

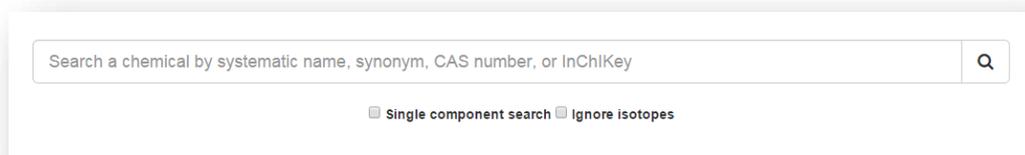
CompTox Chemistry Dashboard

Overview

The CompTox Chemistry Dashboard provides information regarding chemical compounds and substances of potential interest to environmental scientists. It contains information about substances, associated chemical structures, experimental and predicted physicochemical and toxicity data, bioassay data, exposure data and additional links to relevant websites and applications. The dashboard provides information for ~750,000 chemical substances and continues to expand in terms of the number of chemicals represented. Iterative review of the data is ongoing and additional data types are introduced with each release.

Basic Search

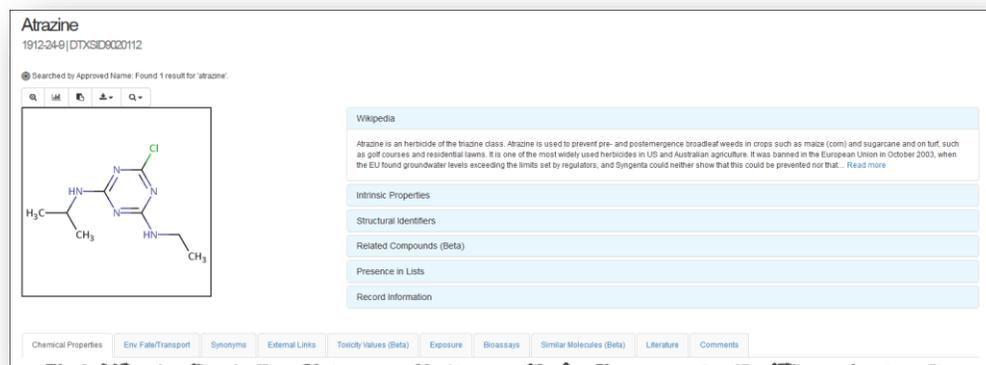
There are a variety of search capabilities presently available on the dashboard including by chemical name or identifier, by mass or molecular formula and a batch search capability for searching larger collections of data. Future work will introduce structure, substructure and similarity searching. The text search box allows a user to search using a number of chemical "identifiers" including chemical name, common name, [CAS Number](#) or [InChIKey](#) (SMILES and InChIString searching will be introduced in a later version). For the time being, the search is for an EXACT Search only (but can be filtered using the checkboxes below the entry box to return only chemical entities that have a single component or exclude isotopically-labeled compounds (e.g. no deuterium- or ¹³C-labeled compounds).



If a hit is identified in the database then the search will return a detailed results page with associated information for the chemical. For example, a search for "atrazine" returns the chemical at <http://comptox.epa.gov/dashboard/DTXSID9020112>, discussed in more detail below in the Chemical Results Page section.

Chemical Results Page

The chemical results page for atrazine is given at <http://comptox.epa.gov/dashboard/DTXSID9020112>. An image of the results page is shown below.



The page shows an image of the chemical structure and associated information. When a Wikipedia article is available then a snippet of that article is shown with a link out via the “Read More” link. There are ~750,000 substances on the dashboard and around 15,000 substances linked to Wikipedia only.

The intrinsic properties include molecular formula, average mass and monoisotopic mass, properties that are valuable to analytical scientists involved in structure identification and, in particular, to support targeted and non-targeted screening identification of environmental chemicals (for example, as [reported by Sobus *et al.*](#)). “Find All Chemicals” will perform a formula search of the dashboard and will display all results in a Tile or Table view depending on the user selection. This will be covered in more detail later in this manual. All properties can be copied to the clipboard, individually, using the Copy button.

Intrinsic Properties

Molecular Formula: C8H14ClN5

Average Mass: 215.69 g/mol

Monoisotopic Mass: 215.093773 g/mol

The structural identifiers include the IUPAC Name, SMILES, InChIString and InChIKey.

Structural Identifiers

IUPAC Name: 6-Chloro-N²-ethyl-N⁴-(propan-2-yl)-1,3,5-triazine-2,4-diamine

SMILES: CCNC1=NC(NC(C)C)=NC(Cl)=N1

InChI String: InChI=1S/C8H14ClN5/c1-4-10-7-12-6(9)13-8(14-7)11-5(2)3/h5H,4H2,1-3H3,(H2,10,11,12,13,14)

InChIKey: MXWJVTOOROXGIU-UHFFFAOYSA-N

Search Google for:

The InChIKey can be used to perform a search across the internet using the Google Search Engine. For example, for the chemical structure of Atrazine the InChIKey displayed above results in over 500 "exact structure" hits online: <https://www.google.com/#q=MXWJVTOOROXGIU-UHFFFAOYSA-N>. An InChIkey skeleton search ignores stereochemistry, charge and isotopes when searching for a particular chemical.

The Relate Compounds tab includes...

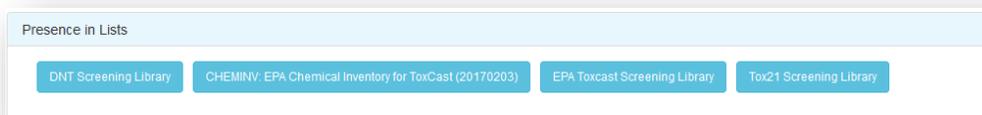
Related Compounds

Same Connectivity: 4 records (based on first layer of InChI)

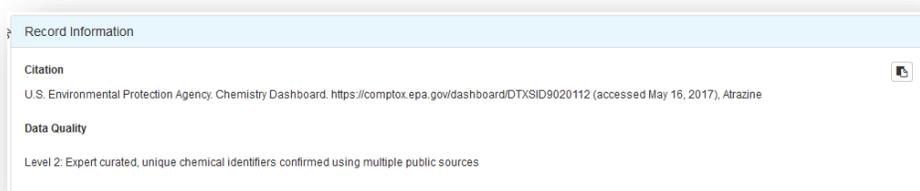
Mixtures, Components, and Neutralized Forms: 20 records (based on QSAR ready mappings and with the compound as a component of a mixture)

Similar Compounds: 63 records (based on Tanimoto coefficient > 0.8)

The Presence in Lists tab lists specific lists that the chemical is part of. Relative to work performed in NCCT this will include our ToxCast dataset and our Chemical Inventory list. For more details regarding the individual lists hover over the blue button to see a short description and to examine the list in more detail simply click on a blue button to open up a new tab containing the list.



The Record Information tab includes a citation that can be utilized when reporting a record, as well as information regarding data quality.



