


CSS DASHBOARD



Dashboards

Using EPA's web-based interactive Dashboard, decision-makers will access summary information derived from chemical exposure, hazard data, decision-rules and predictive models. Dashboards will include information from these diverse sources in order to provide more integrative, holistic information for use in risk assessment and risk management decisions. The "Dashboard" will be customized based on the queries of the decision maker using the web-based tool.

More information available at:
<http://css.epa.gov/>

 EPA
www.epa.gov/research

science in ACTION

INNOVATIVE RESEARCH FOR A SUSTAINABLE FUTURE

CHEMICAL SAFETY FOR SUSTAINABILITY RESEARCH

Background
Chemical safety is a major priority of research and decision making at EPA. EPA's Chemical Safety for Sustainability (CSS) research program is:

- Improving protection of human health and the environment by providing scientific approaches and information on chemical exposure, hazard and risk.
- Evaluating chemicals for potential risks to human health and the environment.
- Targeting nanomaterials and endocrine disrupting chemicals research.
- Moving toward a more sustainable environment by producing new and existing chemicals in safer ways.

Research Focus Areas
CSS research includes eight research focus areas:

Inherency
Inherency is the physico-chemical characteristics of a chemical that influences exposure and toxicity potential. Inherency research will compile and share chemical property information that will lead to a better understanding of the relationships between chemical properties and specific disease outcomes.

Systems Models
Systems Models research investigates the entire process of how a chemical interacts with human and wildlife biological processes. The investigation starts with research on chemical exposures. It then follows the subsequent interactions between chemical exposures and resulting

adverse effects to improve the understanding of environmentally caused diseases. Innovative chemical screening technologies, such as automated, rapid screening will be used to generate chemical data on the biological effects of large numbers of chemicals.

Biomarkers
Biomarkers are biological responses that indicate exposure to a chemical, an effect from exposure to a chemical or susceptibility to adverse effects from a chemical. The research will use linkages to develop biomarker-based predictive tools to understand chemical exposure events and predict outcomes that may result.

Cumulative Risk
Real world chemical exposures are rarely due to a single chemical. *Cumulative Risk* research helps identify, predict, assess and prioritize chemical mixtures and the associated human and wildlife adverse outcomes in real-world settings. The research will assess the potential human health and environmental outcomes that may occur due to multiple and continuous exposures to chemicals and mixtures, especially those found in consumer products.

Life Cycle Considerations
Green chemistry applies across all the life cycle considerations of a chemical product, including its design, manufacture, and use. By examining the environmental exposures and human and ecological health impacts of a chemical, *Life Cycle Considerations* research will provide data to inform the design of more sustainable/greener chemicals.

Extrapolation
Extrapolation research aims to provide data-driven decisions and to develop consistent, appropriate methods for extrapolating measured data to respond to chemicals at other doses, in other species, etc. This research will use available data to develop approaches that extrapolate between test organisms and human or ecological responses, test and real-world exposure durations, and from laboratory to field conditions.

Dashboards
Using EPA's web-based interactive *Dashboard*, decision-makers will access summary information derived from chemical exposure, hazard data, decision-rules and predictive models. Dashboards will include information from these diverse sources in order to provide more integrative, holistic information for use in risk assessment and risk management decisions. The "Dashboard" will be customized based on the queries of the decision maker using the web-based tool.

Evaluation
Evaluation will develop the tools needed to evaluate and characterize the reliability and uncertainty of data, methods, and models that are developed in the other CSS research areas.

Collaboration
EPA Program Offices and Regions as well as external stakeholders have participated in the CSS research planning process since its inception. Collaboration is vital for the success of CSS. EPA will continue to seek input to continuously enhance CSS research.

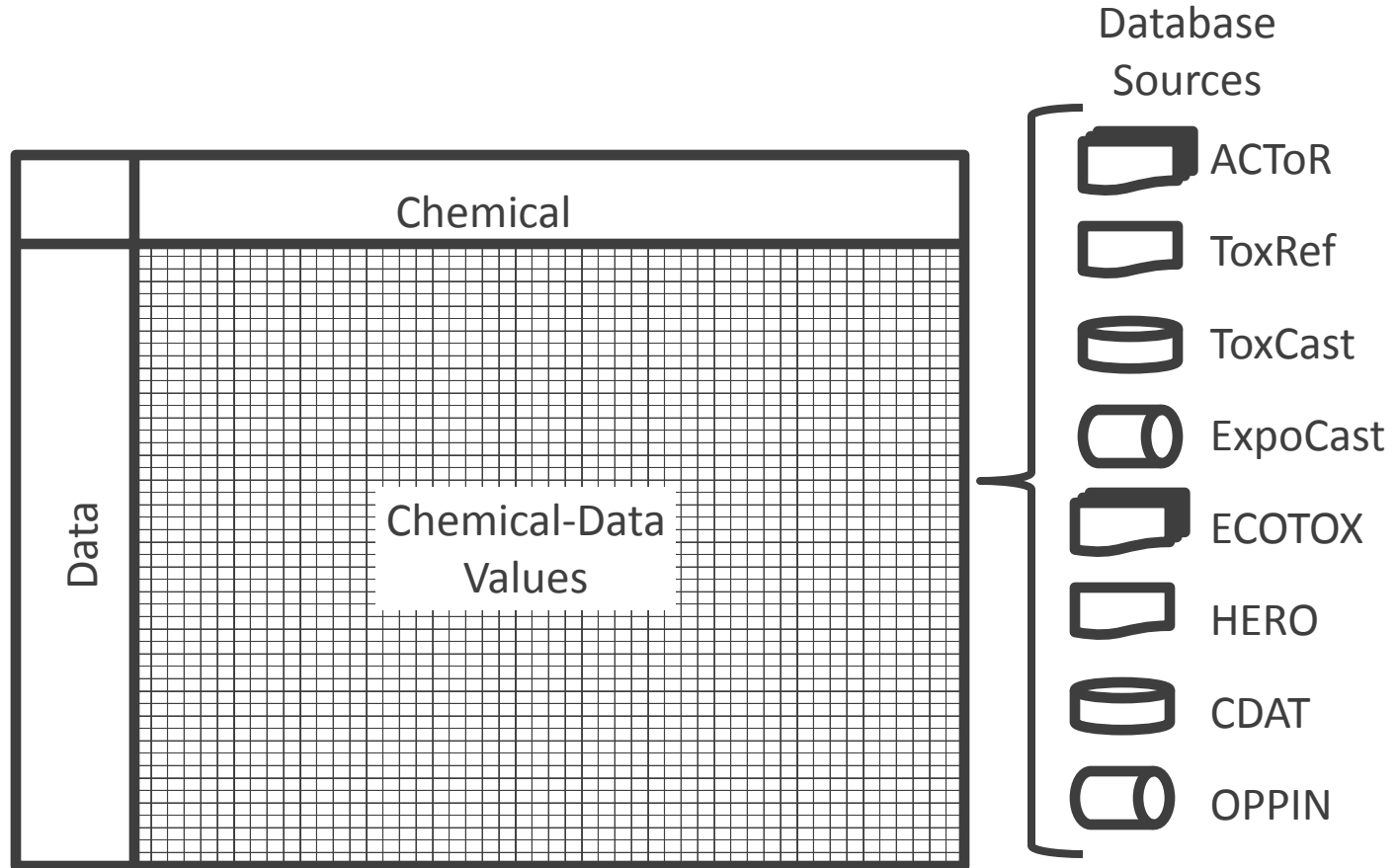
1 U.S. Environmental Protection Agency
Office of Research and Development

www.epa.gov/research
Contact: Monica Linnenbrink
Linnenbrink_monica@epa.gov
919-541-1522

Dashboards key concepts

- The purpose is to provide an interface that allows access to both ORD and PO research/tools and synthesis for integrated decision support
- User-driven design concepts
 - Transparent, retraceable, updatable, interactive, modular, flexible, secure
- Leveraging resources
 - Data: Integration of diverse databases that facilitates continued growth
 - Research: Access to computational tools and models
 - People: Smart design means that a focused team can have far-reaching effects
 - Communication: Distributed, shareable web interface (internal/external)
- Current Dashboard has 3 major interactive modes
 - Data Explorer: Selecting relevant data/models/chemicals
 - Chemical Explorer: Integrating evidence and scoring chemicals
 - Prioritization: Formalized, yet flexible, schemes for decision support

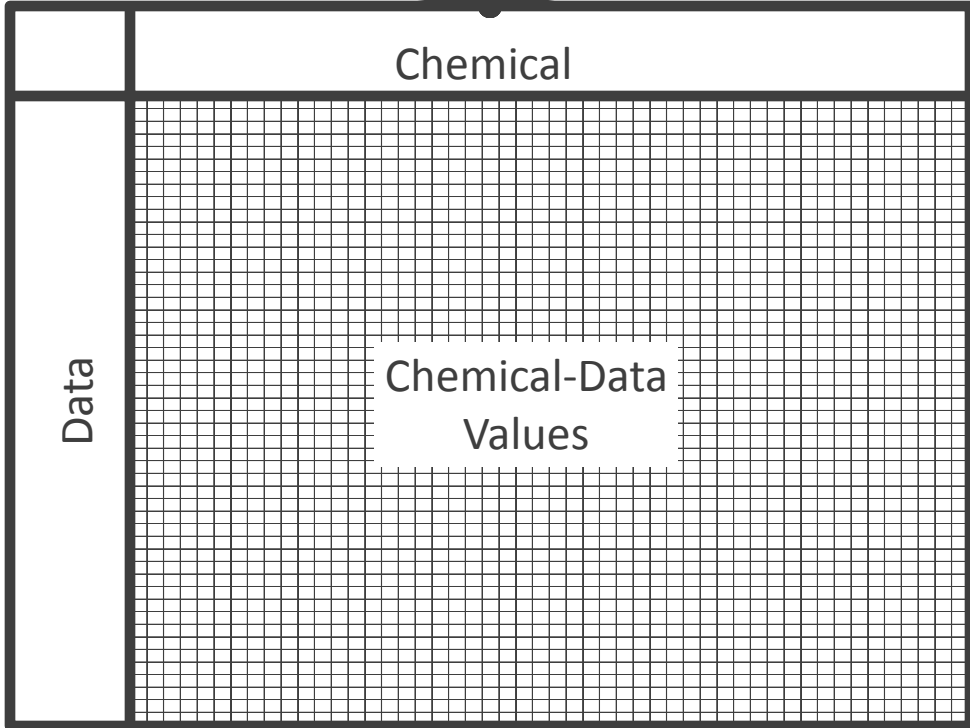
- Near-term priorities:
 - Data Explorer: Provide interactivity to PO partners for “tagging” data
 - Chemical Explorer: Development and expansion of widget library
 - Prioritization: Development and expansion of widget library
 - Assure that development allows seamless transition to public-facing Dashboard
 - Explore incorporation of non-ORD data sources (e.g. PO databases)
- Release schedule for PO partners: OW21, EDSP21 & TSCA21 Dashboards
 - [Dec. 2012] Data source identification & Case study development
 - [March. 2013] PO-driven Data Explorer
 - Using Dashboard to further identify & evaluate data sources
 - Early beta testing of single Dashboard component (Data explorer)
 - Evaluation of case study success
 - [July 2012] Beta-testing of remaining Dashboard components
Chemical explorer & Prioritization mode
 - [Sep. 2013] Internal/External (public) version of Dashboard released



Metadata/Filters/Descriptors

<u>Class</u> OP Carbamate Plasticizer	<u>Availability</u> ToxCast ToxRefDB ACToR	<u>Regulatory</u> TSCA SDWA FIFRA	<u>Structure</u> Chlorine Benzene Azole	<u>Property</u> logP PSA MW	<u>Other</u> XXX YYY ZZZ
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Database Sources



