmv rather than the existing option of μM .

Exposure Predictions:

- ICE tools integrate exposure predictions from the EPA's SEEM3 (Systematic Empirical Evaluation of Models) model (Ring et al. 2019).
- Exposure predictions can be accessed through a download file in the ICE Data Sets page and the ICE REST API. These predicted exposure data can also be compared to the equivalent administered doses (EADs) predicted by the IVIVE tool.

Search Results Redesign (BETA):

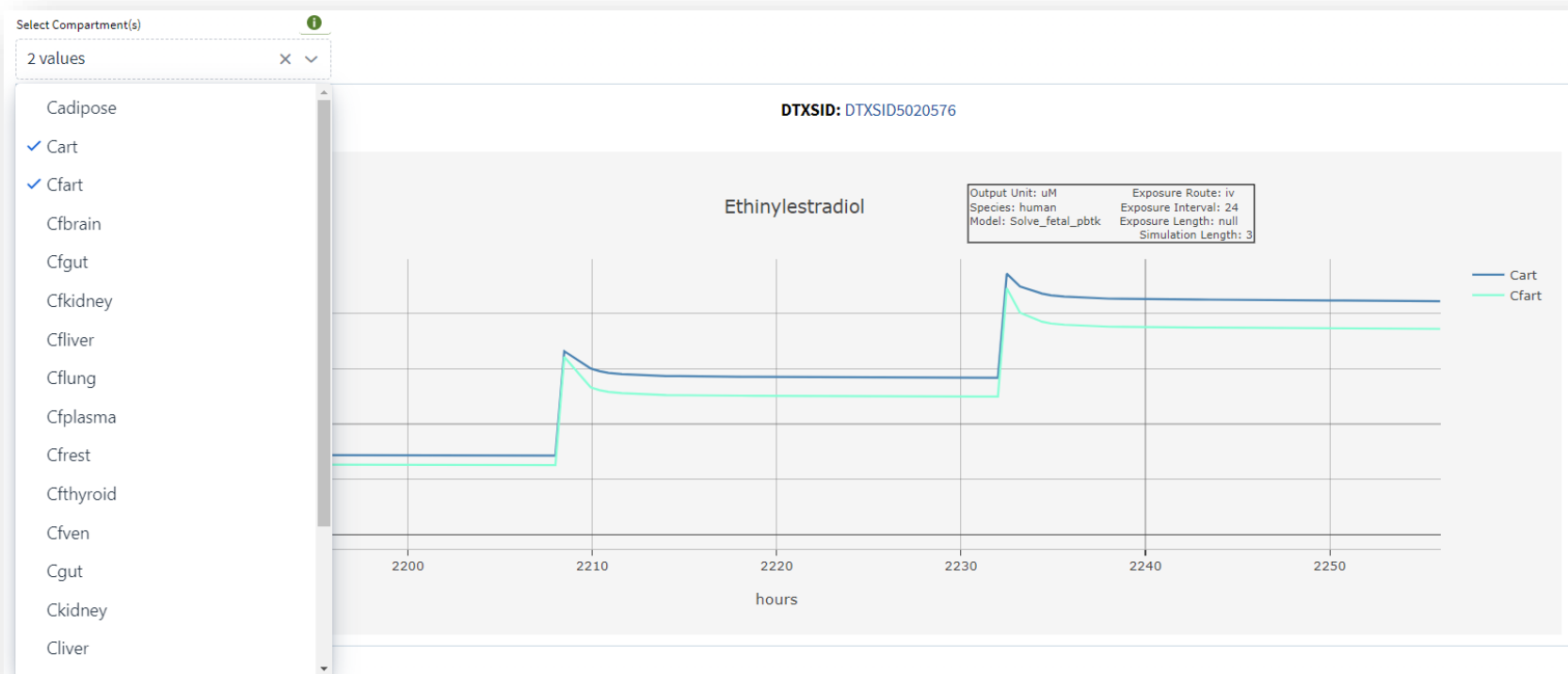
- A completely redesigned Search results interface features new summary interactive visualizations.

Chemical Name Input Option:

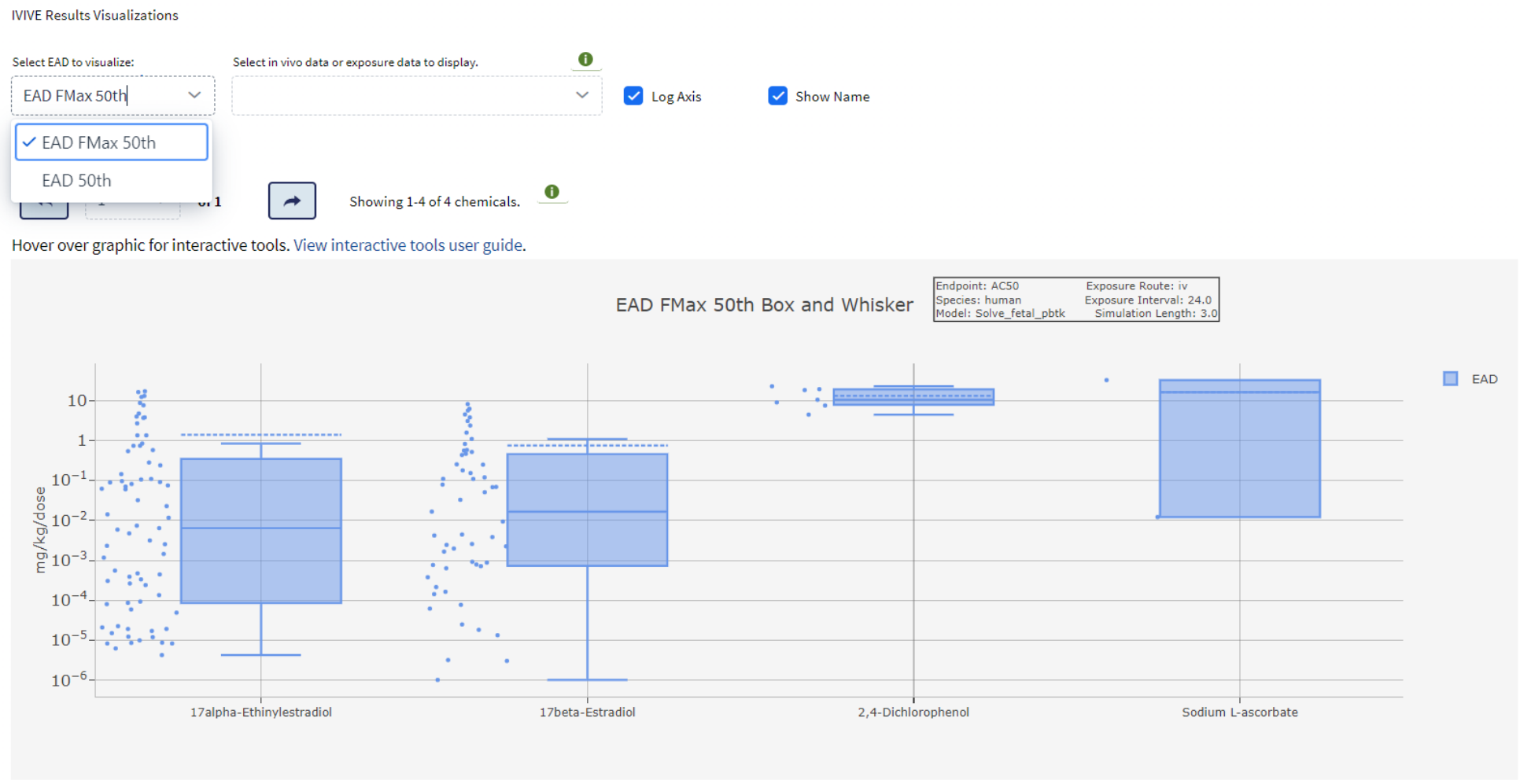
- ICE tools and the ICE REST API now accept chemical names and synonyms as input along with other pre-existing input options like CASRN, DTXSID, SMILES, and InChIKeys. This enhances comprehensive data retrieval to meet growing data needs in NAMs development.

- Human PBPK model yields concentration-time profiles in various maternal and fetal compartments (e.g., kidney, liver, plasma, thyroid, etc.)
- Users can provide gestation day when exposure starts (anywhere from 13 to 40 weeks)

Results visualizations provides filtering options to select maternal and/or fetal compartments for plotting to facilitate comparisons



IVIVE tool can predict maternal and/or fetal EADs for multiple chemicals based on in vitro inputs (using ICE data or user-provided values)



Exposure Overlay in IVIVE Tool

IVIVE Results Visualizations

Select EAD to visualize: EAD 50th

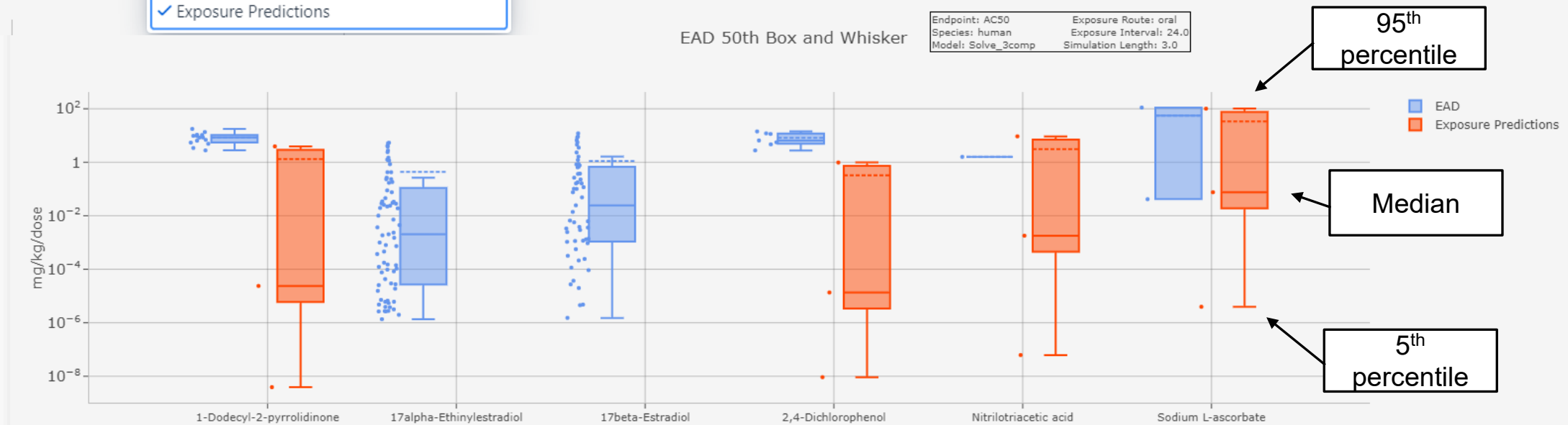
Select in vivo data or exposure data to display: Exposure Predictions Log Axis