The different levels that can be listed are as follows:

Data Quality	Definition
Level 1	Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers
Level 2	Expert curated, unique chemical identifiers confirmed using multiple public sources
Level 3	Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem
Level 4	Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem
Level 5	Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source

Chemical Search Results Page

For each chemical, a series of tabs are displayed providing access to additional information about the chemical. The list of tabs is shown below. Each of these will be discussed in order.



Chemical Properties

The Chemical Properties listed in the table include both experimental and predicted property data. The experimental data are sourced from various sources including data curated from PHYSPROP downloadable files (explained in detail in the paper by [Mansouri et al](#)) as well as data from other public websites. Five forms of predicted property data are available. These include data from [EPISuite](#), from the OPERA models (Mansouri et al. publication in preparation), from the NICEATM models (Zang et al, manuscript accepted for publication), from the [Toxicity Estimation Software](#)

Tool (TEST) Models and harvested from the [Open PHACTS project](#) as predicted by [ACD/Labs](#). The summary tab displays a table with a list of all available properties and, if available, the average experimental property and range of experimental properties. The numbers in parentheses indicate the number of each of the properties available.

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	2.61 (1)	2.76 (4)	2.61	2.76	2.61	2.50 to 3.05	-
Water Solubility	1.30e-04 (1)	1.46e-02 (4)	1.30e-04	1.46e-02	1.30e-04	1.50e-04 to 5.71e-02	mol/L
Density	-	1.27 (1)	-	1.27	-	-	g/cm ³
Melting Point	174 (6)	151 (3)	175	151	173 to 177	114 to 185	°C
Boiling Point	-	312 (3)	-	312	-	284 to 339	°C
Surface Tension	-	53.8 (1)	-	53.8	-	-	dyn/cm
Vapor Pressure	7.21e-11 (1)	4.47e-06 (3)	7.21e-11	4.47e-06	7.21e-11	2.06e-07 to 1.27e-05	mmHg
LogKoa: Octanol-Air	-	8.38 (1)	-	8.38	-	-	-
Henry's Law	-	4.20e-10 (1)	-	4.20e-10	-	-	atm-m ³ /mole
Index of Refraction	-	1.61 (1)	-	1.61	-	-	-
Molar Refractivity	-	58.5 (1)	-	58.5	-	-	cm ³
pKa Basic Apparent	-	2.27 (1)	-	2.27	-	-	-
Molar Volume	-	170 (1)	-	170	-	-	cm ³
Polarizability	-	23.2 (1)	-	23.2	-	-	Å ³

For the example above, the Average Melting Point is listed as 174 (6) indicating that there are 6 melting points available covering a range of 173 to 177 degrees. Clicking on the individual property button on the left hand side opens up a detailed property table for review. The table of Melting Points listed below shows the information for Atrazine. Hovering over the Source names will display details regarding the Source information.

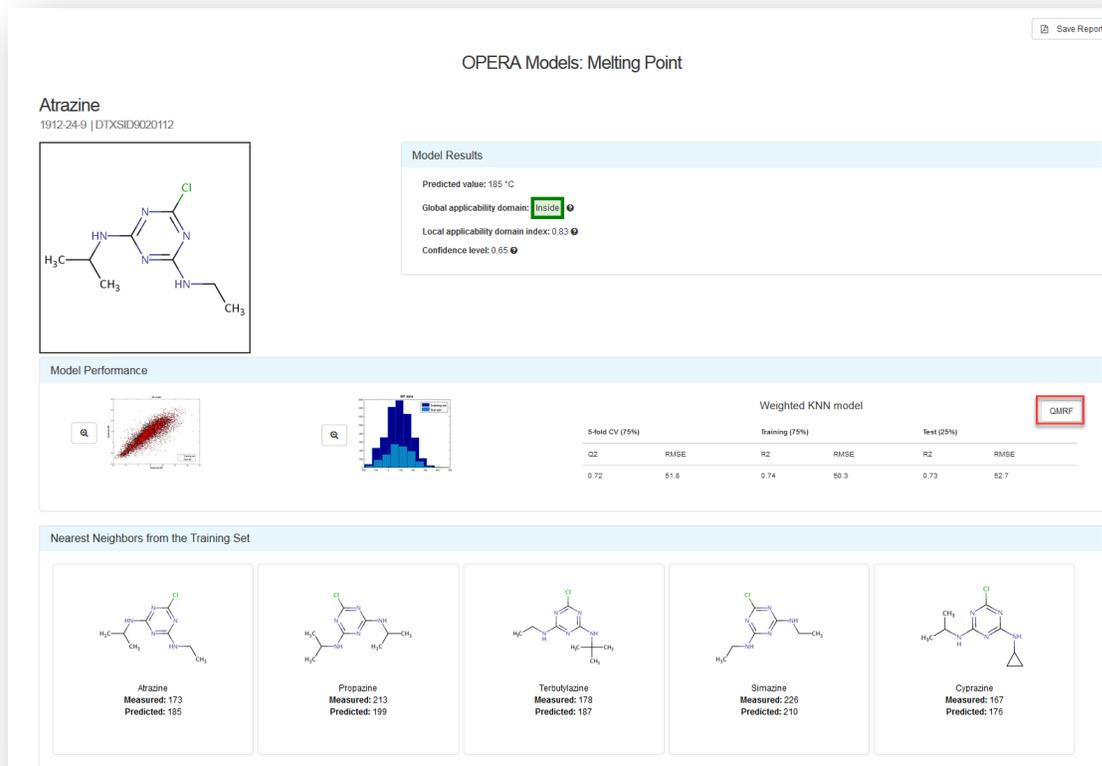
Melting Point			
	Average	Median	Range
Experimental	174 (6)	175	173 to 177
Predicted	151 (3)	151	114 to 185

Experimental			
Source	Result		
Jean-Claude Bradley Open Melting Point Dataset	173 °C		
Jean-Claude Bradley Open Melting Point Dataset	173 °C		
Jean-Claude Bradley Open Melting Point Dataset	175 °C		
Jean-Claude Bradley Open Melting Point Dataset	177 °C		
TCI	175 °C		
PhysPropNCCT	173 °C		

Predicted			
Source	Result	Calculation Details	QMRF
EPISUITE	114 °C	Not Available	Not Available
OPERA	185 °C	OPERA Model Report	Available
NICEATM	153 °C	Not Available	Available

In both cases, the summary table of properties and the detailed table of values, it is possible to download the file in either tab-separated value (TSV), Excel table format or as a Structure Data File (SDF).

In order to deliver total transparency in terms of how the property predictions are performed a report regarding the *Calculation Details* is available for the OPERA calculations. An example is [shown here for Atrazine](#) and is displayed below.



The details regarding how the prediction models were developed are given in the QMRF report that is directly available as a PDF file that can be downloaded. Each of the available OPERA models has its own QMRF detailing the software used to develop the models as well as the individual descriptors parameterizing a specific property. In the Calculation Report shown above the predicted value is the value produced by the prediction model and the Global Applicability Domain describes whether the chemical structure is contained Inside or Outside of the domain. The Local Applicability Domain Index is a value between 0 and 1 based on the similarity between the structure and its five nearest neighbors. The Confidence level, a value between 0 and 1, is an accuracy index of prediction based on the five nearest neighbors. More details are contained within the QMRF report.