- ACToR
- ToxRef
- ToxCast
- ExpoCast
- ECOTOX
- HERO
- CDAT
- OPPIN

Metadata/Filters/Descriptors

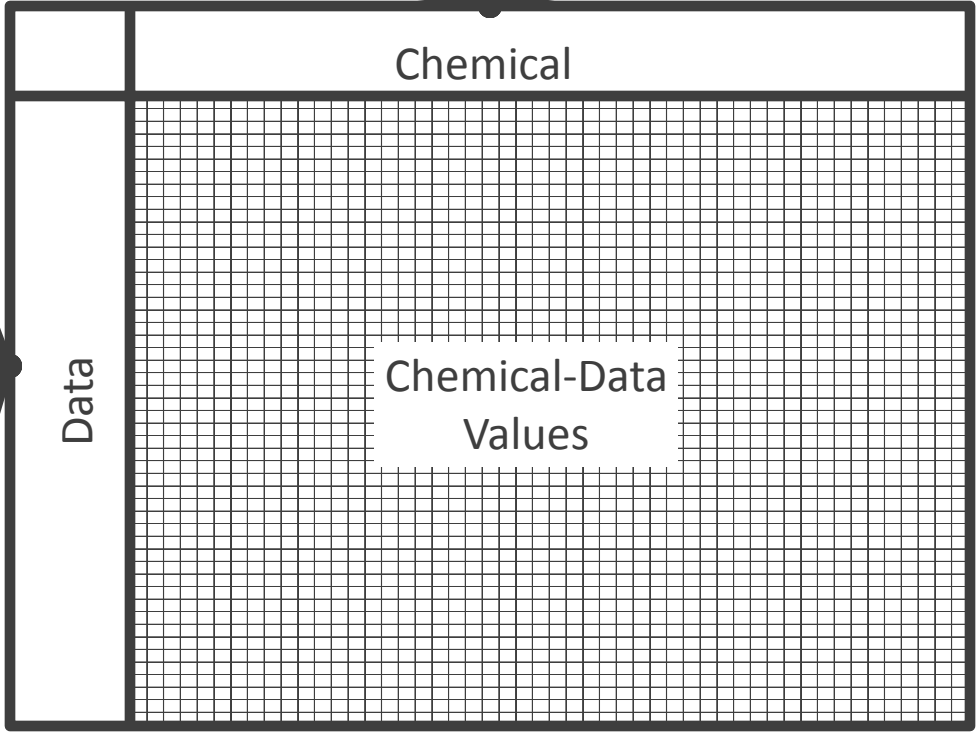
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-  CDAT
-  OPPIN

Metadata/Filters/Descriptors

- Value Type
Quantitative
Qualitative
Link
- Type
Hazard
Exposure
Product
- Hazard Type
In Vivo
In Vitro
In Silico
- Quality
Good
Bad
Ugly
- Source
EPA
FDA
NTP
- Other
XXX
YYY
ZZZ

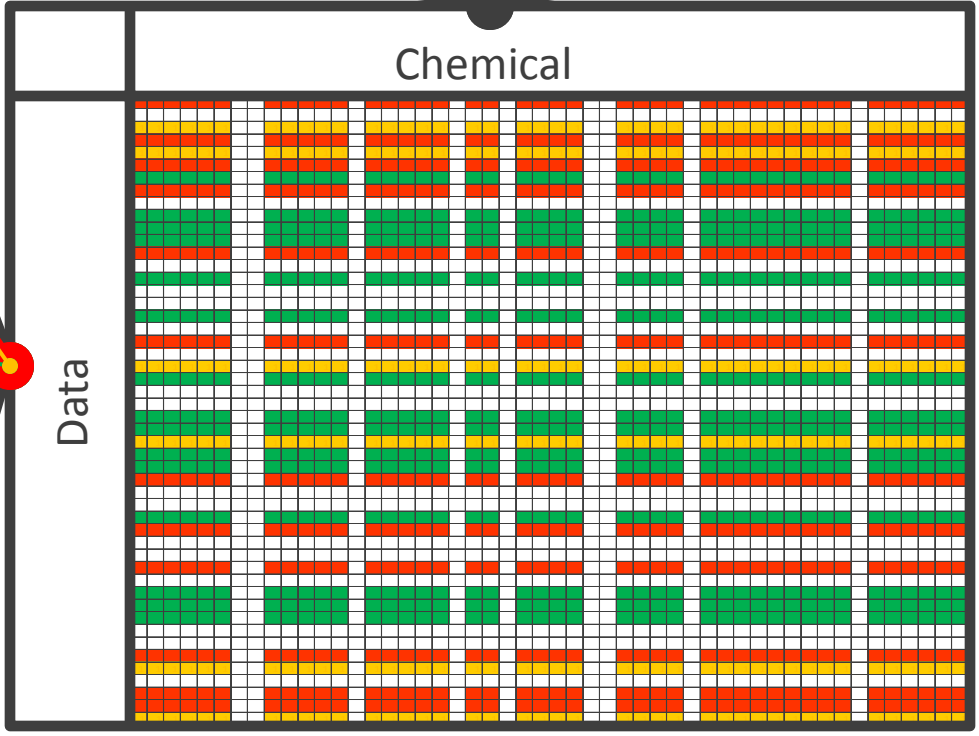


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Metadata/Filters/Descriptors

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Qualitative
Link

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Hazard
Exposure
Product

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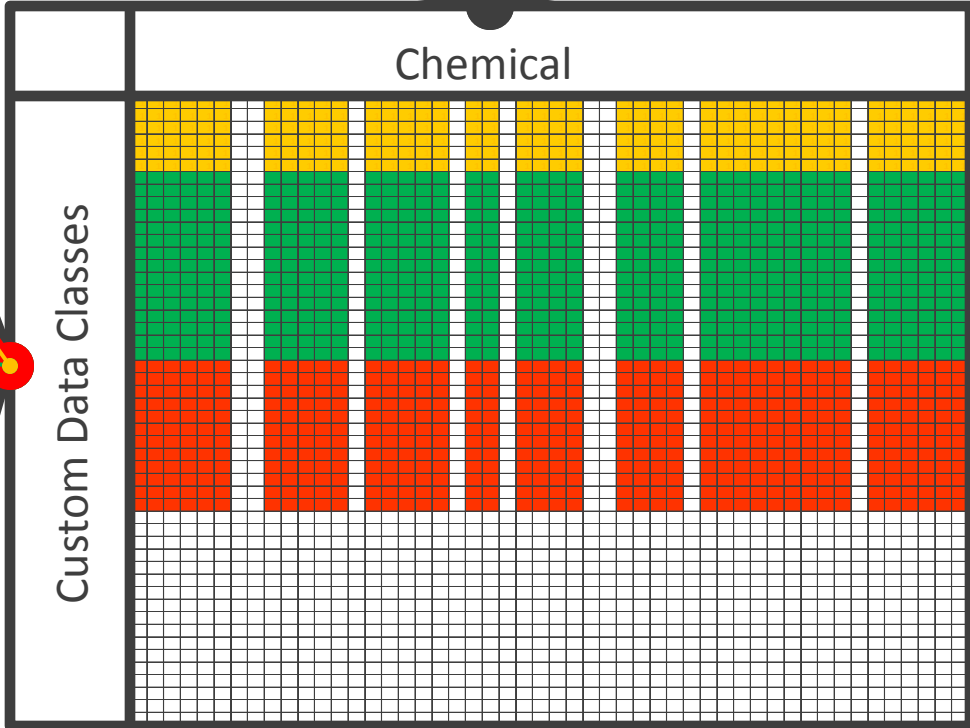
Other
XXX
YYY
ZZZ

Metadata/Filters/Descriptors

<u>Class</u> OP Carbamate Plasticizer	<u>Availability</u> ToxCast ToxRefDB ACToR	<u>Regulatory</u> TSCA SDWA FIFRA	<u>Structure</u> Chlorine Benzene Azole	<u>Property</u> logP PSA MW	<u>Other</u> XXX YYY ZZZ
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Metadata/Filters/Descriptors

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Qualitative
Link

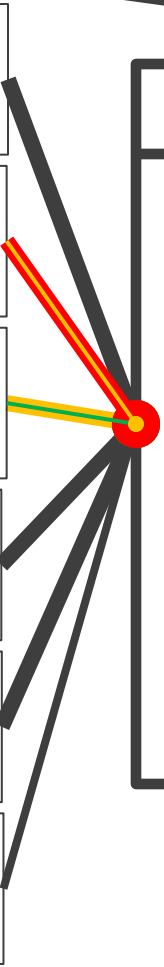
Type
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Exposure
Product

Hazard Type
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FDA
NTP

Other
XXX
YYY
ZZZ



Metadata/Filters/Descriptors

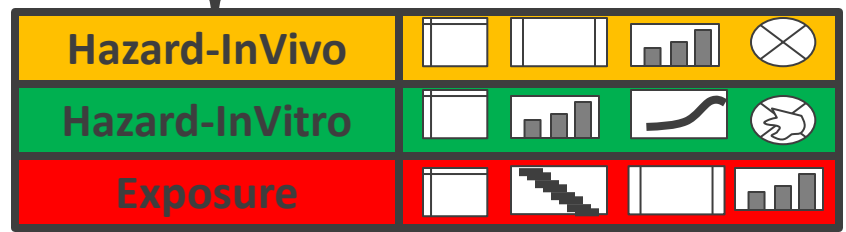
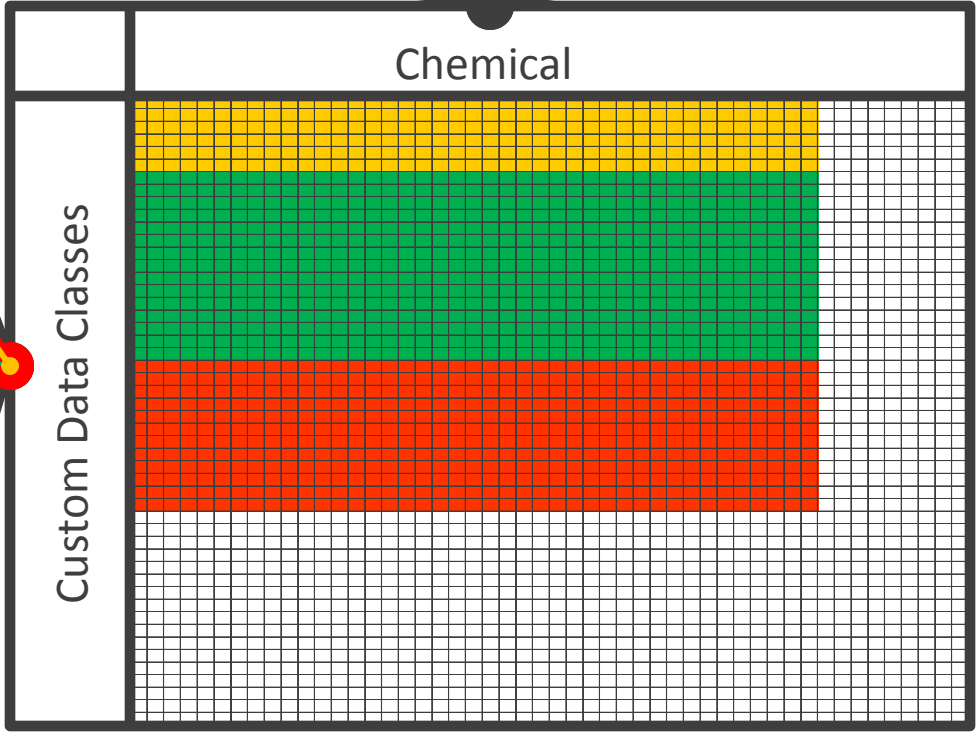
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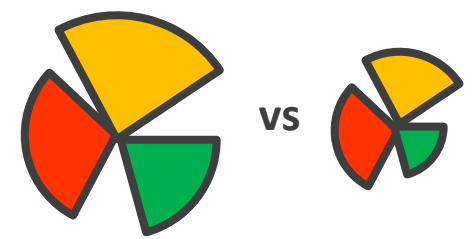
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Qualitative
Link
- Type
Hazard
Exposure
Product
- Hazard Type
In Vivo
In Vitro
In Silico
- Quality
Good
Bad
Ugly
- Source
EPA
FDA
NTP
- Other
XXX
YYY
ZZZ



Chemical Data Explorer

Prioritization



Dashboards workflow: Dynamic, Recordable, Reversible

1 – Login: Username + secure password determines user's specific access

2 – Dashboard select: Choose Dashboard (e.g. default "OW21" or saved user session)

3 – Data Explorer: Choose data sources and organization; set rules for batch ("auto") chemical scoring

4 – Chemical Explorer: Explore data on chemicals; choose chemical subset lists; manually adjust chemical scores

5 – Prioritization: Translate chemical scores into decisions

The image is a collage of screenshots from the EPA's Dashboard workflow, illustrating the five steps described in the text. The screenshots are arranged in a layered, overlapping fashion, showing the progression from login to prioritization.