Select Page: 1 of 1

Hover over graphic for interaction

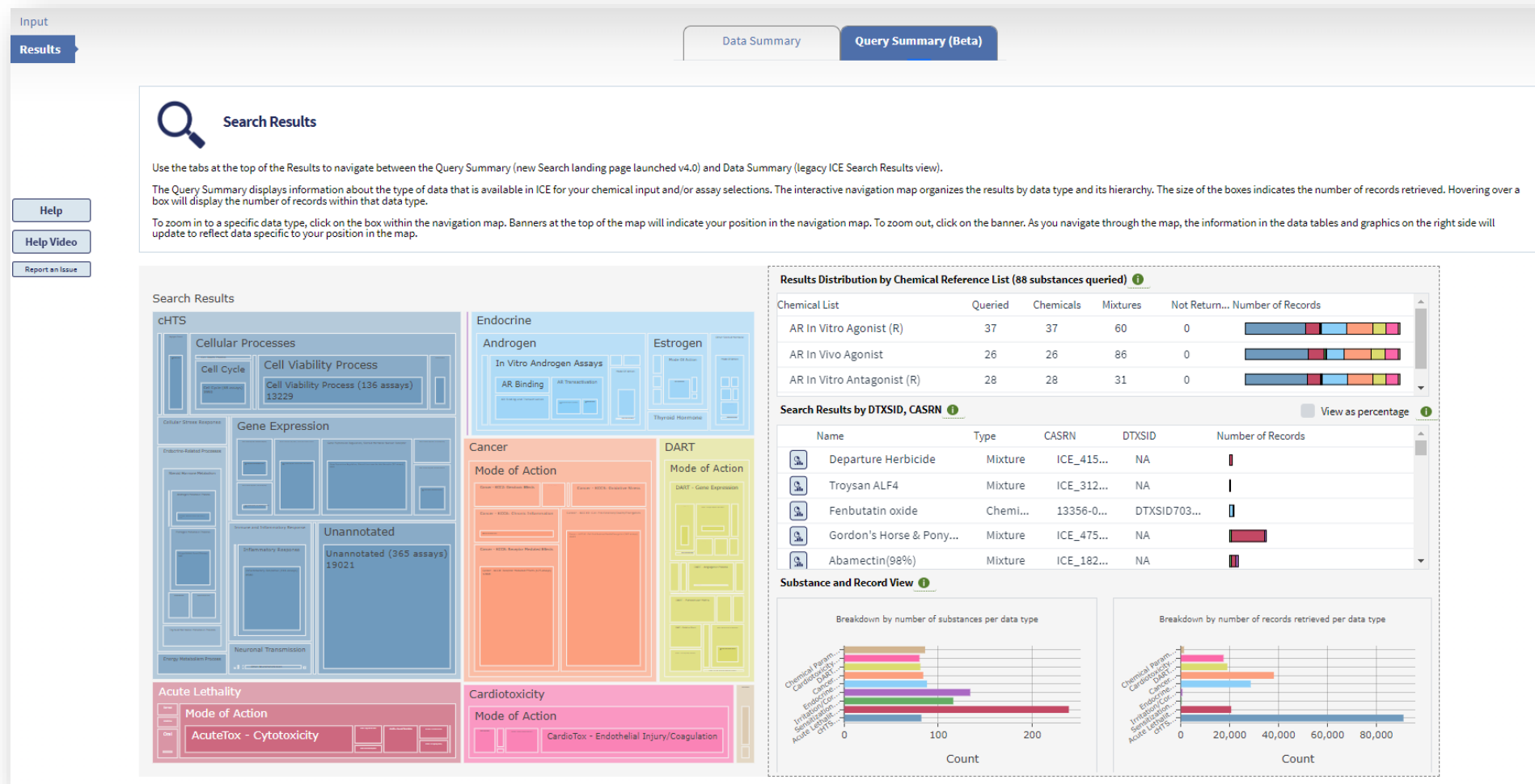
- Estrogen Modulation (Uterotrophic LEL)
- Acute Lethality (Acute Oral Toxicity Assay LD50)
- Androgen Modulation (Hershberger, rat agonist LEL)
- Androgen Modulation (Hershberger, rat antagonist LEL)
- Exposure Predictions

- There is now an overlay option for population-level exposure predictions derived from EPA's SEEM3
- It considers exposure from consumer, dietary, industrial, and pesticide pathways
- To ensure fair comparisons, IVIVE models should be run with 24-hour dosing interval since exposure predictions are in units of mg/kg/day



Interactive visualizations allow you to see the scope and breakdown of your query.

The Data Summary that used to appear for Search in previous versions of ICE is available in the “Data Summary” tab.



Input
Results | **Data Summary** | **Query Summary (Beta)**

Search Results

Use the tabs at the top of the Results to navigate between the Query Summary (new Search landing page launched v4.0) and Data Summary (legacy ICE Search Results view).
 The Query Summary displays information about the type of data that is available in ICE for your chemical input and/or assay selections. The interactive navigation map organizes the results by data type and its hierarchy. The size of the boxes indicates the number of records retrieved. Hovering over a box will display the number of records within that data type.
 To zoom in to a specific data type, click on the box within the navigation map. Banners at the top of the map will indicate your position in the navigation map. To zoom out, click on the banner. As you navigate through the map, the information in the data tables and graphics on the right side will update to reflect data specific to your position in the map.

Search Results

CHTS

- Cellular Processes
 - Cell Cycle
 - Cell Viability Process (136 assays) 13229
- Gene Expression
- Unannotated (365 assays) 19021

Endocrine

- Androgen
 - In Vitro Androgen Assays
 - AR Binding
 - AR Transactivation
- Estrogen
 - Thyroid Hormone

Cancer

- Mode of Action

DART

- Mode of Action
- DART - Gene Expression

Acute Lethality

- Mode of Action
- AcuteTox - Cytotoxicity

Cardiotoxicity

- Mode of Action
- CardioTox - Endothelial Injury/Coagulation

Results Distribution by Chemical Reference List (88 substances queried)

Chemical List	Queried	Chemicals	Mixtures	Not Return...	Number of Records
AR In Vitro Agonist (R)	37	37	60	0	
AR In Vivo Agonist	26	26	86	0	
AR In Vitro Antagonist (R)	28	28	31	0	