Detailed prediction reports are available from the TEST predictors. An example is [shown here](#).

Melting Point		Experimental	
Source	Result	Source	Result
Boiling Point		NCBI	40.0 °C
Surface Tension		Jean-Claude Brodeur Open Melting Point Database	40.0 °C
Thermal Conductivity		Jean-Claude Brodeur Open Melting Point Database	-13.8 °C
Vapor Pressure		Jean-Claude Brodeur Open Melting Point Database	-18.5 °C
Viscosity		Jean-Claude Brodeur Open Melting Point Database	40.0 °C
LogP _{ow} Octanol-Water		Jean-Claude Brodeur Open Melting Point Database	-18.0 °C
LogP _{ow} Octanol-Water		Jean-Claude Brodeur Open Melting Point Database	-17.0 °C
Henry's Law		Oxford University Chemical Safety Data (no longer updated)	40.0 °C
Index of Refraction		Alfa Aesar	40.0 °C
Molar Refractivity		Alfa Aesar	40.0 °C
Molar Volume		Alfa Aesar	-18.0 °C
Polarizability		PhosphorGIC	42.8 °C

Predicted		Calculated	
Source	Result	Calculation Details	QMRF
TEST	185.0 °C	TEST Report	Not Available
ERDFUTL	82.0 °C	Not Available	Not Available
OPERA	51.3 °C	QMRF Report	Available

The Environmental and Transport properties listed in the table is similar to the PhysChem properties in terms of functionality and is simply a segregation of the different types of endpoints.

Summary							
Download as: <input type="button" value="TSV"/> <input type="button" value="Excel"/> <input type="button" value="SDF"/>							
Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
Soil Adsorp. Coeff.	174 (1)	194 (2)	174	194	174	144 to 244	L/kg
Atmos. Hydroxylation Rate	-	1.71e-11 (1)	-	1.71e-11	-	-	cm ³ /molecule*sec
Biodeg. Half-Life	-	4.92 (1)	-	4.92	-	-	days
Fish Biotrans. Half-Life (Km)	8.91e-02 (1)	1.34e-01 (1)	8.91e-02	1.34e-01	-	-	days
Bioaccumulation Factor	-	18.9 (1)	-	18.9	-	-	-
Bioconcentration Factor	7.94 (1)	55.3 (4)	7.94	55.3	7.94	7.45 to 186	-

Synonyms

The database contains over a million synonyms obtained from various resources. These are displayed with the relevant quality flags as shown below. The list of synonyms can be copied to the clipboard using the "Copy All Synonyms" button. **Valid Synonyms** are those that have been manually curated by members of our curation team. *Good Synonyms* have been obtained from a variety of sources and using complex workflows for cross-referencing are ranked as being of higher quality than the remaining collection of "Other Synonyms". The synonyms are not warranted as perfect or complete but are the results of our best efforts.

Found 101 synonyms							
Legend: Valid Synonyms Good Synonyms Other Synonyms <input type="button" value="Copy all Synonyms"/>							
Atrazine							
6-Chloro-N ² -ethyl-N ⁴ -(propan-2-yl)-1,3,5-triazine-2,4-diamine							
1,3,5-triazine-2,4-diamine, 6-chloro-N ² -ethyl-N ⁴ -(1-methylethyl)-							
1912-24-9 Active CAS RN							
1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-N ⁴ -(1-methylethyl)-							
1,3,5-Triazine-2,4-diamine, 6-chloro-N ² -ethyl-N ⁴ -(1-methylethyl)-							
1-Chloro-3-ethylamino-5-isopropylamino-2,4,6-triazine							
2-Chloro-4-(ethylamino)-6-(2-propylamino)-s-triazine							
2-Chloro-4-(ethylamino)-6-(isopropylamino)-s-triazine							
2-Chloro-4-(ethylamino)-6-(isopropylamino)triazine							
2-Chloro-4-ethylaminoisopropylamine-s-triazine							
2-Chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine							
2-Chloro-4-ethylamino-6-isopropylamino-s-triazine							
2-Ethylamino-4-isopropylamino-6-chloro-s-triazine							
6-Chloro-4-(ethylamino)-2-(isopropylamino)-s-triazine							
6-Chloro-N-ethyl-N ⁴ -(1-methylethyl)-1,3,5-triazine-2,4-diamine							
AAtrex Nine-O							
Akticon							
Aktikon							
Aktikon PK							
Aktinit A							
Aktinit PK							

External Links

There is an abundance of information available for many of the chemicals contained within the CompTox Dashboard. In order to assist the user in navigating to these external links we have produced a click-through integration allowing the user to navigate directly to the site. Hovering over the names of the sources will display a tooltip with information about the specific resource. When links cannot be identified then the appropriate resource is grayed out and not linked. In the example below, there is no information for the particular chemical in the NIST Chemistry Webbook or

Household Products Database. This approach is not exhaustive however and some of the links may not have data associated. We continue to invest in approaches to improve these external links.

The screenshot shows the 'External Links' tab with the following categories and links:

- General:** EPA Substance Registry Service, NIST Chemistry Webbook, Household Products Database, PubChem, Chemspider, HMDB, Wikipedia, MSDS Lookup, ToxPlanet, ChemHat: Hazards and Alternat..., ChEMBL, Consumer Product Information..., ECHA Brief Profile, ECHA Infocard, Sigma-Aldrich Chemicals, Wikidata, Wolfram Alpha, WebWISER, ECHA Dossier, ScrubChem.
- Toxicology:** ACToR, DrugPortal, CCRIS, ChemView, CTD, eChemPortal, EDSP Dashboard, Gene-Tox, HSDB, ToxCast Dashboard 2, LacMed, International Toxicity Estimates f..., ACToR PDF Report.
- Publications:** Toxline, NIEHS, National Toxicology Program, Google Books, Google Scholar, Google Patents, PubMed, BioCaddie DataMed, Federal Register, Regulations.gov, RSC Publications, Springer Materials, IRIS Assessments, CORE Literature Search, Bielefeld Academic Search Eng..., Environmental Health Perspecti...
- Analytical:** RSC Analytical Abstracts, FOR-IDENT, MONA: MassBank North America, NEM: National Environmental..., Tox21 Analytical Data.
- Prediction:** Chemicalize, Proton NMR Prediction, Carbon-13 NMR Prediction, 2D NMR HSQC/HMBC Prediction, ChemRTP Predictor.

Toxicity Values (Beta)

The Toxicity Values (Beta) tab provides Toxicity Value data that have been assembled from a number of EPA agency resources as well as many other public sources. When toxicity data is available it is shown under a set of subtabs, shown on the left hand side of the table. Selecting the appropriate subtab shows a table of data. Each column heading can be selected for ordering in the interface. Hovering over the Type, Details and Source provides a detail hover with information. The Details link will open the detailed table under Toxval for that chemical.

The screenshot shows the 'Toxicity Values (Beta)' tab with a table of exposure limits. The table has the following columns: Grouping ID, Priority, Type, Subtype, Value, Units, Study Type, Exposure Route, Study Duration, Species, Media, Details, and Source. The table is filtered by 'Exposure Limit' and 'Point Of Departure'. The table contains 15 rows of data.