- Step 1 (Login):** Shows the EPA website's login page with fields for Username and Password, and a Login button.
- Step 2 (Dashboard select):** Shows the user's dashboard after login, with a navigation menu and a 'Select User Session' dropdown menu.
- Step 3 (Data Explorer):** Shows the 'Data Explorer' interface, where a chemical class (Estrogen) is selected, and a list of chemical names and their associated data points is displayed.
- Step 4 (Chemical Explorer):** Shows the 'Chemical Explorer' interface, where a specific chemical (CAS# 83-62-7) is selected, and its properties, literature results, and a 'Toxicity Score vs Chemical Rank' graph are displayed.
- Step 5 (Prioritization):** Shows the 'Prioritization' interface, where a grid of chemical scores is displayed, and a 'Toxicity Score vs Chemical Rank' graph is used to visualize the data.

Dashboard components in the 'Chemical Explorer' mode

Modular design facilitates development: This includes new data types (e.g. ExpoCast), widget development (e.g. hazard banding or chemical profile read-across), alternate modes (e.g. HH Risk Assessment), evidence translation, etc.

Dashboard mode selector

Information display tabs
(widget collections for main canvas area)

Widget selector

Main chemical

Data types

Comparison chemical list

Chemical selection and evidence summary (searchable, sortable, saveable)

Main canvas
(contains interactive widgets)

Summary evidence buttons

Dashboard components in the 'Prioritization Mode': ToxPi widget

The organization of information is user-group specific (e.g. The Dashboard below has chemical information organized into endocrine-relevant data classes to support EDSP decisions)

Select User Session ✕

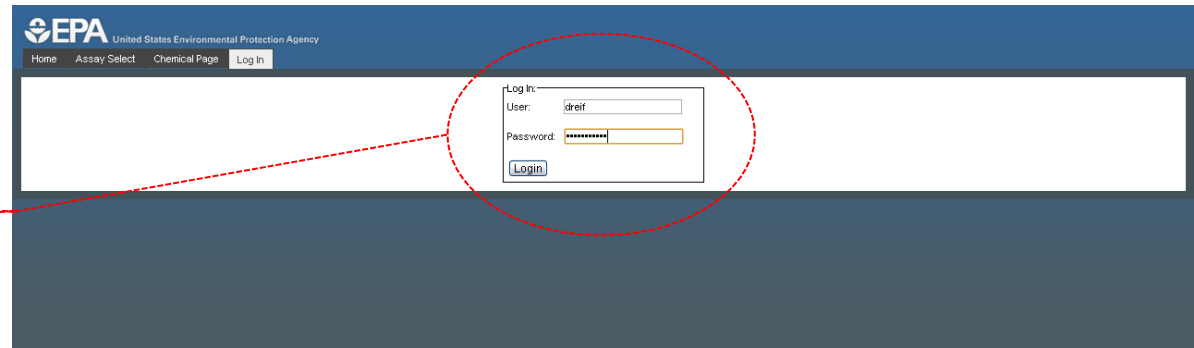
EDSP21

- EDSP21
- TSCA21
- OW21
- OPP21
- Demo
- Test

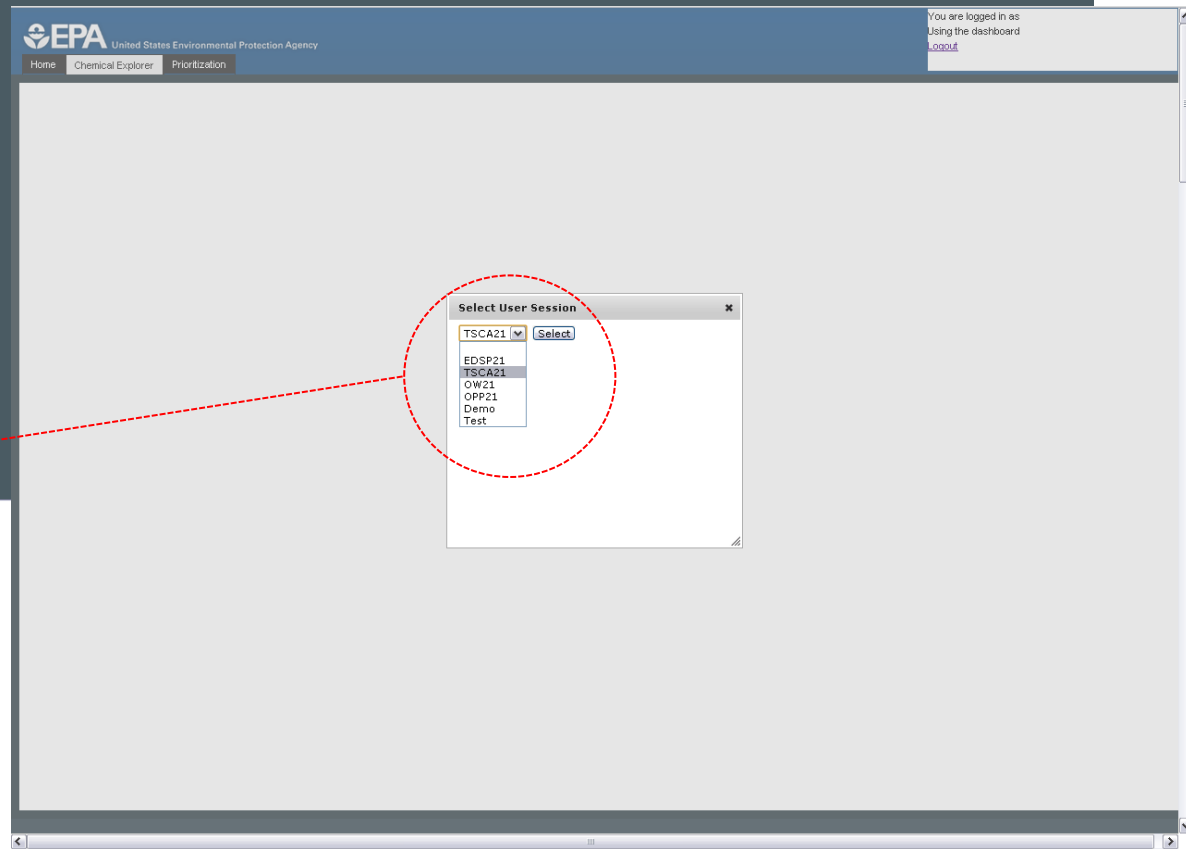


Chemical Explorer mode: Exploring assay results (Screenshot from prototype Dashboard)

Users login to gain access to specific Dashboards. This allows control over protected information and setting of various roles (e.g. division manager, specific assessor) to facilitate oversight or sharing.

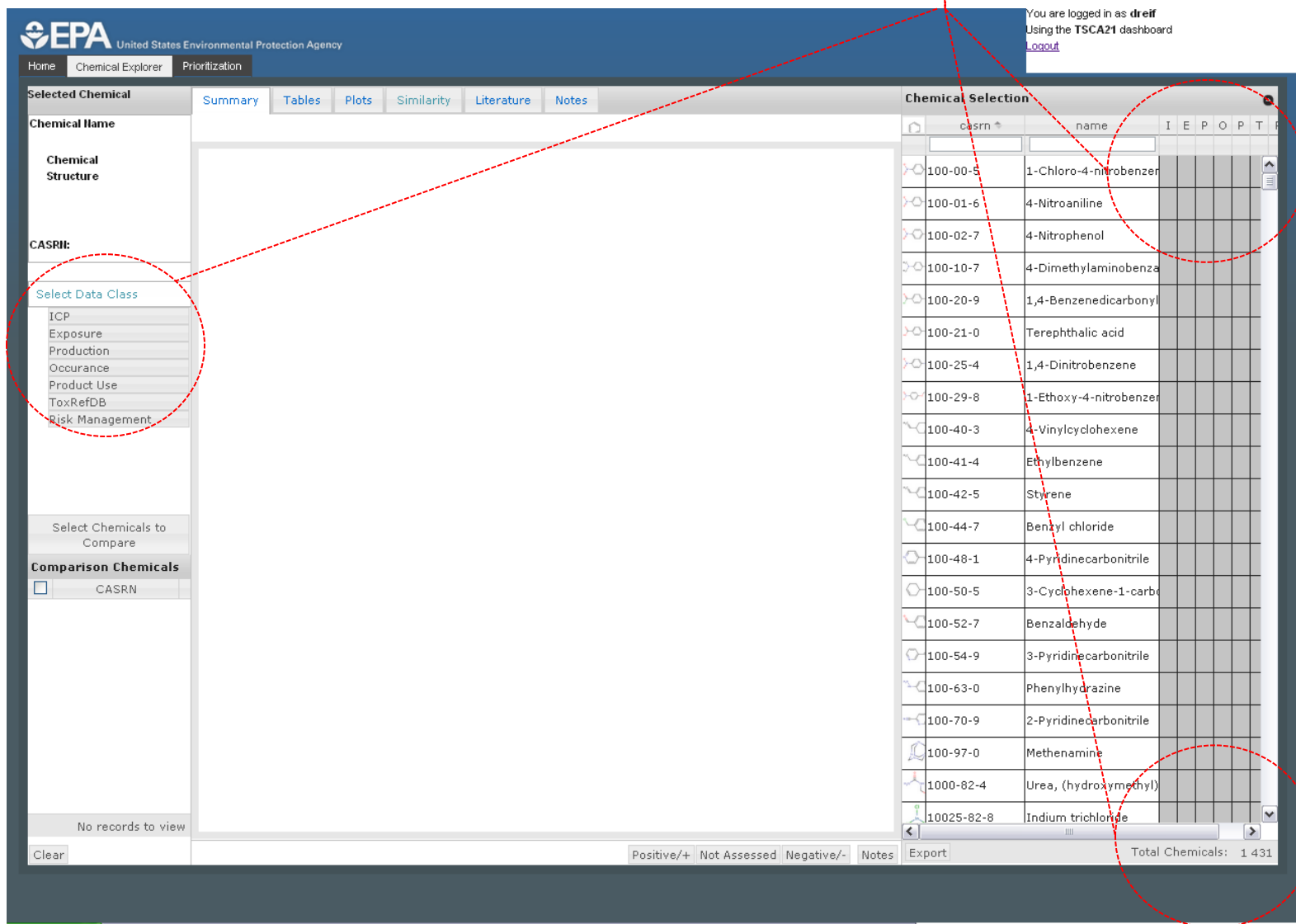


Login grants access to a menu of available Dashboards for that user.