Search Results by DTXSID, CASRN | View as percentage

Name	Type	CASRN	DTXSID	Number of Records
Departure Herbicide	Mixture	ICE_415...	NA	
Troysan ALF4	Mixture	ICE_312...	NA	
Fenbutatin oxide	Chemi...	13356-0...	DTXSID703...	
Gordon's Horse & Pony...	Mixture	ICE_475...	NA	
Abamectin(98%)	Mixture	ICE_182...	NA	

Substance and Record View

Breakdown by number of substances per data type

Breakdown by number of records retrieved per data type

- ICE now offers a chemical name and synonym matching option in all its tools

The screenshot shows the 'Chemical Quest' tool interface. At the top, it says 'National Toxicology Program U.S. Department of Health and Human Services' and 'Integrated Chemical Environment'. Below that are navigation tabs: 'Home', 'Search', 'Tools', 'Data', 'About', 'Help'. The 'Chemical Quest' tab is active. On the left, there are buttons for 'Input', 'Results', 'Help', and 'Report an Issue'. The main area contains a description: 'The Chemical Quest tool uses fingerprints to predict structure similarity.' Below this, it states: 'This tool uses fingerprints generated using Saagar features. Only 50 input chemical ids/structures allowed at a time.' There are 'Run' and 'Reset' buttons, and a checkbox for 'Search Custom Chemical List'. Below that, there are input fields for 'Max hits per input: 10' and 'Tanimoto Coefficient: 0.7 or greater'. At the bottom, there is a text area for 'Chemical ID input (one per line)' containing the following text: Ethynylestradiol, Ethinyl estradiol, Ethinyl oestradiol, 17 α -Ethinylestradiol.

Input any synonyms for 17 alpha-Ethinylestradiol

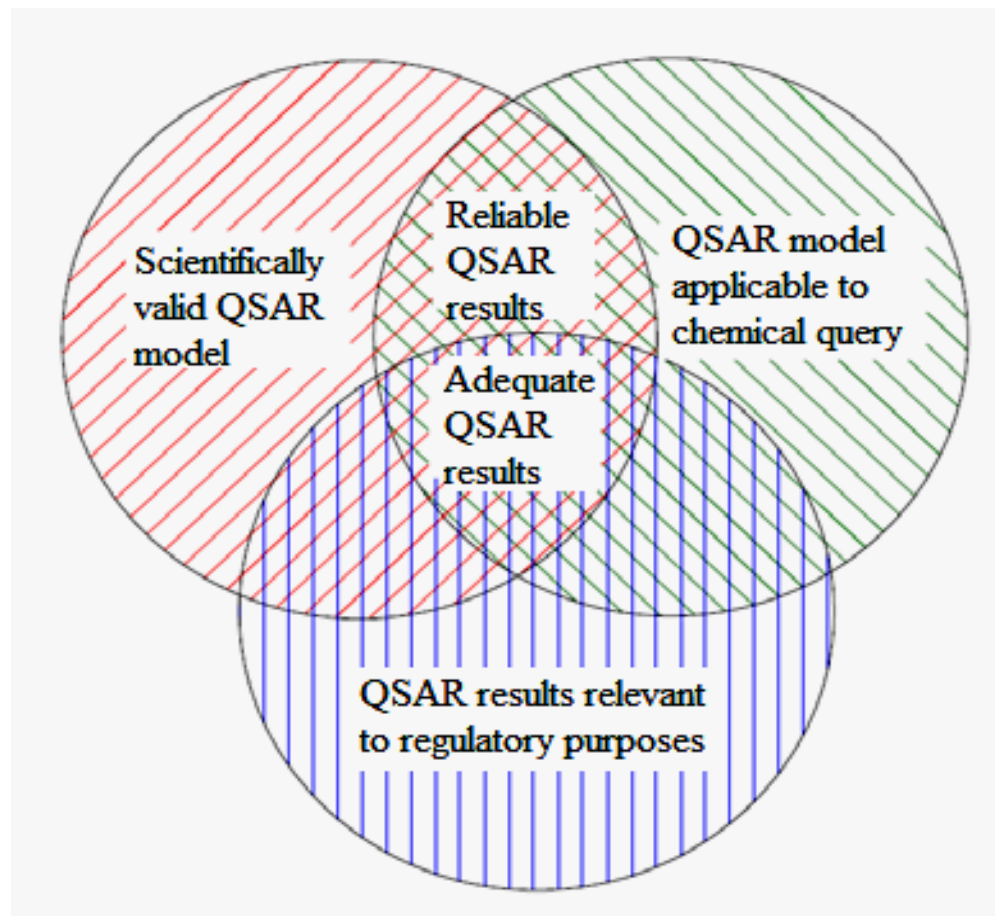
The screenshot shows the 'Chemical Quest Results' interface. At the top, there are buttons for 'Input' and 'Results'. Below that, there are icons for 'TXT', 'XLSX', and 'SDF' and a 'Send filtered results to:' dropdown menu with a 'Clear Filter' button. The main area displays the following information: 'Chemical Name: 17alpha-Ethinylestradiol', 'CASRN: 57-63-6', 'DTXSID: DTXSID5020576', 'Tanimoto: top 10 hits and >0.7', 'Hit Count: 10', 'Passed Filter(s): 10/10', and 'Selected Item(s): 0/10'. There is a 'View Results' button. Below this, there is a chemical structure diagram of 17 α -Ethinylestradiol. A callout box points to the structure with the text: 'Result will display 17 alpha-Ethinylestradiol'.