Grouping ID	Priority	Type	Subtype	Value	Units	Study Type	Exposure Route	Study Duration	Species	Media	Details	Source
5966	6	tolerable d...	-	2.00	ul/kg-day	-	oral	-	-	-	RIVM details	RIVM
5967	6	tolerable d...	-	5.00	ul/kg-day	-	oral	-	-	-	RIVM details	RIVM
48903	2	MCL-base...	-	1.90e-03	mg/kg-day	-	-	-	-	-	RSL details	RSL
176188	3	water qualit...	drinking wa...	0.7	mg/L	-	oral	chronic	-	drinking wa...	EPA Drinki...	ACToR
176190	3	MCL goal	drinking wa...	3.00e-03	mg/L	-	oral	-	-	drinking wa...	EPA Drinki...	ACToR
176191	3	MCL	drinking wa...	3.00e-03	mg/L	-	oral	-	-	drinking wa...	EPA Drinki...	ACToR
176192	2	MCL	drinking wa...	1.00e-03	mg/L	-	oral	-	-	drinking wa...	California ...	ACToR
176193	2	MCL	drinking wa...	3.00e-03	mg/L	-	oral	-	-	drinking wa...	California ...	ACToR
176194	2	MCL	drinking wa...	3.00e-03	mg/L	-	oral	-	-	drinking wa...	California ...	ACToR
176195	3	MCL goal	drinking wa...	3.00e-03	mg/L	-	oral	-	-	drinking wa...	EPA Drinki...	ACToR
176196	3	MCL	drinking wa...	3.00e-03	mg/L	-	oral	-	-	drinking wa...	EPA Drinki...	ACToR
176197	2	water qualit...	drinking wa...	0.5	g/L	-	oral	-	-	drinking wa...	California ...	ACToR
176198	2	MCL	drinking wa...	1.00	g/L	-	oral	-	-	drinking wa...	California ...	ACToR
176199	3	MCL	drinking wa...	3.00e-03	mg/L	-	oral	-	-	drinking wa...	EPA Nation...	ACToR

Exposure

The Exposure tab provides a listing of products containing the chemical, percent composition of the chemical in the product and associated suppliers from the [CPCat Database](#). The data can be downloaded in either TSV or Excel format. For details regarding each of the tables and how the data are sourced click on the informational icon adjacent to the title for details.

The screenshot shows the 'Exposure' tab in the CPCat Database. The table is titled 'Chemical Weight Fractions' and includes columns for Product Name, Product Use Category, Minimum Weight Fraction, Maximum Weight Fraction, Data Type, and Source. The data is as follows:

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
bonus s max + fireant killer 12...	pesticides: insecticide	0	0.011	MSDS	Retail Product Categories/Wal...
bonus s max 10m 1	landscape/yard: lawn fertilizer	0	0.011	MSDS	Retail Product Categories/Wal...
bonus s max 5m 1	landscape/yard: lawn fertilizer	-	-	MSDS	Retail Product Categories/Wal...
expert gardener st augustine w...	landscape/yard: garden fertilizer	0.013	0.013	MSDS	Retail Product Categories/Wal...
expert gardener st augustine ...	landscape/yard: garden fertilizer	0.013	0.013	MSDS	Retail Product Categories/Wal...
scotts bonus s max with fire an...	pesticides: insecticide	-	-	MSDS	Retail Product Categories/Wal...
scotts bonus s 29-3-4 1	landscape/yard: lawn fertilizer	0.011	0.011	MSDS	Retail Product Categories/Wal...
scotts bonus s max wfireant Nr...	pesticides: insecticide	0.014	0.014	MSDS	Retail Product Categories/Wal...
scotts bonus s, 538-18 1	landscape/yard: lawn fertilizer	0.013	0.013	MSDS	Retail Product Categories/Wal...

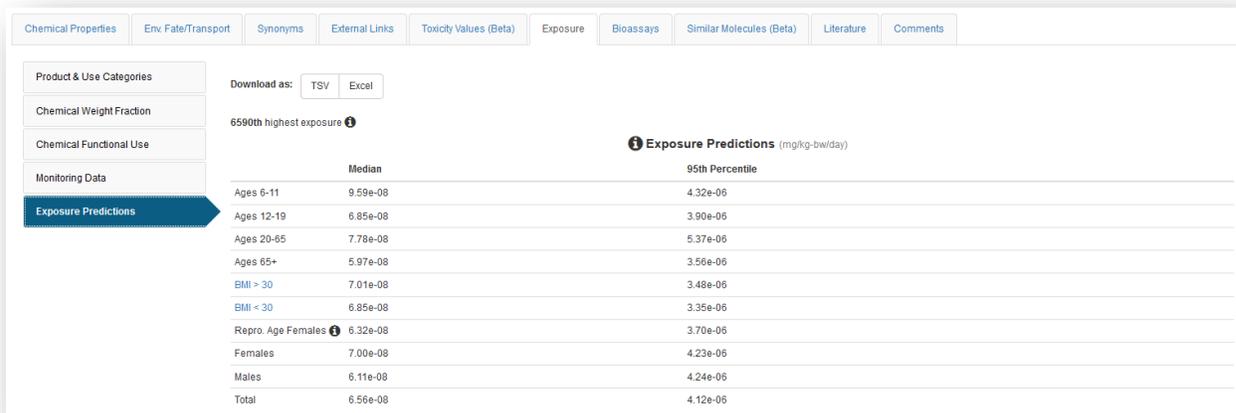
NHANES: The Centers for Disease Control (CDC) National Health and Nutrition Examination Survey (NHANES) is a program of studies designed to assess the health and nutritional status of adults and children in the United States. As part of the [NHANES](#), the CDC monitors [biomarkers of chemical exposure](#) (chiefly metabolites) in the blood and urine to quantify the levels of chemical compounds present in U.S. residents. Each two-year study cycle comprises approximately 10,000 individuals, with exposure biomarker data for any given chemical available from only a subset of roughly 1/3 of the individuals in the study. In the 2014 publication "[High Throughput Heuristics for Prioritizing Human Exposure to Environmental Chemicals](#)" EPA scientists inferred steady state exposure rates (mg/kg bodyweight) for **106 chemicals** from the NHANES urine samples.