Chemical Explorer mode: Exploring assay results (Screenshot from prototype Dashboard)

The specific dashboard chosen affects the chemical set, organization of data classes, and defaults for the evidence table.



The screenshot displays the EPA Chemical Explorer interface. The top navigation bar includes "Home", "Chemical Explorer", and "Prioritization". The main content area is divided into a left sidebar and a right main panel. The sidebar contains a "Selected Chemical" section with tabs for "Summary", "Tables", "Plots", "Similarity", "Literature", and "Notes". Below this is a "Chemical Name" field, a "Chemical Structure" field, and a "CASRN:" field. A "Select Data Class" dropdown menu is highlighted with a red circle, showing options: "ICP", "Exposure", "Production", "Occurance", "Product Use", "ToxRefDB", and "Risk Management". Below the dropdown is a "Select Chemicals to Compare" section with a "Comparison Chemicals" table containing a "CASRN" column and a "No records to view" message. The main panel is titled "Chemical Selection" and features a table with columns for "casrn", "name", and a grid of evidence categories: "I", "E", "P", "O", "P", "T". The table lists 20 chemicals, including 1-Chloro-4-nitrobenzene, 4-Nitroaniline, 4-Nitrophenol, 4-Dimethylaminobenzene, 1,4-Benzenedicarbonyl, Terephthalic acid, 1,4-Dinitrobenzene, 1-Ethoxy-4-nitrobenzene, 4-Vinylcyclohexene, Ethylbenzene, Styrene, Benzyl chloride, 4-Pyridinecarbonitrile, 3-Cyclohexene-1-carbonyl, Benzaldehyde, 3-Pyridinecarbonitrile, Phenylhydrazine, 2-Pyridinecarbonitrile, Methenamine, Urea, (hydroxymethyl), and Indium trichloride. A red dashed line connects the "Select Data Class" dropdown to the "I" column header in the table. At the bottom right, a "Total Chemicals: 1 431" label is also circled in red. The bottom navigation bar includes "Clear", "Positive/+", "Not Assessed", "Negative/-", "Notes", "Export", and "Total Chemicals: 1 431".

You are logged in as dreif
Using the TSCA21 dashboard
[Logout](#)

Home Chemical Explorer Prioritization

Selected Chemical Summary Tables Plots Similarity Literature Notes

Chemical Name

Chemical Structure

CASRN:

Select Data Class

- ICP
- Exposure
- Production
- Occurance
- Product Use
- ToxRefDB
- Risk Management

Select Chemicals to Compare


Comparison Chemicals

CASRN	Name	I	E	P	O	P	T
100-00-5	1-Chloro-4-nitrobenzene						
100-01-6	4-Nitroaniline						
100-02-7	4-Nitrophenol						
100-10-7	4-Dimethylaminobenzene						
100-20-9	1,4-Benzenedicarbonyl						
100-21-0	Terephthalic acid						
100-25-4	1,4-Dinitrobenzene						
100-29-8	1-Ethoxy-4-nitrobenzene						
100-40-3	4-Vinylcyclohexene						
100-41-4	Ethylbenzene						
100-42-5	Styrene						
100-44-7	Benzyl chloride						
100-48-1	4-Pyridinecarbonitrile						
100-50-5	3-Cyclohexene-1-carbonyl						
100-52-7	Benzaldehyde						
100-54-9	3-Pyridinecarbonitrile						
100-63-0	Phenylhydrazine						
100-70-9	2-Pyridinecarbonitrile						
100-97-0	Methenamine						
1000-82-4	Urea, (hydroxymethyl)						
10025-82-8	Indium trichloride						

Clear Positive/+ Not Assessed Negative/- Notes Export Total Chemicals: 1 431

Chemical Explorer mode: Exploring assay results

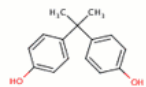
(Screenshot from prototype EDSP Dashboard for a HTS assay probing Estrogen Receptor activity)


United States Environmental Protection Agency

Home
Chemical Page
Prioritization

Selected Chemical

Bisphenol A



CASRN: 80-05-7

Select Data Class

- Estrogen
- Androgen
- Thyroid
- Steroidogenesis

Select Chemicals to Compare

Comparison Chemicals


CASRN

No records to view

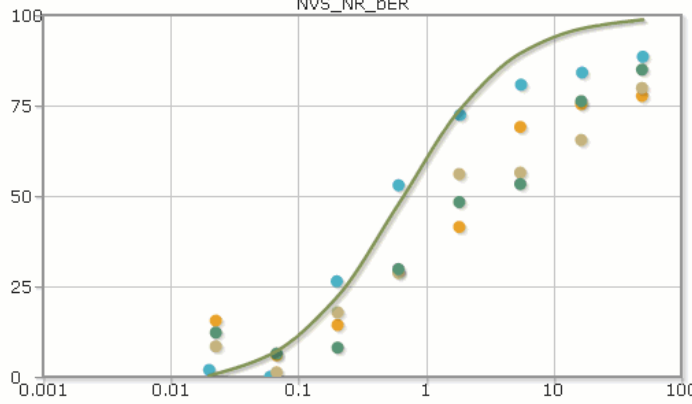
Clear

Summary | Tables | Plots | Similarity | Literature | Notes

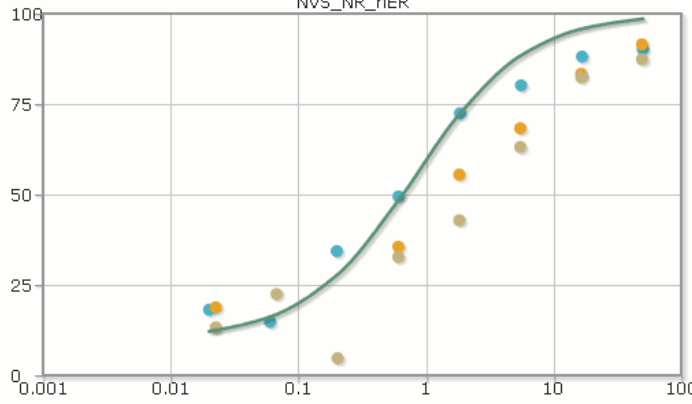
Estrogen



NVS_NR_ber



NVS_NR_her



Chemical Selection


CASRN	NAME	E	A	T	S
1001-32-1	Chloroform				
1861-40-1	Benfluralin				
1897-45-6	Chlorothalonil				
1912-24-9	Atrazine				
2921-88-2	Chlorpyrifos				
30560-19-1	Acephate				
333-41-5	Diazinon				
52315-07-8	Cypermethrin				
60-51-5	Dimethoate				
63-25-2	Carbaryl				
67-64-1	Acetone				
68359-37-5	Cyfluthrin				
71751-41-2	Abamectin				
759-94-4	S-Ethyl dipropylthiocarbamate				
80-05-7	Bisphenol A				
82657-04-3	Bifenthrin				
84-66-2	Diethyl phthalate				
84-74-2	Dibutyl phthalate				
85-68-7	Butyl benzyl phthalate				
94-75-7	2,4-Dichlorophenoxyacetic acid				

Positive/+ | Not Assessed | Negative/- | Notes

Total Chemicals: 26

Chemical Explorer mode: Exploring structural similarity

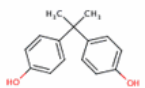
(Screenshot from prototype EDSP Dashboard using a chemoinformatic model to find structurally similar chemicals)


United States Environmental Protection Agency

Home
Chemical Page
Prioritization

Selected Chemical

Bisphenol A



CASRN: 80-05-7

Select Data Class

- Estrogen
- Androgen
- Thyroid
- Steroidogenesis

Select Chemicals to Compare

Comparison Chemicals


CASRN

No records to view

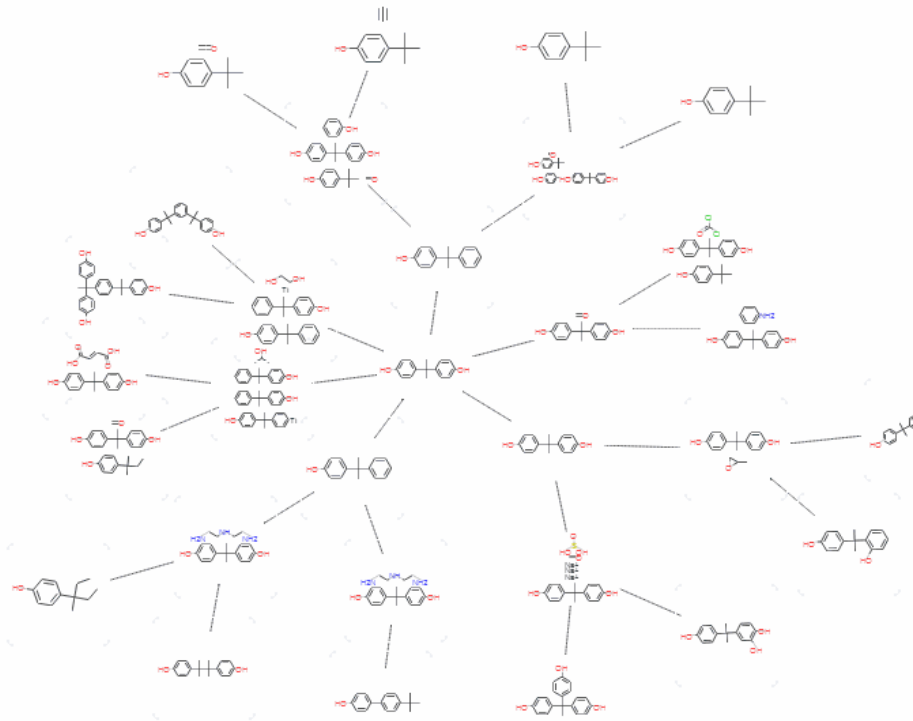
Clear

Estrogen

Similarity Range: 75 - 300



Bisphenol A



Chemical Selection

CASRN	NAME	E	A	T	S
1861-40-1	Benfluralin				
1897-45-6	Chlorothalonil				
1912-24-9	Atrazine				
2921-88-2	Chlorpyrifos				
30560-19-1	Acephate				
333-41-5	Diazinon				
52315-07-8	Cypermethrin				
60-51-5	Dimethoate				
63-25-2	Carbaryl				
67-64-1	Acetone				
68359-37-5	Cyfluthrin				
71751-41-2	Abamectin				
759-94-4	S-Ethyl dipropylthiocarbamate				
80-05-7	Bisphenol A				
82657-04-3	Bifenthrin				
84-66-2	Diethyl phthalate				
84-74-2	Dibutyl phthalate				
85-68-7	Butyl benzyl phthalate				
94-75-7	2,4-Dichlorophenoxyacetic acid				