Result will display 17 alpha-Ethinylestradiol



The 5 OECD Principles

- 1) A defined endpoint
- 2) An unambiguous algorithm
- 3) A defined domain of applicability
- 4) Appropriate measures of goodness-of-fit, robustness and predictivity
- 5) Mechanistic interpretation, if possible



[Journal of Cheminformatics](#)
December 2018, 10:10 | [Cite as](#)

OPERA models for predicting physicochemical properties and environmental fate endpoints



OPERA approach

- Curated **open** access datasets (<https://doi.org/10.1186/s13321-018-0263-1>)
- **Open-source** code (github.com/NIEHS/OPERA)
- **Transparent** unambiguous algorithms (<https://qsardb.jrc.ec.europa.eu/qmrf/>)
- **Transparent** validated performances (<https://doi.org/10.1080/1062936X.2016.1253611>)
- **Defined** applicability domain and limitations of the models
- Predictions **available** through:
 - NICEATM's Integrated Chemical Environment (<https://ice.ntp.niehs.nih.gov/>)
 - The EPA's CompTox Dashboard (<https://comptox.epa.gov/dashboard>)
 - Free and open-source standalone application (github.com/NIEHS/OPERA)



Integrated
Chemical
Environment

OPERA models (version 2.9)

Physchem properties		Chemicals	Version
BP	Boiling Point	7860	2.9
HL	Henry's Law Constant	2233	2.9
LogP	Octanol-water Partition Coefficient	18154	2.9
MP	Melting Point	22554	2.9
VP	Vapor Pressure	6764	2.9
WS	Water Solubility	9943	2.9
pKa	Acid Dissociation Constant	6503	2.6
KOA	Octanol/Air Partition Coefficient	270	2.6

Environmental fate		Chemicals	Version
AOH	Atmospheric Hydroxylation Rate	692	2.6
BCF	Bioconcentration Factor	626	2.6
BioHL	Biodegradation Half-life	150	2.6
RB	Ready Biodegradability	1603	2.6
KM	Fish Biotransformation Half-life	541	2.6
KOC	Soil Adsorption Coefficient	728	2.6

Toxicity endpoints		Chemicals	Version
ER	Estrogen Receptor Activity	32464	2.6
AR	Androgen Receptor Activity	47673	2.6
AcuteTox	Acute Oral Systemic Toxicity	50660	2.6

ADME properties		Chemicals	Version
FUB	Fraction unbound	3229	2.8
Clint	Intrinsic clearance	1346	2.8
CACO2	Caco-2 permeability	4601	2.8

New/updated since 2021

PFAS in OPERA models

Models		PFAS/Total
BP	Boiling Point	346/7860
LogP	Octanol-water Partition Coef.	97/18154
MP	Melting Point	409/22554
VP	Vapor Pressure	178/6764
WS	Water Solubility	105/9943

Environmental Chemistry

Property Estimation of Per- and Polyfluoroalkyl Substances: A Comparative Assessment of Estimation Methods

Alina Lampic and J. Mark Pamis*

Chemical Properties Research Group (Canadian Environmental Modelling Centre), Department of Chemistry, Trent University, Peterborough, Ontario, Canada

VP Vapor Pressure

Deviation of \log_{10} (Pa) estimates from experimental measurements at 25 °C

	COSMOtherm	EPI Suite	NICEATM	ACD/Labs	TEST	OPERA
MAE	1.22	1.08	1.46	1.53	1.31	0.95
RMSE	1.48	1.48	2.06	1.99	1.91	1.26

LogP Octanol-water Coef

Deviation of octanol-water partition ratio ($\log K_{OW}$) estimates from experimental measurements at 25 °C

	COSMOtherm	EPI Suite	NICEATM	ACD/Labs	OPERA	LSER
MAE	0.41	0.25	0.68	0.61	0.21	0.33
RMSE	0.50	0.29	1.13	0.70	0.28	0.36

WS Water solubility

Deviation of water solubility ($\log S$; mg/L) estimates from experimental measurements at 25 °C

	COSMOtherm	EPI Suite	NICEATM	TEST*	OPERA
MAE	0.35	1.82	2.38	0.95	0.23
RMSE	0.41	2.20	2.55	1.36	0.36

Source code

Packaged installers

Updates notifications

NIH / OPERA Public

forked from kmansouri/OPERA

<> Code Pull requests Actions Projects Wiki Security Insights Settings

master 3 branches 34 tags

This branch is 37 commits ahead of kmansouri:master.

kmansouri Merge pull request #34 from kmansouri/master 77e9221 on Sep 8, 2022 210 commits

OPERA_Source_code	v2.9	9 months ago
Icon.png	OPERA 1.2 icon	6 years ago
Install_guide.pdf	v2.9	8 months ago
LICENSE	Initial commit	7 years ago
Logo.png	Added logo and icon	7 years ago
OPERA1.5_Source_code.zip	MATLAB source code for OPERA1.5	5 years ago
OPERA2.0_Source_code.zip	MATLAB source code for OPERA 2.0	5 years ago
OPERA_Data.zip	v2.9	9 months ago
OPERA_models_2.9.xlsx	v2.9	9 months ago
QMRFS.zip	v2.8.1	last year
README.md	Update README.md	9 months ago
icons.zip	OPERA 1.2 icons different sizes	6 years ago

Releases 5

OPERA 2.9 (64bit) Latest on Sep 1, 2022

NIH / OPERA Public

forked from kmansouri/OPERA

<> Code Pull requests Actions Projects Wiki Security Insights Settings

Releases / v2.9.1

OPERA 2.9 (64bit) Latest

kmansouri released this Sep 1, 2022 · 6 commits to master since this release v2.9.1 1e6d5e2

OPERA v2.9.1

(See the install and quick run guide pdf file in the zip file for more info and input options)

Clarifications about log4j concerns:

1. The presence of a log4j jar file on a computer does not imply a vulnerability in itself. It's a very common file in java-based tools. It is only when log4j is used on an exposed server that the vulnerability can be a problem.
2. We do not use log4j in OPERA software. OPERA runs locally and does not connect to the internet. Our testing thus far indicates that the removal of the log4j jar file will not affect OPERA software. OPERA should work normally with or without the log4j file as it does not depend on it.
3. OPERA uses two main tools: KNIME and MATLAB. In OPERA 2.9, both KNIME and Matlab were updated to the latest version of the log4j file to deal with the vulnerability. For more details see <https://www.knime.com/changelog-v45>. For the MATLAB runtime, MathWorks has published the following in the Trust Center (version 3 of 2021-12-18): <https://www.mathworks.com/content/dam/mathworks/policies/mathworks-response-to-cve-2021-44228-log4j-vulnerability.pdf>

To scan and remove any unwanted files/classes you can use: <https://github.com/logpresso/CVE-2021-44228-Scanner>

<https://github.com/NIEHS/OPERA>

<https://github.com/NIEHS/OPERA/releases>

Over 5000 downloads

(<https://tooomm.github.io/github-release-stats/>)

OPERA as a standalone desktop application

OPERA standalone application:

- Free, opensource & open-data
- Single chemical and batch mode
- Multiple platforms (Windows and Linux)
- Embeddable libraries (java, C, C++, Python)
- **Command line & Graphical user interface**

OPERA models:

- Physicochemical properties
- Environmental fate
- ADME properties
- Toxicity endpoints

Input options:

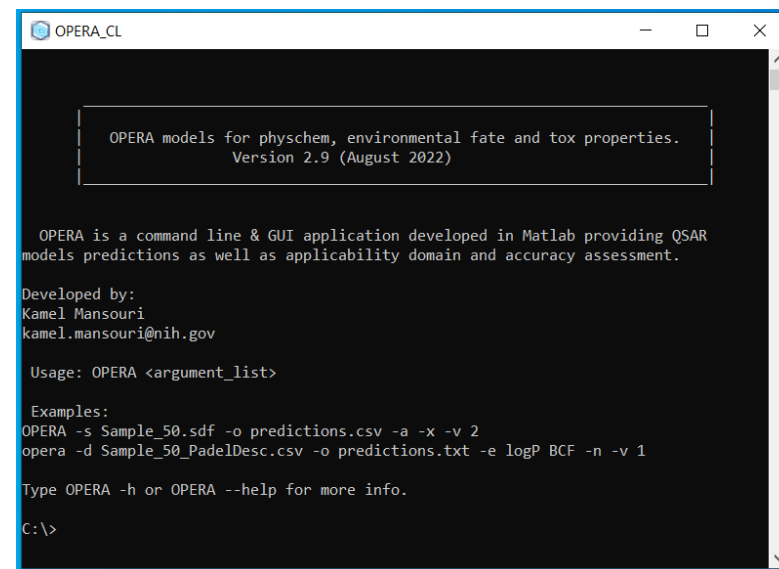
- Structure IDs (CAS, DTXSID, InChIKey)
- Structure files (SMILES, SDF, Mol)

Links:

<https://github.com/NIEHS/OPERA>

<https://ntp.niehs.nih.gov/go/opera>

<https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0263-1>



```
OPERA_CL
-----
OPERA models for physchem, environmental fate and tox properties.
Version 2.9 (August 2022)

OPERA is a command line & GUI application developed in Matlab providing QSAR
models predictions as well as applicability domain and accuracy assessment.

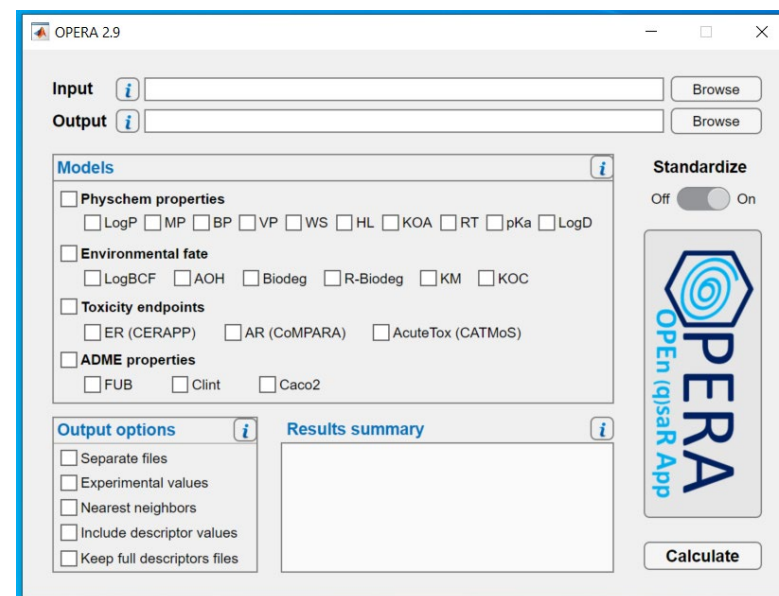
Developed by:
Kamel Mansouri
kamel.mansouri@nih.gov

Usage: OPERA <argument_list>


Examples:
OPERA -s Sample_50.sdf -o predictions.csv -a -x -v 2
opera -d Sample_50_PadelDesc.csv -o predictions.txt -e logP BCF -n -v 1


Type OPERA -h or OPERA --help for more info.


C:\>
```



OPERA 2.9

Input  Browse

Output  Browse

Models 

Physchem properties

LogP MP BP VP WS HL KOA RT pKa LogD

Environmental fate

LogBCF AOH Biodeg R-Biodeg KM KOC

Toxicity endpoints


ER (CERAPP) AR (CoMPARA) AcuteTox (CATMoS)