The screenshot shows the 'Exposure' tab in the CPCat Database. The table is titled 'National Health and Nutrition Examination Survey (NHANES) Inferences (mg/kg-bw/day)' and includes columns for Lower 95th Limit, Upper 95th Limit, and Median. The data is as follows:

	Lower 95th Limit	Upper 95th Limit	Median
Ages 6-11	3.21e-09	4.23e-07	4.79e-08
Ages 12-19	1.84e-09	4.70e-07	5.21e-08
Ages 20-65	5.53e-09	4.38e-07	7.79e-08
Ages 65+	2.42e-09	4.97e-07	6.93e-08
BMI > 30	3.56e-09	4.01e-07	6.19e-08
BMI < 30	3.70e-09	4.63e-07	5.98e-08
Repro. Age Females	3.96e-09	5.39e-07	8.17e-08
Females	4.30e-09	4.34e-07	7.04e-08
Males	1.71e-09	3.75e-07	4.20e-08
Total	2.81e-09	3.81e-07	5.76e-08

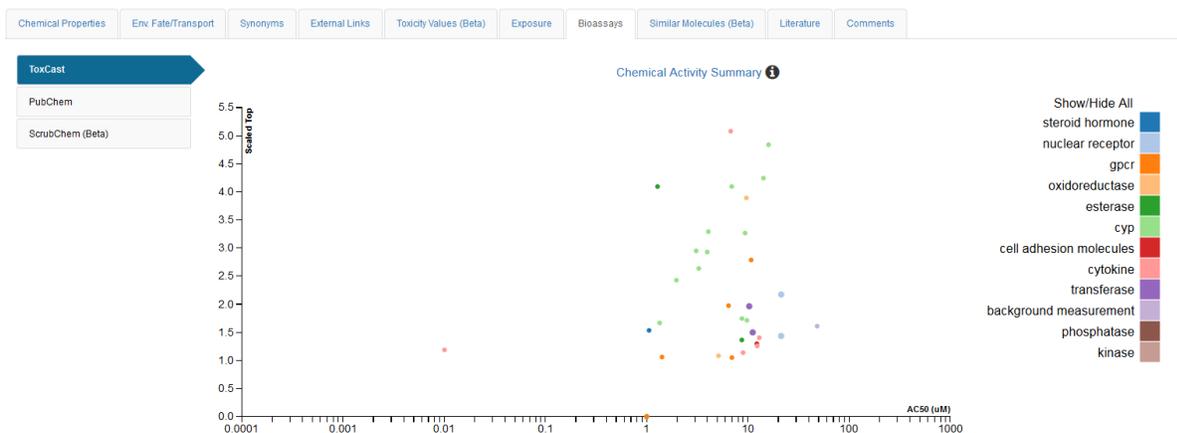
Predicted Exposure Data: The table of Exposure Predictions lists data produced as a result of the work published in Figure 4 of the 2014 publication "[High Throughput Heuristics for Prioritizing Human Exposure to Environmental Chemicals](#)" EPA scientists ranked 7968 chemicals based on the upper (highest) 95th percentile limit on the predicted

average (geometric mean) exposure rate for the total U.S. population. This is one of those 7968 chemicals. The 1st highest would have the highest predicted possible rate, while the 7968th highest would have the lowest predicted possible rate. Note that because of [limited information available on exposure](#) to most chemicals the uncertainties are large and we are only 95% confident that the exposure rate is equal to or lower than the upper 95th percentile limit. The ranking for a chemical is shown on the top left hand side as the XXXXth Highest Exposure out of 7968 chemicals.



Bioassays

The Bioassays tab provides access to three different types of bioassay data. This includes the ToxCast data, an embedded view of PubChem Bioassay data and an embedded view of ScrubChem Bioassay data. The ToxCast data shows the bioassay data represented as a graphic and the target families displayed on the right hand side. These can be displayed one family at a time and switched using Show/Hide All as necessary. The color coding represents the ACTIVE hit calls as a function of target family.



The table below the plot lists the tabular data associated with the ToxCast data. The Inactives and “Background Results” are *not* shown by default but can be displayed by selecting the buttons above the table. The columns can be ranked by selecting the appropriate column header (in blue) and hovering over the assay name provides the details of the assay. Selecting the download in either TSV or Excel will download the file *including* the background results and inactives.

Download as: [TSV](#) [Excel](#) Show: [Inactive](#) [Background](#)

Assay Name	Hit Call ↑	Top	Scaled Top	AC50	log AC50	Intended Target Family
NVS_GPCR_bAdoR_NonSelective	ACTIVE	57.5	2.79	10.8	1.03	gpcr
NVS_ENZ_rMAOAC	ACTIVE	24.5	1.08	5.13	0.710	oxidoreductase
NVS_ENZ_oCOX2	ACTIVE	77.8	3.89	9.66	0.985	oxidoreductase
NVS_ENZ_hPDE5	ACTIVE	27.3	1.36	8.71	0.940	esterase
NVS_ENZ_hPDE4A1	ACTIVE	85.3	4.09	1.28	0.107	esterase
NVS_ADME_hCYP2C19	ACTIVE	34.9	1.74	8.73	0.941	cyp
NVS_ADME_hCYP1A2	ACTIVE	34.3	1.71	9.78	0.990	cyp
BSK_SAg_Eselectin_down	ACTIVE	0.166	1.30	12.2	1.09	cell adhesion molecules

The PubChem selection button displays a PubChem widget allowing the user to navigate through the PubChem data sourced using the embedded widget and real time service calls against PubChem to retrieve the latest data.

ToxCast **PubChem** ScrubChem (Beta)

PubChem Biological Activities

PUBCHEM > COMPOUND > ATRAZINE > BIOLOGICAL TEST RESULTS > BIOASSAY RESULTS >

BioAssay Results

Refine/Analyze Download

All (1,489) Active(23) Inconclusive(35) Inactive(1,280) Unspecified(151)

1 to 10 of 1,489 1 2 3 ... 149 Activity

Activity	Activity Value [μM]	Substance SID	BioAssay AID	BioAssay Name	Target
Inactive		438027	192	NCI In Vivo Anticancer Drug Screen. Data for tumor model B16 Melanoma (intraperitoneal) in B6D2F1 (BDF1) mice	
Inactive		438027	256	NCI In Vivo Anticancer Drug Screen. Data for tumor model L1210 Leukemia (intraperitoneal) in CD2F1 (CDF1) mice	
Inactive		438027	330	NCI In Vivo Anticancer Drug Screen. Data for tumor model P388 Leukemia (intraperitoneal) in CD2F1 (CDF1) mice	
Inactive		17390035	421	Cell Viability - BJ	
Inactive		17390035	426	Cell Viability - Jurkat	
Inactive		17390035	427	Cell Viability - Hek293	
Inactive		17390035	433	Cell Viability - HepG2	
Inactive		17390035	434	Cell Viability - MRC5	

Navigation of the PubChem widget should be fairly self-explanatory

ScrubChem

Filter by 'Justifications'

Records 2,119 Chemicals 1 MolTargets 485 Assays 1,137

Active 63 Inactive 1,802 Inconclusive 32 Unspecified 167 Probe 0

AID (assay ID)	MID (panel ID)	TID (test ID)	SID (substance ID)	CID (compound ID)	Chemical Name	Outcome	TID Qualifier (fixed)	Value (for tid)	TID Unit	TID Name
651548	0	3	56789618	2256	atrazine	inactive		10.044	percent	REPLICATE
651550	0	2	56314826	2256	atrazine	inactive		OC'd by RTI International	none	Compound
651560	0	1	56314826	2256	atrazine	inactive		-1.248	percent	%Activity_Nc
651560	0	2	56314826	2256	atrazine	inactive		-0.7069	percent	%Activity_Cc
651560	0	3	56314826	2256	atrazine	inactive		448.5		Value at 20 t
651572	0	1	56314826	2256	atrazine	inactive		-3.4	percent	Inhibition at

Showing 1 to 100 of 2,119 entries

Similar Molecules (Beta)

The Similar Molecules tab shows a collection of chemicals that match the chemical structure with a Tanimoto of >0.8 or the most similar chemicals to a total of 50 chemicals.