Total Chemicals: 26

Positive/+

Not Assessed

Negative/-

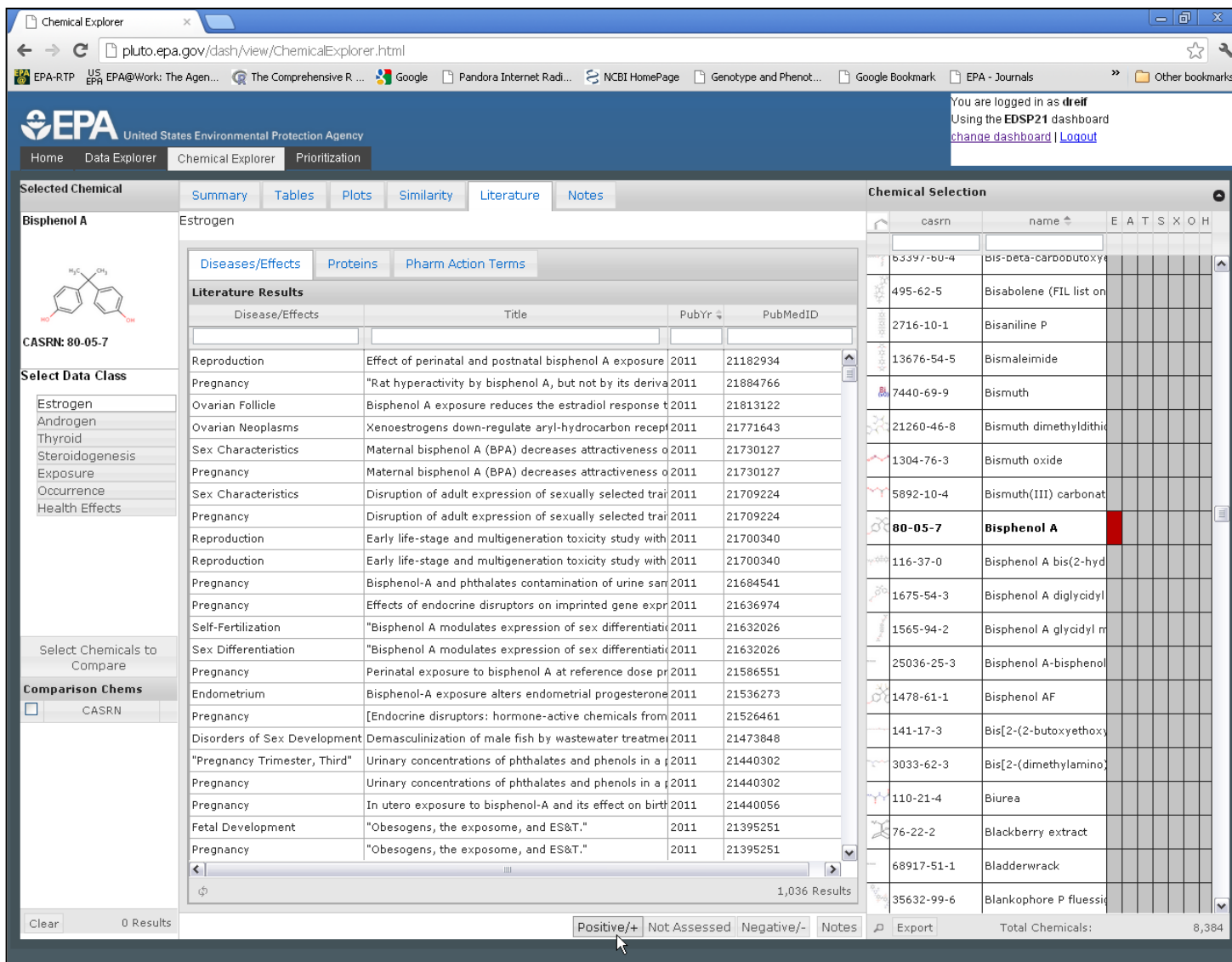
Notes

Integrating information into a web-enabled, interactive 'Dashboard': Literature mining

The Dashboard provides an interactive front-end for (re)organizing information from public databases and recording decisions

This interface was designed to integrate any number of information sources to let users make comprehensive decisions about chemicals

e.g. A user has assigned BPA as having positive evidence of estrogen-related effects in the table at right



The screenshot shows the Chemical Explorer interface. The main content area displays literature results for Bisphenol A, categorized by Disease/Effects, Proteins, and Pharm Action Terms. The 'Disease/Effects' table is expanded, showing a list of results with columns for Disease/Effects, Title, PubYr, and PubMedID. The results are filtered to show 1,036 results. The 'Chemical Selection' table on the right shows a list of chemicals, with Bisphenol A (CASRN: 80-05-7) highlighted in red. The interface includes navigation tabs for Summary, Tables, Plots, Similarity, Literature, and Notes. The top navigation bar includes Home, Data Explorer, Chemical Explorer, and Prioritization. The bottom of the interface has a 'Clear' button, a '0 Results' indicator, and a 'Positive/+' button, along with other filters like 'Not Assessed', 'Negative/-', and 'Notes'. The total number of chemicals is shown as 8,384.

Disease/Effects	Title	PubYr	PubMedID
Reproduction	Effect of perinatal and postnatal bisphenol A exposure	2011	21182934
Pregnancy	"Rat hyperactivity by bisphenol A, but not by its deriva	2011	21884766
Ovarian Follicle	Bisphenol A exposure reduces the estradiol response t	2011	21813122
Ovarian Neoplasms	Xenoestrogens down-regulate aryl-hydrocarbon recep	2011	21771643
Sex Characteristics	Maternal bisphenol A (BPA) decreases attractiveness o	2011	21730127
Pregnancy	Maternal bisphenol A (BPA) decreases attractiveness o	2011	21730127
Sex Characteristics	Disruption of adult expression of sexually selected trai	2011	21709224
Pregnancy	Disruption of adult expression of sexually selected trai	2011	21709224
Reproduction	Early life-stage and multigeneration toxicity study with	2011	21700340
Reproduction	Early life-stage and multigeneration toxicity study with	2011	21700340
Pregnancy	Bisphenol-A and phthalates contamination of urine san	2011	21684541
Pregnancy	Effects of endocrine disruptors on imprinted gene expr	2011	21636974
Self-Fertilization	"Bisphenol A modulates expression of sex differentiat	2011	21632026
Sex Differentiation	"Bisphenol A modulates expression of sex differentiat	2011	21632026
Pregnancy	Perinatal exposure to bisphenol A at reference dose pr	2011	21586551
Endometrium	Bisphenol-A exposure alters endometrial progesterone	2011	21536273
Pregnancy	[Endocrine disruptors: hormone-active chemicals from	2011	21526461
Disorders of Sex Development	Demasculinization of male fish by wastewater treatme	2011	21473848
"Pregnancy Trimester, Third"	Urinary concentrations of phthalates and phenols in a	2011	21440302
Pregnancy	Urinary concentrations of phthalates and phenols in a	2011	21440302
Pregnancy	In utero exposure to bisphenol-A and its effect on birth	2011	21440056
Fetal Development	"Obesogens, the exposome, and ES&T."	2011	21395251
Pregnancy	"Obesogens, the exposome, and ES&T."	2011	21395251

Integrating information into a web-enabled, interactive 'Dashboard': ToxPi implementation

pluto.epa.gov/dash/view/prioritization.html

EPA - RTP US EPA@Work: The Agen... The Comprehensive R ... Google Pandora Internet Radi... NCBI HomePage Genotype and Phenot... Google Bookmark EPA - Journals Other bookmarks

You are logged in as dreif
Using the EDSP21 dashboard
[change dashboard](#) | [Logout](#)

Home Data Explorer Chemical Explorer **Prioritization**

Selected Chemical ToxPi

Silane, dichloroethenylmethyl- Androgen

CASRN: 124-70-9

Select Data Class

- Estrogen Weight: 3
- Androgen Weight: 2
- Thyroid Weight: 2
- Steroidogenesis Weight: 1
- Exposure Weight: 1
- Occurrence Weight: 1
- Health Effects Weight: 1
- Multi Select

ToxPi Score vs Chemical Rank



casrn	name	ts	E	A	T	S	X	O	H
100-01-6	4-Nitroaniline								
124-06-1	Ethyl tetradecan								
15875-13-5	1,3,5-Triazine-1,								
6410-41-9	2-Naphthalenece								
102-09-0	Diphenylcarbona								
5407-87-4	2-Pyridinamine,								
251553-55-6	Alcohols, C>14,								
68422-69-5	Butyl 9(or 10)-(s								
68584-47-4	Poly(oxy-1,2-eth								
732-26-3	2,4,6-Tris(tert-b								
68890-70-0	Sulfuric acid, mo								
299-28-5	Calcium D-glucos								
3520-72-7	C.I. Pigment Ora								
9011-13-6	Styrene - maleic								
35365-94-7	Triethyl ammoni								
102-24-9	Boroxin, trimeth								
13047-13-7	4-(Hydroxymeth								
61725-89-1	Tridecylxypoly(
67762-12-3	Soybean oil, pol								

100-01-6 (3.142) 124-06-1 (2.685) 15875-13-5 (2.619) 6410-41-9 (2.608) 102-09-0 (2.593)

5407-87-4 (2.59) 251553-55-6 (2.573) 68422-69-5 (2.53) 68584-47-4 (2.516) 732-26-3 (2.51)

68890-70-0 (2.505) 299-28-5 (2.493) 3520-72-7 (2.493) 9011-13-6 (2.493) 35365-94-7 (2.482)

102-24-9 (2.462) 13047-13-7 (2.456) 61725-89-1 (2.445) 67762-12-3 (2.442) 72-18-4 (2.439)

Positive/+ Not Assessed Negative/- Notes Page 1 of 420 1-20 of 8,384

Integrating information into a web-enabled, interactive 'Dashboard': ToxPi implementation

The organization of information is user-group specific (e.g. The Dashboard below has chemical information organized into endocrine-relevant data classes to support EDSP decisions)


Select User Session ✕

EDSP21

- EDSP21
- TSCA21
- OW21
- OPP21
- Demo
- Test



Dashboards provide interactive ways to explore and synthesize information (= "Translation")

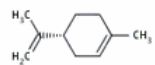


United States Environmental Protection Agency

Home
Chemical Page
Prioritization

Selected Chemical

Structure



CASRN: 5989-27-5

Carcinogenicity

ReproTox

- inVItro (ToxCast)
- inVivo (ToxRef)
- inSilico
- Signatures

DevTox

NeuroTox

AqaticTox

Select Chemicals to Compare

Comparison Chemicals

CASRN

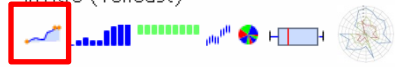
- 126572-80-3
- 23726-91-2
- 100-64-1
- 10482-56-1
- 513-49-5

Total Chemicals: 5

Clear

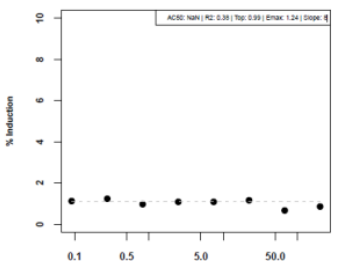
Assay Selection Tables **Plots** Similarity Literature Notes

inVItro (ToxCast)