ADME properties

FUB Clint Caco2

Standardize

Off On

 OPERA
Open (q)SAR App

Output options 


Separate files

Experimental values

Nearest neighbors

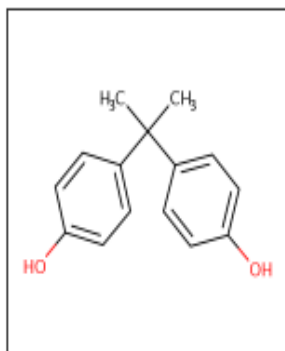
Include descriptor values

Keep full descriptors files

Results summary 

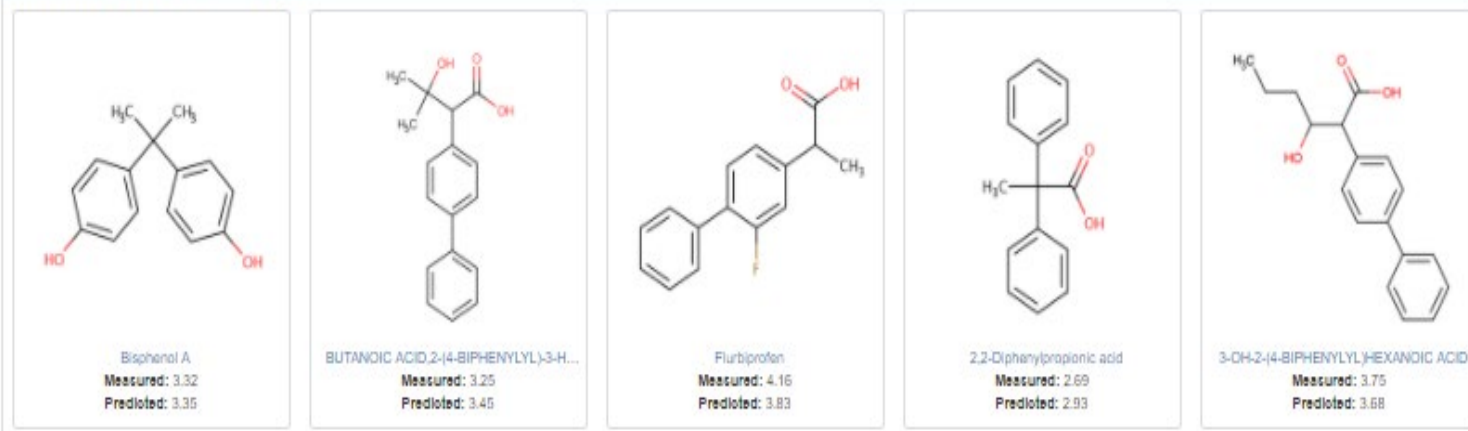
OPERA output

Bisphenol A^{MS}
80-05-7 | DTXSID7020182




- Predicted value
- Experimental value, if available
- Global applicability domain
- Local applicability domain index [0:1]
- Accuracy index [0:1]
- Confidence interval [min:max]
- 5 nearest neighbors:
 - Identifiers (CAS, DTXSID, InChiKey)
 - Experimental values
 - Predicted values
- Molecular descriptors values

Nearest Neighbors from the Training Set



MoleculeID	DTXSID7020182
LogP_exp	3.32
LogP_pred	3.32
LogP_predRange	[3.27:3.37]
AD_LogP	1
AD_index_LogP	1
Conf_index_LogP	0.948
LogP_CAS_neighbor_1	80-05-7
LogP_CAS_neighbor_2	93371-55-2
LogP_CAS_neighbor_3	85-27-8
LogP_CAS_neighbor_4	5104-49-4
LogP_CAS_neighbor_5	5558-66-7
LogP_InChiKey_neighbor_1	IISBACLAFKSPIT-I
LogP_InChiKey_neighbor_2	ZNPAJPOVURPFI
LogP_InChiKey_neighbor_3	PQSXNIMHIHYFE
LogP_InChiKey_neighbor_4	SYTBZMRGLBWN
LogP_InChiKey_neighbor_5	ODELFXJUOVNEF
LogP_DTXSID_neighbor_1	DTXSID7020182
LogP_DTXSID_neighbor_2	DTXSID5087493C
LogP_DTXSID_neighbor_3	DTXSID50100531
LogP_DTXSID_neighbor_4	DTXSID0037231
LogP_DTXSID_neighbor_5	DTXSID40204126
LogP_Exp_neighbor_1	3.32
LogP_Exp_neighbor_2	3.25
LogP_Exp_neighbor_3	2.11
LogP_Exp_neighbor_4	4.16
LogP_Exp_neighbor_5	2.69
LogP_pred_neighbor_1	3.18
LogP_pred_neighbor_2	3.66
LogP_pred_neighbor_3	3.5
LogP_pred_neighbor_4	3.05
LogP_pred_neighbor_5	3.44



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

Calendar & Events | News & Media | Get Involved | Support

SEARCH

News & Events

ICE v3.5 Release


ICE updates include:

New tools and expanded capabilities:

- Saagar Fingerprints (Beta)
- Individually Selected Results - Curve Surfer and Chemical Quest
- SDF Downloads
- AC50 Plots


Learn about ICE updates

UPDATES




OPERA
OPEn (q)saR App


PLAY




Search >





Chemical Quest >



Curve Surfer >

 Download

 Query Mixtures

 Clear Filter

Number of chemicals = 5 ⓘ

Substance Name	CASRN	DTXSID	CATMoS, Rat Acute Oral Toxicity LD50	CoMPARA, AR Agonist Call	CoMPARA, AR Antagonist Call	CoMPARA, AR Binding Call	CERAPP, ER Agonist Call	CERAPP, ER Antagonist Call	CERAPP, ER Binding Call
Acetaminophen	103-90-2	DTXSID2020006	1625	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Endosulfan	115-29-7	DTXSID1020560	2.26	Inactive	Inactive	Inactive	Inactive	Active	Active
3-Phenylprop-2-enal	104-55-2	DTXSID1024835	2568	Inactive	Inactive	Inactive	Inactive	Active	Active
Acrolein	107-02-8	DTXSID5020023	40	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Linalool	78-70-6	DTXSID7025502	2097	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive



Integrated Chemical Environment



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

Input

Union or Intersection
 Union ⌵

Run

Reset

Chemical Input

Select Chemicals ⓘ

Quick List CASRN

User CASRNs

104-55-2

78-70-6

103-90-2

107-02-8

115-29-7

Assay Input

Select Assays ⓘ

Assay

- CERAPP, ER Binding
- CERAPP, ER Antagonist
- CERAPP, ER Agonist
- CoMPARA, AR Binding
- CoMPARA, AR Antagonist
- CoMPARA, AR Agonist
- CATMoS, Rat Acute Oral Toxicity

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

Single chemical

Endosulfan
115-29-7 | DTXSID1020560
Searched by DSSTox Substance Id.