Similar Molecules

Searched with a similarity threshold of 0.82

Download as: TSV Excel

Similarity Value		1	1	1	1	1
LogP, Octanol-Water	Experimental	-	-	1.51	2.61	2.93
	Predicted	-	2.77	1.58	2.76	3.15
Water Solubility	Experimental	-	-	0.00197	0.000130	0.0000374
	Predicted	-	0.0287	0.0108	0.0146	0.000514
Density	Experimental	-	-	-	-	-
	Predicted	-	-	1.38	1.27	1.23
Melting Point	Experimental	-	-	133	175	213
	Predicted	-	169	142	151	160
Boiling Point	Experimental	-	-	-	-	-
	Predicted	-	312	303	312	318

Literature

The Literature Tab provides access to four different ways to access data we class as literature for the purpose of review within the dashboard. It includes access to PubMed literature, searches against Google Scholar, an Abstract Sifter that can be used for specific queries against Pubmed articles using MeSH based searches and access to PubChem Patents.

Google Scholar

The Google Scholar search function allows for terms to be selected from the drop downs. These are appended into a search using the CAS Number and Preferred Name. For the query shown below a search of Google Scholar will return a list of articles with *Atrazine* and *Hazard* in the query results. The query can also be edited in the search box as necessary.



The screenshot shows a web interface with a navigation bar at the top containing tabs: Chemical Properties, Env. Fate/Transport, Synonyms, External Links, Toxicity Values (Beta), Exposure, Bioassays, Similar Molecules (Beta), Literature (selected), and Comments. On the left, a sidebar lists search options: Google Scholar (selected), PubMed Abstract Sifter, PubChem Articles, PubChem Patents, and IRIS. The main search area has a 'Select Term:' label above three dropdown menus. Below these is a text box labeled 'Edit the Query Before Querying (25 Characters)' containing the query '"1912-24-9" OR "Atrazine"'. A green 'Submit' button is located below the text box.

PubMed Abstract Sifter

The abstract sifter functionality uses pre-defined queries to initiate a query against PubMed. The list of queries is:



The screenshot shows a 'Select Term:' dropdown menu. The dropdown is open, displaying a list of query terms. The first item is 'Select a Query Term' (highlighted in blue). The other items are: Hazard, Fate and Transport, Metabolism/PK/PD, Chemical Properties, Exposure, Mixtures, Male Reproduction, Androgen Disruption, Female Reproduction, GeneTox, Embryo and embryonic development, Child (infant through adolescent), and Dust and Exposure.

Selection of one of these queries creates the MeSH query required to perform the search. Retrieve articles (the green button) will return the number of articles that are identified with a maximum of 1000 available for download. For the

example shown below the abstracts are retrieved and the filter boxes can be used to search and mark-up the abstracts based on substring searches. Up to three terms can be searched (using the Search and Count button) and clicking on the individual terms in the table will rank order the results based on the specific search terms. When one or more abstracts are identified for further reading then the PMID can be selected to open up the abstract in the PubMed interface.

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

IRIS

Select Term: Hazard

Retrieve Articles **28 Articles (out of 28)**

Add additional query terms to filter abstracts:

reproduce development

Search and Count

Edit the Query Before Retrieving Articles

(*1912-24-8* OR "Atrazine" OR "Atrazine") AND (NOAEL OR NOEL OR LOEL OR RfD OR "reference dose" OR "reference concentration" OR "adverse effect level"[lab] OR "cancer slope factor"[lab])

repro...	devel...	Term 3	Total	PMID	PubYr	Title
0	0	0	0	25138046	2014	Effect of atrazine and fenitrothion at no-observed-effect-levels (NOEL) on amphibian and mammalian corticosterone-binding-globulin (CBG).
0	0	0	8	24797874	2014	Multigeneration reproduction and male developmental toxicity studies on atrazine in rats.
0	0	0	2	24323408	2013	Evaluation of hydroxyatrazine in the endocrine disruptor screening and testing program's male and female pubertal protocols.
0	0	0	1	23958493	2013	Estimation of placental and lactational transfer and tissue distribution of atrazine and its main metabolites in rodent dams, fetuses, and neonates w...

Record: 5 of 28

Title: Multigeneration reproduction and male developmental toxicity studies on atrazine in rats.

Abstract: Reproductive toxicity of Atrazine (ATR) was evaluated in two rat multigenerational studies. Development of male reproductive parameters was evaluated in separate studies after prenatal or postnatal exposure. In multigenerational studies, rats received dietary concentrations of 0, 10, 50, 100 or 500 ppm ATR. In separate studies in female rats, ATR was administered by gavage at 0, 1, 5, 25 or 125 mg/kg/day during pregnancy (GD6-21) or lactation (LD2-21). Plasma testosterone concentration, testicular and epididymal weights, and sperm counts were measured in male offspring on PND70 and 170 in the multigenerational studies, parental systemic toxicity occurred at 500 ppm (38.7 mg/kg/day), but reproductive endpoints were unaffected. In the prenatal study, maternal toxicity and embryo-fetal mortality occurred at 125 mg/kg/day. In male offspring, testosterone levels and sperm counts were unaffected, although the percentage of abnormal sperm increased at 125 mg/kg/day (PND 70) and 25 mg/kg/day (PND 170). In the postnatal study, maternal toxicity and reduced body weights of male offspring occurred at 125 mg/kg/day. Additionally, reduced testicular (PND70, PND170) and epididymal (PND70) weights and increased numbers of abnormal sperm (PND70, PND170) were seen, but no changes in plasma testosterone or sperm counts. Dietary administration of ATR did not affect rat reproduction on up to a parentally toxic dose of 38.7 mg/kg/day. Some effects on male reproductive system development occurred after high dose, bolus administration to dams, but doses were much higher than expected under normal use conditions. Thus, oral RfDs for ATR would be protective for reproductive effects.

PubChem Articles

The [PubMed widget](#) provides access to the latest articles reported in Pubmed with the chemical in question flagged for inclusion using the [MeSH Ontology](#) mappings in PubChem. The articles are ranked with most recent listed first.