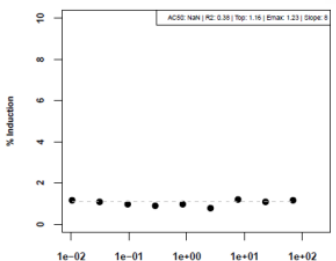


Attagene (Transcription Factor Activation): PPARg_TRANS

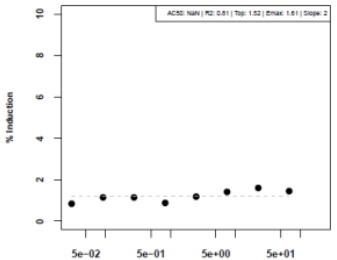
5989-27-5



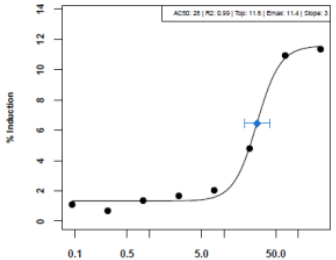
126572-80-3



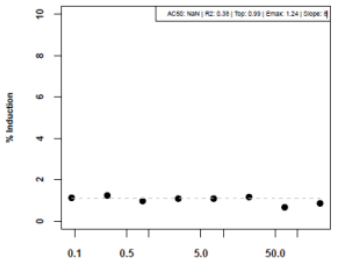
23726-91-2



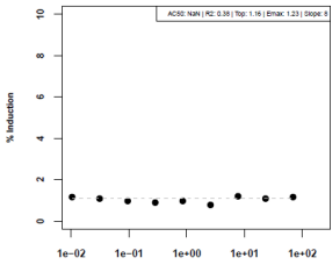
100-64-1



10482-56-1



513-49-5



Positive/+ Not Assessed Negative/- Notes

Chemical Selection

CASRN	NAME	C	R	D	N	A
3388-04-3	((Epoxy)cyclohexyl)ethyl)trimethc					
81-13-0	(+)-Panthenol					
1139-30-6	(-)-beta-Caryophyllene epoxide					
6485-40-1	(-)-Carvone					
989-51-5	(-)-Epigallocatechin gallate (85 p					
27193-28-8	(1,1,3,3-Tetramethylbutyl)phenol					
5039-78-1	(2-(Methacryloyloxy)ethyl)trimetl					
109-58-0	(2-Aminoethyl)carbamic acid					
4584-46-7	(2-Chloroethyl)dimethylamine, h					
150-39-0	(2-Hydroxyethyl)ethylenediamine					
132059-51-9	(BMX-1) 3-Chloro-4-(bromochlor					
132059-52-0	(BMX-2) 3-Chloro-4-(dibromome					
132059-53-1	(BMX-3) 3-Bromo-4-(dibromome					
5989-27-5	(d)-Limonene					
126572-80-3	(E)-2-Chloro-3-(dichlorometl					
115340-67-5	(E)-3-Formyl-2,4,4-trichloro-2-bu					
23726-91-2	(E)-beta-Damascone					
100-64-1	(Hydroxyimino)cyclohexane					
10482-56-1	(L)-alpha-Terpineol					
513-49-5	(S)-2-Aminobutane					
100-86-7	.alpha.,.alpha.-Dimethylbenzene					
94-91-7	.alpha.,.alpha."-(Propylenedinitr					
959-98-8	.alpha.-Endosulfan					
101-86-0	.alpha.-Hexylcinnamaldehyde					

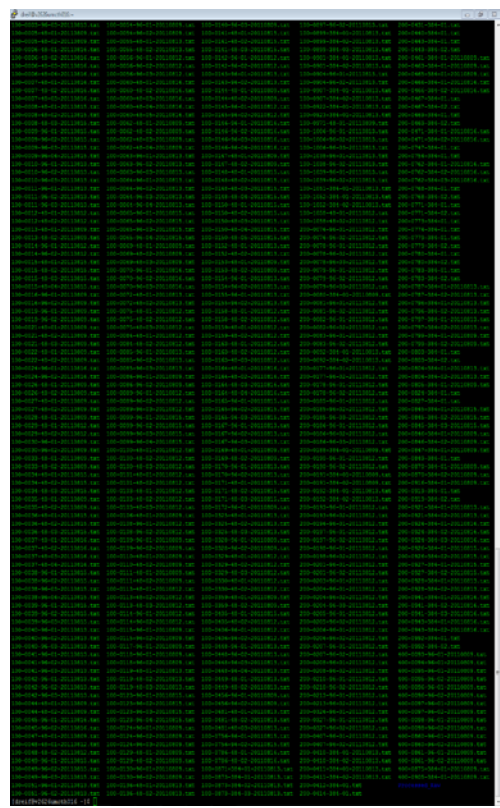
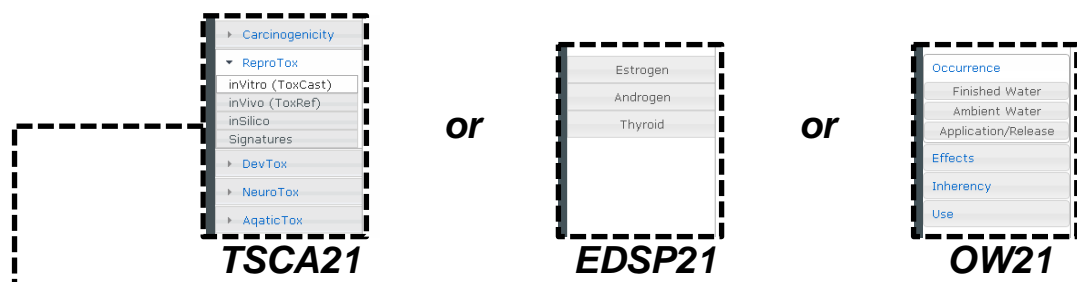
Total Chemicals: 5 683

“Collaboration” means Dashboards are customized for particular needs

Leverage resources by repackaging the same data for custom uses

Components are modular, so the Dashboards infrastructure can be customized to translate data according to particular use cases

Single Source Database (e.g. ACToR)



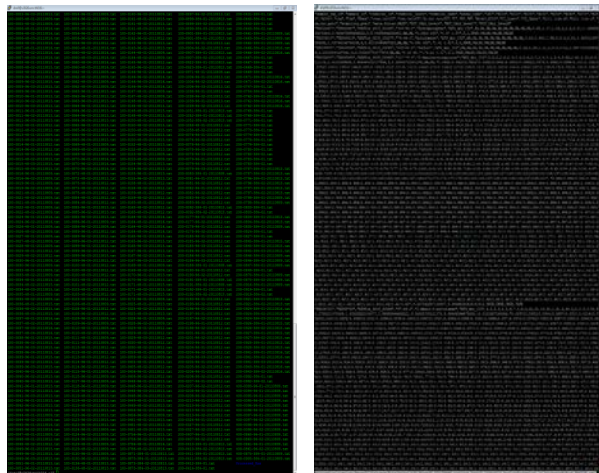
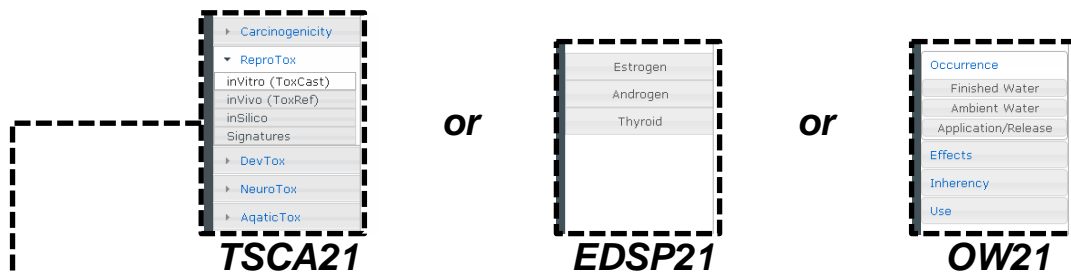
The screenshot shows the EPA Chemical Dashboard interface. At the top, it says "EPA United States Environmental Protection Agency" and "Home Chemical Page Prioritization". Below this, there are tabs for "Selected Chemical", "Assay Selection", "Tables", "Plots", "Similarity", "Literature", and "Notes". The "Assay Selection" tab is active, showing "inVivo (ToxCast)" and "Attagene (Transcription Factor Activation): PPARg_TRANS". A red box highlights the "inVivo (ToxCast)" assay. Below this, there are six plots showing "% Inhibition" vs. "Concentration" for different chemicals: 5989-27-5, 126572-80-3, 23726-91-2, 100-64-1, 10482-56-1, and 513-49-5. On the right side, there is a "Chemical Selection" table with columns for CASRN, NAME, and C R D N A. The table lists various chemicals, including (d)-Limonene, (E)-2-Chloro-3-(dichloromethyl)-2-methylbutane, (E)-beta-Damascone, (Hydroxyimino)cyclohexane, (L)-alpha-Terpineol, (S)-2-Aminobutane, and Hexylcinnamaldehyde. At the bottom, there are buttons for "Clear", "Positive/+ ", "Not Assessed", "Negative/-", and "Notes".

“Collaboration” means Dashboards are customized for particular needs

Specialized data may be needed for certain uses

Components are modular, so the Dashboards infrastructure can be customized to translate data according to particular use cases


Multiple Source Databases
(e.g. ACToR + PO-specific DB)



The screenshot shows the EPA Chemical Dashboard interface. The top navigation bar includes Home, Chemical Page, and Prioritization. The main content area is divided into several sections:

- Selected Chemical**: Shows the chemical structure of 5989-27-5 (Limonene) with its CASRN: 5989-27-5.
- Assay Selection**: A red box highlights the "inVivo (ToxCast)" assay.
- Plots**: A grid of six graphs showing "% Inhibition" vs. concentration for various chemicals. The top-left graph is for 5989-27-5, and the top-right graph is for 126572-80-3.
- Chemical Selection**: A table listing various chemicals with their CASRN, names, and a grid of red and white cells indicating their status. The table includes columns for CASRN, NAME, and C, R, D, N, A.

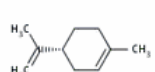
Dashboards provide interactive ways to explore and synthesize data (e.g. many chemicals by single data source)


United States Environmental Protection Agency

Home
Chemical Page
Prioritization

Selected Chemical

Structure



CASRN: 5989-27-5

Carcinogenicity

ReproTox

- inVitro (ToxCast)
- inVivo (ToxRef)
- inSilico
- Signatures

DevTox

NeuroTox

AqaticTox

Select Chemicals to Compare

Comparison Chemicals

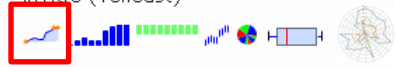
<input type="checkbox"/>	CASRN
<input checked="" type="checkbox"/>	126572-80-3
<input type="checkbox"/>	23726-91-2
<input checked="" type="checkbox"/>	100-64-1
<input checked="" type="checkbox"/>	10482-56-1
<input type="checkbox"/>	513-49-5

Total Chemicals: 5

Clear

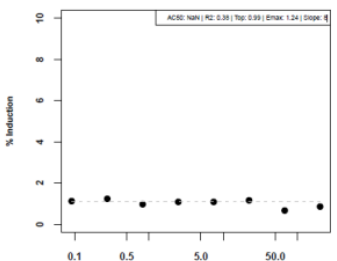
Assay Selection Tables **Plots** Similarity Literature Notes

inVitro (ToxCast)

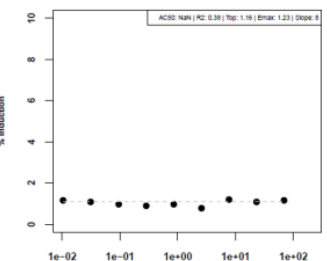


Attagene (Transcription Factor Activation): PPARg_TRANS

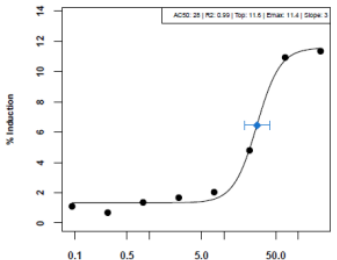
5989-27-5



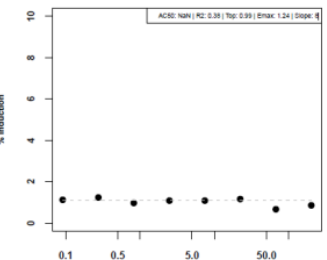
126572-80-3



100-64-1



10482-56-1




Chemical Selection

CASRN	NAME	C	R	D	N	A
3388-04-3	((Epoxy)cyclohexyl)ethyl)trimetho					
81-13-0	(+)-Panthenol					
1139-30-6	(-)-beta-Caryophyllene epoxide					
6485-40-1	(-)-Carvone					
989-51-5	(-)-Epigallocatechin gallate (85 p					
27193-28-8	(1,1,3,3-Tetramethylbutyl)phenol					
5039-78-1	(2-(Methacryloyloxy)ethyl)trimetl					
109-58-0	(2-Aminoethyl)carbamic acid					
4584-46-7	(2-Chloroethyl)dimethylamine, h					
150-39-0	(2-Hydroxyethyl)ethylenediamine					
132059-51-9	(BMX-1) 3-Chloro-4-(bromochlor					
132059-52-0	(BMX-2) 3-Chloro-4-(dibromome					
132059-53-1	(BMX-3) 3-Bromo-4-(dibromome					
5989-27-5	(d)-Limonene					
126572-80-3	(E)-2-Chloro-3-(dichlorometl					
115340-67-5	(E)-3-Formyl-2,4,4-trichloro-2-bu					
23726-91-2	(E)-beta-Damascone					
100-64-1	(Hydroxyimino)cyclohexane					
10482-56-1	(L)-alpha-Terpineol					
513-49-5	(S)-2-Aminobutane					
100-86-7	.alpha.,.alpha.-Dimethylbenzene					
94-91-7	.alpha.,.alpha.\'--(Propylenedinitr					
959-98-8	.alpha.-Endosulfan					
101-86-0	.alpha.-Hexylcinnamaldehyde					