ToxCast: Models
ToxCast Model Predictions

Download ToxCast Model Predictions

Model	Receptor	Agonist	Antagonist	Binding
ToxCast Pathway Model (AUC)	Androgen	0.00	7.34e-2	-
ToxCast Pathway Model (AUC)	Estrogen	2.95e-2	0.00	-
COMPARA (Consensus)	Androgen	Inactive	inactive	Inactive
CERAPP Potency Level (From Literature)	Estrogen	-	inactive (NaN)	Active (Weak)
CERAPP Potency Level (Consensus)	Estrogen	Inactive (Inactive)	Active (VeryWeak)	Active (VeryWeak)

<https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID1020560#bioactivity-toxcast-models>

Batch search

Batch Search

Step 1 Step 2 Step 3

Step Five: Click "Download"

Please enter one identifier per line

Select Input Type(s)

- Identifiers
 - Chemical Name
 - CASRN
 - InChIKey
 - DSSTox Substance ID
 - DSSTox Compound ID
 - InChIKey Skeleton
 - MS-Ready Formula(e)
 - Exact Formula(e)
 - Monoisotopic Mass

Enter Identifiers to Search

104-55-2
78-70-6
103-90-2
107-02-8
115-29-7

Display All Chemicals Download Chemical Data

Select Output Format: Excel Download

Customize Results

- Select All
- Select All in Lists

Chemical Identifiers

- DTXSID
- Chemical Name
- DTXCID
- CAS-RN
- InChIKey
- IUPAC Name

Structures

- Mol File
- SMILES
- InChI String
- MS-Ready SMILES
- QSAR-Ready SMILES

Intrinsic And Predicted Properties

- Molecular Formula
- Average Mass
- Monoisotopic Mass
- TEST Model Predictions
- OPERA Model Predictions

Presence in Lists:

- DRUGS(NORMAN): Pharr
- 40CFR995: Extremely Ha
- AEGUS: Acute Exposure
- Amphibole Minerals
- ANDROGEN: Androgen
- ARTICLE: Bench-Mark Di
- ARTICLE: Collaborative E
- ARTICLE: Collaborative E
- ATSDR: Minimal Risk Lev
- ATSDR: Toxic Substance
- CalEPA Office of Environ
- Canadian Domestic Sub
- Chemicals in human blo
- DRUGS: Antibiotics
- DRUGS: DrugBank data
- DRUGS: Opioids and rel
- DRUGS: Statin drugs
- DRUGS(NORMAN): ITNA
- DRUGS(NORMAN): Pharr
- DRUGS(NORMAN): Targe
- DRUGSIWIKILIST: Veterir

https://comptox.epa.gov/dashboard/dsstoxdb/batch_search

Predictions on FDA's precision platform

precisionFDA

A secure, collaborative, high-performance computing platform that builds a community of experts around the analysis of biological datasets in order to advance precision medicine.

The screenshot displays the precisionFDA web interface for the OPERA v2.9 application. The browser address bar shows the URL: <https://precision.fda.gov/home/apps/app-GGk23K8035gy3KxgGkJXQ8jF-1>. The left sidebar contains navigation options: Apps (189), Databases (0), Assets (200), Workflows (0), and Executions (1203). The main content area shows the application details for OPERA v2.9, including a 'Revision: 5 Latest' dropdown, a table with columns for LOCATION, NAME, ID, ADDED BY, and CREATED ON, and tabs for Spec, Executions (10), and Readme. The configuration section includes 'DEFAULT INSTANCE TYPE' (baseline-4) and 'HAS INTERNET ACCESS' (No). The 'INPUTS' section lists: 'Input file format' (string, REQUIRED, Default: sdf, Choices: [sdf, mol, smi, descriptor]), 'Input file' (file, REQUIRED), 'Output prefix' (string, Default: outputs), 'Output prediction file format' (string, REQUIRED, Default: csv, Choices: [csv, txt]), and 'Extra arguments' (string, Default: -a -x -v 2). The 'OUTPUTS' section lists: 'OPERA output tarball' (file, REQUIRED). A URL <https://precision.fda.gov> is displayed in the bottom right corner of the interface.

At this position:	Count
QSARs	2
Automated workflows	0
Standardized workflows	0

Toolbox Repository

Tools / QSARs / OPERA models

OPERA models

Current version:	1.0
Supported Toolbox versions:	4.5
Developer:	NIEHS
Category:	QSARs
Downloads:	57
Rating:	☆☆☆☆☆ 0

Description:
OPERA is a free and open-source/open-data suite of tools for predicting physicochemical properties, environmental fate, ADME and toxicological information including applicability domain and accuracy. It includes a user-friendly graphical interface for Windows and Linux operating systems.

<https://repository.qsartoolbox.org/>

Acknowledgments

The NICEATM Group



Integrated
Chemical
Environment

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



[https://ntp.niehs.nih.gov/go/
2021iccvamreport](https://ntp.niehs.nih.gov/go/2021iccvamreport)



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