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

IRIS

PubChem Articles

PUBCHEM > COMPOUND > ATRAZINE > LITERATURE > DEPOSITOR PROVIDED PUBMED CITATIONS >

Depositor Provided PubMed Citations

Download

1 to 10 of 2,470 1 2 3 ... 247 Date

PMID	Date	Title	Journal
26962873	2016-07-01	A High-Throughput Screening Strategy to Identify Protein-Protein Interaction Inhibitors That Block the Fanconi Anemia DNA Repair Pathway.	Journal of biomolecular screening
18378257	2008-05-09	Univariate method for background correction in liquid chromatography-Fourier transform infrared spectrometry.	Journal of chromatography, A
1430	1976-01-01	Hydrolysis of a chloro-s-triazine herbicide.	Journal of agricultural and food chemistry
5165	1976-03-01	N-nitrosamine formation from atrazine.	Bulletin of environmental contamination and toxicology
119497	1979-01-01	Sorption and desorption of atrazine by three bacterial species isolated from aquatic systems.	Archives of environmental contamination and toxicology
218588	1979-01-01	Increases in rat liver cyclic AMP and glycogen phosphorylase activity caused by the herbicide atrazine.	Biochemical pharmacology
239812	1975-06-01	The effects of some herbicides and pesticides on sodium uptake by isolated perfused gills from the carp <i>Cyprinus carpio</i> .	Comparative biochemistry and physiology. C: Comparative pharmacology
412980	1977-11-01	Mutagenicity of the triazine herbicides atrazine, cyanazine, and simazine in <i>Drosophila melanogaster</i> .	Journal of toxicology and environmental health
429685	1979-03-01	Metabolism of atrazine by the soluble fraction (105000g) from chicken liver homogenates.	Journal of agricultural and food chemistry
461116	1979-03-01	Pesticide residue levels in soils and crops from 37 states, 1972--National Soils Monitoring Program (IV).	Pesticides monitoring journal

PubChem Patents

The [PubChem Patent Widget](#) lists patents associated with a particular chemical and indexed through PubChem. The list of patents is ranked with most recent patent listed first. The data can be downloaded directly from the widget using the Download Button at the top right hand corner.

Patent ID	Patent Title	Submitted Date	Granted Date
EP0000002	TETRAHYDROFURANE DERIVATIVES, PROCESSES FOR THEIR PREPARATION AND THEIR USE AS HERBICIDES	1978-12-20	1981-08-26
EP0000681	AMINO-2 (OR -4) ALKYLTHIO-5 PYRIMIDINES, PROCESSES FOR THEIR PREPARATION, THEIR USE AS HERBICIDES AND COMPOSITION CONTAINING THEM	1979-02-07	1981-08-26
EP0000852	TREATMENT OF HERBICID CONTAINING CULTURES WITH DERIVATIVES OF DICHLOROACETAMIDE OR OF TRICHLOROACETAMIDE, NOVEL DERIVATIVES OF DICHLOROACETAMIDE OR TRICHLOROACETAMIDE AND PROCESS FOR THEIR PREPARATION	1979-02-21	1982-08-25
EP0001519	WATER-DISPERSIBLE HERBICIDAL COMPOSITIONS AND USE THEREOF	1979-04-18	1982-01-06
EP0002881	5-Isoxazolylurea derivatives, their preparation, their use and compositions containing them.	1979-07-11	
EP0003877	HERBICIDAL DERIVATIVES OF 2-(4(2-PYRIDYLOXY)PHENOXY)PROPANE, PROCESSES FOR PREPARING THEM, AND HERBICIDAL COMPOSITIONS CONTAINING THEM	1979-09-05	1988-02-03
EP0003890	HERBICIDAL PYRIDINE COMPOUNDS AND HERBICIDAL COMPOSITIONS CONTAINING THEM HERBICIDAL PYRIDINE COMPOUNDS, PROCESSES FOR PREPARING THEM AND HERBICIDAL PROCESSES AND COMPOSITIONS UTILISING THEM	1979-09-05	1990-04-04
EP0004171	PYRAZOLOTRIAZINEDIONE DERIVATIVES, PROCESS FOR THEIR PREPARATION AND HERBICIDAL COMPOSITIONS CONTAINING	1979-09-19	1981-02-11

Iris

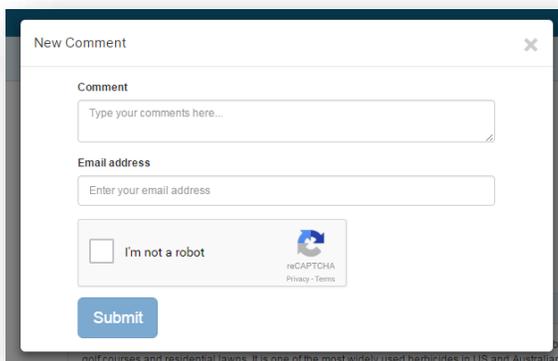
Iris shows the Integrated Risk Information System report associated with a chemical, if available.

RfD (mg/kg-day)	System	Basis	PoD	Composite UF	Confidence
			NOAEL		

Comments

The comments tab will list any comments made by users of the system in terms of potential data issues. Each chemical record can be annotated with comments regarding incorrect synonyms, quality of experimental property data etc. This allows crowd sourcing curation of the data on the database and engages the community of users in

facilitating expansion and validation of the data. Comments can be submitted by selecting the Select Comment button on the top right hand side of the interface. This opens up a modal dialog box for the user to add their comments. The users email must be included in order to submit a comment as this will allow us to respond. The email will not be displayed on the record and will be kept private. A captcha is included to prevent spamming.



The image shows a 'New Comment' modal dialog box. It has a title bar with a close button (X). The form includes a text area for 'Comment' with the placeholder 'Type your comments here...'. Below that is an input field for 'Email address' with the placeholder 'Enter your email address'. There is a checkbox labeled 'I'm not a robot' next to a CAPTCHA image. At the bottom left is a blue 'Submit' button.

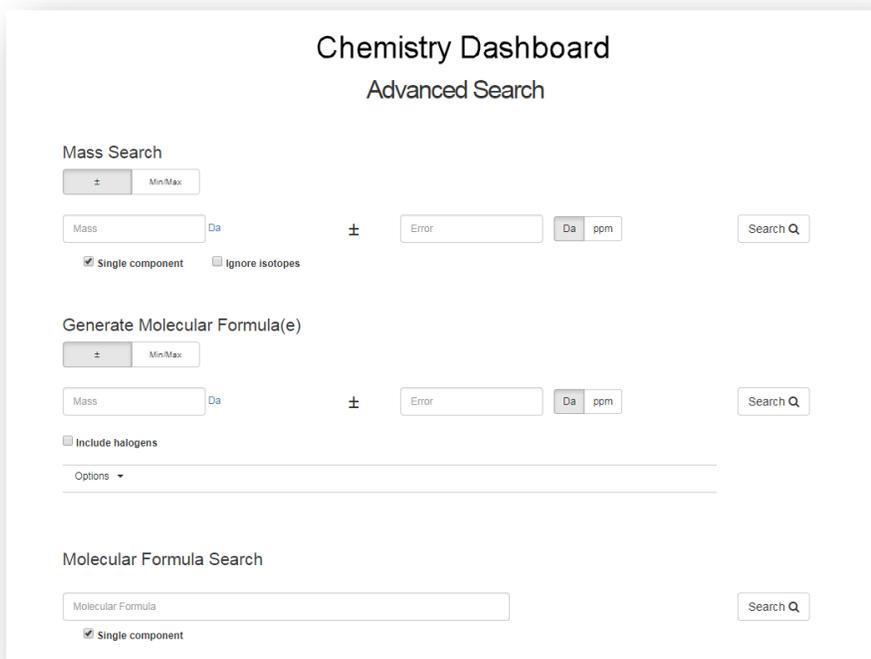
Advanced Searches

A number of additional searches are possible the Advanced Search page located at http://comptox.epa.gov/dashboard/dsstoxdb/advanced_search, or accessed on the top left hand side of the page. Here the user can perform searches to support Mass spectrometry (formula and mass)

There is also a batch-based search located https://comptox.epa.gov/dashboard/dsstoxdb/batch_search or accessed on the top left hand side of the page.