Total Chemicals: 5 683

Positive/+
Not Assessed
Negative/-
Notes

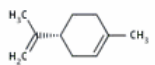
Dashboards provide interactive ways to explore and synthesize data (e.g. many data sources by single chemical)


United States Environmental Protection Agency

Home
Chemical Page
Prioritization

Selected Chemical

Structure



CASRN: 5989-27-5

Carcinogenicity

ReproTox

- inVitro (ToxCast)
- inVivo (ToxRef)
- inSilico
- Signatures

DevTox

NeuroTox

AqaticTox

Select Chemicals to Compare

Comparison Chemicals


<input type="checkbox"/>	CASRN

No records to view

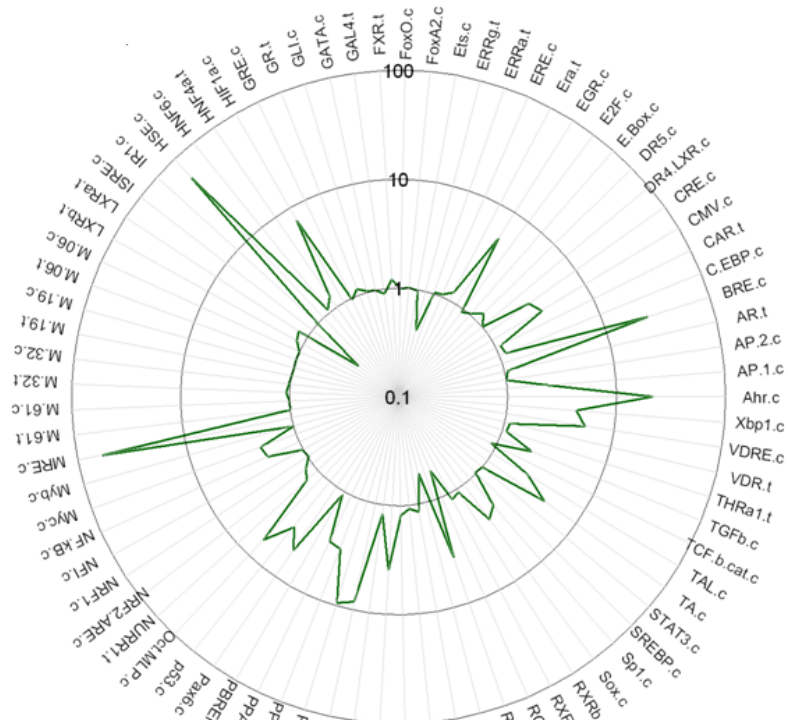
Clear

Assay Selection Tables **Plots** Similarity Literature Notes

inVitro (ToxCast)



Attagene (Transcription Factor Activation): All assays



Concentration: 1nM, 1uM, 1mM


Chemical Selection

CASRN	NAME	C	R	D	N	A
3388-04-3	((Epoxy)cyclohexyl)ethyl)trimeth...					
81-13-0	(+)-Panthenol					
1139-30-6	(-)-beta-Caryophyllene epoxide					
6485-40-1	(-)-Carvone					
989-51-5	(-)-Epigallocatechin gallate (85 p...					
27193-28-8	(1,1,3,3-Tetramethylbutyl)phenol					
5039-78-1	(2-(Methacryloyloxy)ethyl)trimetl...					
109-58-0	(2-Aminoethyl)carbamic acid					
4584-46-7	(2-Chloroethyl)dimethylamine, h...					
150-39-0	(2-Hydroxyethyl)ethylenediamine					
132059-51-9	(BMX-1) 3-Chloro-4-(bromochlor...					
132059-52-0	(BMX-2) 3-Chloro-4-(dibromome...					
132059-53-1	(BMX-3) 3-Bromo-4-(dibromome...					
5989-27-5	(d)-Limonene					
126572-80-3	(E)-2-Chloro-3-(dichloromethyl)b...					
115340-67-5	(E)-3-Formyl-2,4,4-trichloro-2-bu...					
23726-91-2	(E)-beta-Damascone					
100-64-1	(Hydroxyimino)cyclohexane					
10482-56-1	(L)-alpha-Terpineol					
513-49-5	(S)-2-Aminobutane					
100-86-7	.alpha.,.alpha.-Dimethylbenzene					
94-91-7	.alpha.,.alpha.'-(Propylenedinitr...					
959-98-8	.alpha.-Endosulfan					
101-86-0	.alpha.-Hexylcinnamaldehyde					

Total Chemicals: 5 683

Positive/+
Not Assessed
Negative/-
Notes

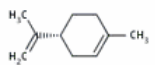
Dashboards provide interactive ways to explore and synthesize data (e.g. many data sources by single chemical)


United States Environmental Protection Agency

Home
Chemical Page
Prioritization

Selected Chemical

Structure



CASRN: 5989-27-5

Carcinogenicity

ReproTox

- inVitro (ToxCast)
- inVivo (ToxRef)
- inSilico
- Signatures

DevTox

NeuroTox

AqaticTox

Select Chemicals to Compare

Comparison Chemicals


<input type="checkbox"/>	CASRN

No records to view

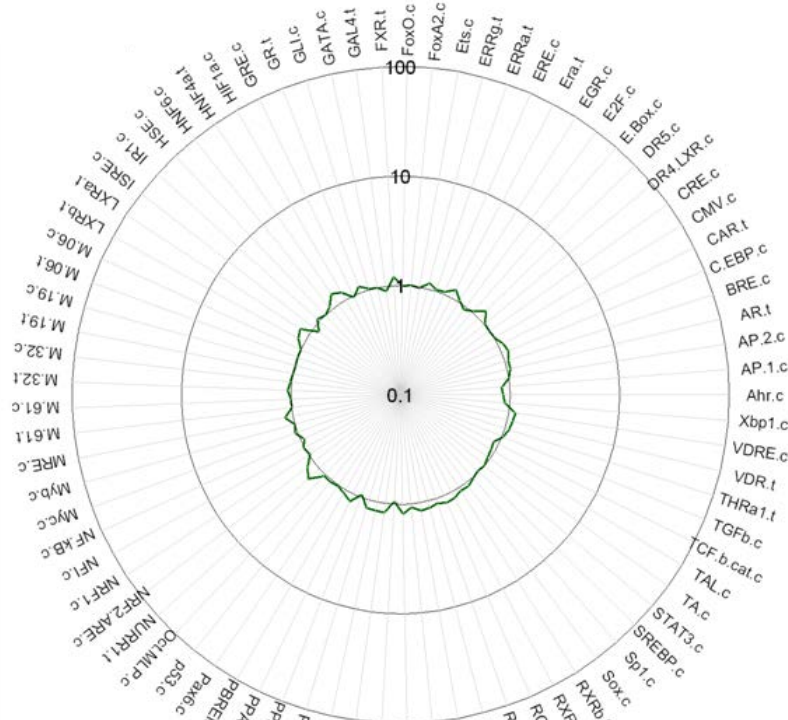
Clear

Assay Selection Tables **Plots** Similarity Literature Notes

inVitro (ToxCast)



Attagene (Transcription Factor Activation): All assays



Concentration: 1nM, 1uM, 1mM

Chemical Selection

CASRN	NAME	C	R	D	N	A
3388-04-3	((Epoxy)cyclohexyl)ethyl)trimethc					
81-13-0	(+)-Panthenol					
1139-30-6	(-)-beta-Caryophyllene epoxide					
6485-40-1	(-)-Carvone					
989-51-5	(-)-Epigallocatechin gallate (85 p					
27193-28-8	(1,1,3,3-Tetramethylbutyl)phenol					
5039-78-1	(2-(Methacryloyloxy)ethyl)trimetl					
109-58-0	(2-Aminoethyl)carbamic acid					
4584-46-7	(2-Chloroethyl)dimethylamine, h					
150-39-0	(2-Hydroxyethyl)ethylenediamine					
132059-51-9	(BMX-1) 3-Chloro-4-(bromochlor					
132059-52-0	(BMX-2) 3-Chloro-4-(dibromome					
132059-53-1	(BMX-3) 3-Bromo-4-(dibromome					
5989-27-5	(d)-Limonene					
126572-80-3	(E)-2-Chloro-3-(dichloromethyl)b					
115340-67-5	(E)-3-Formyl-2,4,4-trichloro-2-bu					
23726-91-2	(E)-beta-Damascone					
100-64-1	(Hydroxyimino)cyclohexane					
10482-56-1	(L)-alpha-Terpineol					
513-49-5	(S)-2-Aminobutane					
100-86-7	.alpha.,.alpha.-Dimethylbenzene					
94-91-7	.alpha.,.alpha.\'--(Propylenedinitr					
959-98-8	.alpha.-Endosulfan					
101-86-0	.alpha.-Hexylcinnamaldehyde					

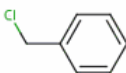
Total Chemicals: 5 683

What kind of information is available for selected chemical sets?

EPA United States Environmental Protection Agency
Home | Chemical Page | **Prioritization**

Selected Chemical

Structure



CASRN: 100-44-7

Carcinogenicity

ReproTox

DevTox

NeuroTox

AqaticTox

Select Chemicals to Compare

Comparison Chemicals

CASRN

100-46-9

100-47-0

100-51-6

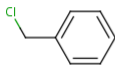
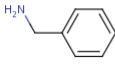
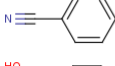
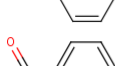

100-52-7

Total Chemicals: 4

Clear

Assay Selection | **Tables** | Plots | Similarity | Literature | Notes

Data summary

	100-44-7	Benzyl chloride	Carc	Repro	Dev	Neuro	Aq
	100-46-9	Benzylamine	Carc		Dev		
	100-47-0	Benzonitrile	Carc	Repro	Dev		
	100-51-6	Benzyl alcohol	Carc	Repro	Dev		Aq
	100-52-7	Benzaldehyde	Carc	Repro	Dev	Neuro	Aq

Chemical Selection

CASRN	NAME	C	R	D	N	A
100-00-5	p-Chloronitrobenzene					
100-01-6	p-Nitroaniline					
100-02-7	p-Nitrophenol					
100-06-1	Ethanone, 1-(4-methoxyphenyl)-					
100-09-4	Benzoic acid, 4-methoxy-					
100-10-7	Benzaldehyde, 4-(dimethylamino)					
100-18-5	Benzene, 1,4-bis(1-methylethyl)-					
100-20-9	1,4-Benzenedicarbonyl dichloride					
100-21-0	Terephthalic acid					
100-25-4	p-Dinitrobenzene					
100-27-6	4-Nitrobenzeneethanol					
100-29-8	Benzene, 1-ethoxy-4-nitro-					
100-36-7	1,2-Ethanediamine, N,N-diethyl-					
100-37-8	Ethanol, 2-(diethylamino)-					
100-39-0	Benzene, (bromomethyl)-					
100-40-3	4-Vinylcyclohexene					
100-43-6	4-Vinylpyridine					
100-44-7	Benzyl chloride					
100-46-9	Benzylamine					
100-47-0	Benzonitrile					
100-50-5	3-Cyclohexene-1-carboxaldehyde					
100-51-6	Benzyl alcohol					
100-52-7	Benzaldehyde					
100-53-8	Benzenemethanethiol					

Total Chemicals: 5 683

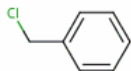
Positive/+ | Not Assessed | Negative/- | Notes

Annotated literature searches for specific effects by chemical

Home Chemical Page Prioritization

Selected Chemical

Structure



CASRN: 100-44-7

Carcinogenicity

ReproTox

DevTox

NeuroTox

AqaticTox

Select Chemicals to Compare

Comparison Chemicals

CASRN

No records to view

Clear

Assay Selection Tables Plots Similarity Literature Notes

PubMed: Neurological Effects

Link to PubMed Tox Env Flag Flag Pub Yr Title

Link to PubMed	Tox Flag	Env Flag	Pub Yr	Title
10560777	1	0	1999	Developmental effects of intermittent prenatal exposure to 1,1,1-trichloroethane in the rat.
10910995	1	0	2000	Biphasic effects of 1,1,1-trichloroethane on the locomotor activity of mice: relationship to blood and brain solvent concentrations.
10912586	1	0	2000	Effects of inhaled 1,1,1-trichloroethane on the regional brain cyclic GMP levels in mice and rats.
11003972	1	0	2000	Acute effects of 200 ppm 1,1,1-trichloroethane on the human EEG.
11552300	1	0	2001	Inhibitory effect of 1,1,1-trichloroethane on calcium channels of neurons.
11779060	1	0	2001	Effect of 1,1,1-trichloroethane on calcium current of rat dorsal root ganglion neurons.
12194155	1	1	2002	Is neurotoxicity associated with environmental trichloroethylene (TCE)?
12681521	1	0	2003	Inhaled drugs of abuse enhance serotonin-3 receptor function. Tolerance and sensitization to inhaled 1,1,1-trichloroethane in mice: results from open-field behavior and a functional observational battery.
16541244	1	0	2006	[The use of 1,1,1-trichloroethane (methylchloroform) in industrial operations: the neurotoxicity risk].
1865846	1	1	1991	Time course of the ethanol-like discriminative stimulus effects of abused inhalants in mice.
18722399	0	0	2009	Discriminative stimulus effects of inhaled 1,1,1-trichloroethane in mice: comparison to other hydrocarbon vapors and volatile anesthetics.
18972104	1	1	2009	Toluene and TCE decrease binding to mu-opioid receptors, but not to benzodiazepine and NMDA receptors in mouse brain.
18991886	0	1	2008	Exposure of rats to high concentrations of 1,1,1-trichloroethane and its effects on brain lipid and fatty acid composition.
2096382	1	0	1990	Fatal cerebral oedema following trichloroethane abuse.
2231588	1	0	1990	Diagnosis and treatment of acute poisoning with volatile substances.
2777267	1	0	1989	Chronic non-neurological toxicity from volatile substance abuse.
2777269	1	1	1989	Peripheral neuropathy in two workers exposed to 1,1,1-trichloroethane.
2845159	1	0	1988	Effects of low-dose inhalation of three chlorinated aliphatic organic solvents on deoxyribonucleic acid in gerbil brain.
3433047	1	0	1987	Effect of 1,1,1-trichloroethane inhalation on heart rate and its mechanism: a role of autonomic nervous system.
3606210	1	0	1987	Respiratory disorders following 1,1,1-trichloroethane inhalation: a role of reflex mechanism arising from lungs.
3740953	1	0	1986	Death associated with the abuse of typewriter correction fluid.
3784854	1	0	1986	Developmental neurotoxicology of in utero exposure to industrial solvents in experimental animals.
3785760	1	0	1986	Behavioral changes during exposure to 1,1,1-trichloroethane: time-course and relationship to blood solvent levels.
3826081	1	0	1987	Sudden death in adolescents resulting from the inhalation of typewriter correction fluid.
3974043	1	0	1985	[The mechanism of respiratory arrest following 1,1,1-trichloroethane inhalation].
4087498	1	0	1985	Fatal poisoning by 1,1,1-trichloroethane after prolonged survival.
6662442	1	0	1983	Comparison of unconditioned reflex and conditioned avoidance tests in rats exposed by inhalation to carbon monoxide, 1,1,1-trichloroethane, toluene or ethanol.
6890184	1	0	1982	Short-term exposure of human subjects to m-xylene and 1,1,1-trichloroethane.
6954923	1	0	1982	Effects of 1,1,1-trichloroethane on a match-to-sample discrimination task in the baboon.
7120510	0	0	1982	[A role of the autonomic nervous system in alterations of blood pressure and heart rate induced by 1, 1, 1-trichloroethane (author's transl)].
7321285	1	0	1981	Toxic encephalopathy due to 1,1,1-trichloroethane exposure.
7605490	1	1	1995	Solvents in the workplace.
7770278	1	1	1995	

Positive/+ Not Assessed Negative/- Notes

Chemical Selection

CASRN	NAME	C	R	D	N	A
100-00-5	p-Chloronitrobenzene					
100-01-6	p-Nitroaniline					
100-02-7	p-Nitrophenol					
100-06-1	Ethanone, 1-(4-methoxyphenyl)-					
100-09-4	Benzoic acid, 4-methoxy-					
100-10-7	Benzaldehyde, 4-(dimethylamino)					
100-18-5	Benzene, 1,4-bis(1-methylethyl)-					
100-20-9	1,4-Benzenedicarbonyl dichloride					
100-21-0	Terephthalic acid					
100-25-4	p-Dinitrobenzene					
100-27-6	4-Nitrobenzeneethanol					
100-29-8	Benzene, 1-ethoxy-4-nitro-					
100-36-7	1,2-Ethanediamine, N,N-diethyl-					
100-37-8	Ethanol, 2-(diethylamino)-					
100-39-0	Benzene, (bromomethyl)-					
100-40-3	4-Vinylcyclohexene					
100-43-6	4-Vinylpyridine					
100-44-7	Benzyl chloride					
100-46-9	Benzylamine					
100-47-0	Benzonitrile					
100-50-5	3-Cyclohexene-1-carboxaldehyde					
100-51-6	Benzyl alcohol					
100-52-7	Benzaldehyde					
100-53-8	Benzenemethanethiol					

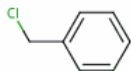
Total Chemicals: 5 683

Annotated literature searches for specific effects by chemical: interactive browsing

Home Chemical Page Prioritization

Selected Chemical

Structure



CASRN: 100-44-7

Carcinogenicity

ReproTox

DevTox

NeuroTox

AqaticTox

Select Chemicals to
Compare

Comparison Chemicals

CASRN

No records to view

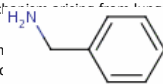
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Assay Selection Tables Plots Similarity Literature Notes

PubMed: Neurological Effects

Link to
PubMed Tox Env
Flag Flag Pub Yr Title

Link to PubMed	Tox Flag	Env Flag	Pub Yr	Title
10560777	1	0	1999	Developmental effects of intermittent prenatal exposure to 1,1,1-trichloroethane in the rat.
10910995	1	0	2000	Biphasic effects of 1,1,1-trichloroethane on the locomotor activity of mice: relationship to blood and brain solvent concentrations.
10912586	1	0	2000	Effects of inhaled 1,1,1-trichloroethane on the regional brain cyclic GMP levels in mice and rats.
11003972	1	0	2000	Acute effects of 200 ppm 1,1,1-trichloroethane on the human EEG.
11552300	1	0	2001	Inhibitory effect of 1,1,1-trichloroethane on calcium channels of neurons.
11779060	1	0	2001	Effect of 1,1,1-trichloroethane on calcium current of rat dorsal root ganglion neurons.
12194155	1	1	2002	Is neurotoxicity associated with environmental trichloroethylene (TCE)?
12681521	1	0	2003	Inhaled drugs of abuse enhance serotonin-3 receptor function.
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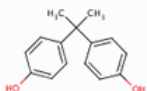
Positive/+ Not Assessed Negative/- Notes

Total Chemicals: 5 683

Predictive signatures connect *in vitro* assays to *in vivo* endpoints

Selected Chemical

Structure



CASRN: 80-05-7

Carcinogenicity

ReproTox

- inVitro (ToxCast)
- inVivo (ToxRef)
- inSilico
- Signatures

DevTox

NeuroTox

AqaticTox

Select Chemicals to Compare

Comparison Chemicals

CASRN

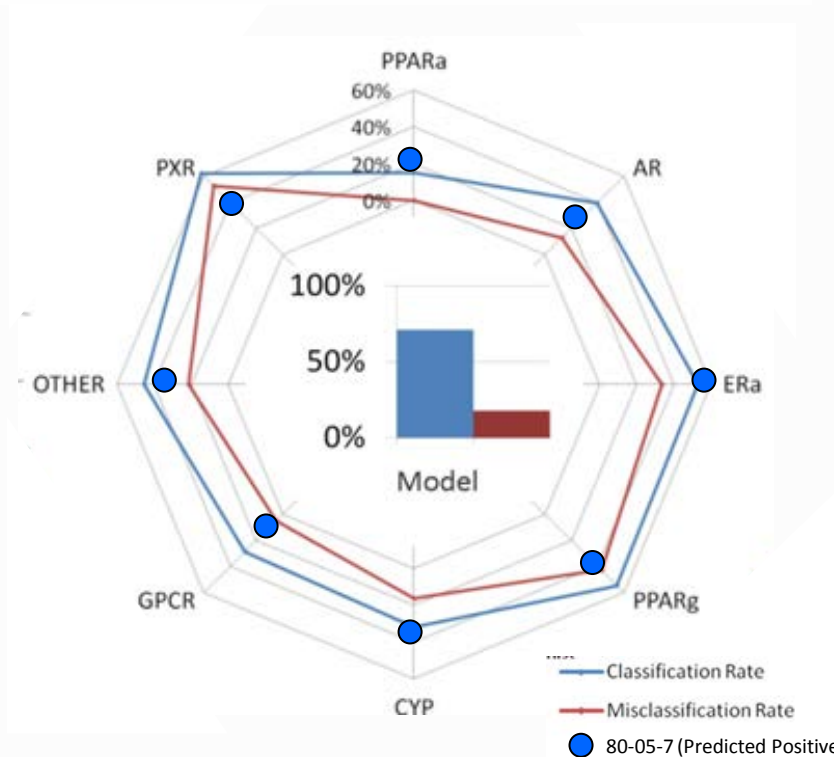
No records to view

Clear

Assay Selection Tables Plots Similarity Literature Notes

Signatures

- [Predictive model of rat reproductive toxicity from ToxCast high throughput screening \[Martin et al., Biol Reprod. 2011 Aug;85\(2\):327-39\]](#)
- [Economic benefits of using adaptive predictive models of reproductive toxicity in the context of a tiered testing program \[Martin et al., Syst Biol Reprod Med. 2012 Feb;58\(1\):3-9\]](#)
- [Profiling the reproductive toxicity of chemicals from multigeneration studies in the toxicity reference database \[Martin et al., Toxicol Sci. 2009 Jul;110\(1\):181-90\]](#)



Chemical Selection

CASRN	NAME	C	R	D	N	A
	Bisp					
80-05-7	Bisphenol A (4,4'-Isopropylidenebisphenol A)					
116-37-0	Bisphenol A bis(2-hydroxypropyl) ether					
1675-54-3	Bisphenol A diglycidyl ether					
1565-94-2	Bisphenol A-glycidyl methacrylate					

Dashboard/Workflow Conceptual Framework