Mass Spectrometry Based Searches

The MS-based searches allow for searches based on inputting masses or formulae as shown in the interface entry forms below.



The image shows the 'Chemistry Dashboard Advanced Search' interface. It has a title 'Chemistry Dashboard' and subtitle 'Advanced Search'. There are three main search sections:

- Mass Search:** Includes a range selector (± Min/Max), an input field for 'Mass' (Da), a tolerance input field (Error), a unit selector (Da ppm), and a 'Search Q' button. It also has checkboxes for 'Single component' (checked) and 'Ignore isotopes'.
- Generate Molecular Formula(e):** Includes a range selector (± Min/Max), an input field for 'Mass' (Da), a tolerance input field (Error), a unit selector (Da ppm), and a 'Search Q' button. It has a checkbox for 'Include halogens' and an 'Options' dropdown menu.
- Molecular Formula Search:** Includes an input field for 'Molecular Formula' and a 'Search Q' button. It has a checked checkbox for 'Single component'.

Mass Search

This search is primarily incorporated to allow a user to search the database for chemicals matching a particular monoisotopic mass. This search will be of particular value for screening and non-targeted analysis users. A search can be performed on a single mass +/- error, either in Da or ppm. The search can be performed ignoring multicomponent structures and ignoring isotopes. An example search such as 228.1 +/- 5 ppm gives 215 results in a Table or Tile format. Selection of the single component or ignore isotopes filters means that only chemicals containing one component will be returned (i.e. no multi component mixtures, no compounds with solvents of hydration, etc.) Pre-selection of the isotope filter removes all isotopically labeled compounds from the search results.

Generate Molecular Formulae

Generating one or more molecular formulae from a mass and error (a maximum error of 0.05 Da is allowed) generates all possible formulae depending on the elemental option settings and then ranks these formulae based on the number of matching hits in the database. For example, the search below for 162.116 Da +/- 5ppm produces a hit list of six formulae with only one matching formula as shown below.

Molecular Formulae	Hits
<input checked="" type="checkbox"/> C12H13BrO4	19
<input checked="" type="checkbox"/> C13H9BrN4	6
<input checked="" type="checkbox"/> C9H8N4O4S2	3
<input checked="" type="checkbox"/> C6H3F11O	3
<input checked="" type="checkbox"/> C10H4N8S2	1
<input checked="" type="checkbox"/> C8H13CN2O4S2	1
<input checked="" type="checkbox"/> C12H13IO	1
<input checked="" type="checkbox"/> C16H9ClO2S	1
<input type="checkbox"/> C25	0
<input type="checkbox"/> C9H10N4O2P2S	0
<input type="checkbox"/> C11H10NO5S2	0
<input type="checkbox"/> C8H16O4P4	0
<input type="checkbox"/> CH24N2O4P4S3	0
<input type="checkbox"/> C4H12O13S	0
<input type="checkbox"/> C3H6N7O8S	0
<input type="checkbox"/> C2N14O3S	0
<input type="checkbox"/> C2H21F2NO5S	0

Selecting on a particular formula will open a new tab with the associated chemical structures shown. It is possible to View All Hits also by selecting the button (top right hand side)

The pre-defined options for the molecular formulae are as shown below. The default options ignore halogens. Other elements can be included by adding to the options input box.

Include halogens

Options ▾

C to

H to

O to

N to

P to

S to

Other options

Molecular Formula Search

This search is primarily incorporated to allow a user to search the database for chemicals matching a particular molecular formula. This search will be of particular value for non-targeted analysis users who have already generated a potential molecular formula from an unknown observed chemical. As with a mass-based search it can be performed on a molecular formula for a single component and multicomponent structures can be ignored. An example search such as C₁₅H₁₆O₂ yields 207 results.

Advanced Search Results Display

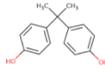
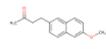
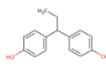
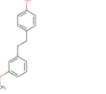
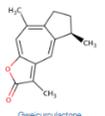
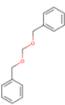
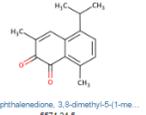
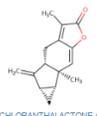
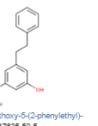
The results from a hit list can be shown as either a Table or in Tile form. The tile form of the hit list form is shown below. The tile list can be pruned using the check box below the structure and choosing the "View Selected" button. The hit list can be downloaded in the form of a TSV file, an Excel spreadsheet or an SDF file.

Chemistry Dashboard

View Selected Hide Multicomponent Chemicals

Searched by Molecular Formula, ignoring isotopes: Found 207 results for C₁₅H₁₆O₂

Download as: TSV Excel SDF

ID	Preferred Name	CAS-RN	QC Level	Number of Sources	PubChem Data Source Count
	Bisphenol A	80-05-7	<input type="checkbox"/>		
	Nabumetone	42024-03-0	<input type="checkbox"/>		
	4,4'-Propane-1,1'-diyl(diphenol)	1570-13-2	<input type="checkbox"/>		
	4-Hydroxy-3-methoxybibenzyl	95566-27-5	<input type="checkbox"/>		
	Gwercuculactone	123814-43-2	<input type="checkbox"/>		
	Preventol D2	2746-70-4	<input type="checkbox"/>		
	1,2-Naphthalenedione, 3,8-dimethyl-5-(1-methyl-2-propenyl)-	5574-34-5	<input type="checkbox"/>		
	Stahliarthusone	87018-25-6	<input type="checkbox"/>		
	CHLORANTHALACTONE A	06395-02-6	<input type="checkbox"/>		
	Phenol, 3-methoxy-5-(2-phenylethyl)-	17635-58-6	<input type="checkbox"/>		

epa.gov Privacy AccessAbility Downloads

Using the buttons on the top right hand side allows the user to switch between table and tile mode and to show or hide multicomponent chemicals.

Searched by Molecular Formula and single component chemicals: Found 207 results for 'C15H16O2'.

Download as: TSV Excel SDF

ID	Structure	Preferred Name	CAS-RN	QC Level	CPCat Count	Number of S...	PubChem Da...	Monoisotopic Mass
DTXSID7020182 ToxCast™		Bisphenol A	80-05-7	Level 1: Expert curate...	259	96	161	228.115030
DTXSID4045472 ToxCast™		Nabumetone	42924-53-8	Level 2: Expert curate...	0	32	138	228.115030
DTXSID60181905		Preventol D2	2749-70-4	Level 4: Programmati...	0	8	32	228.115030
DTXSID3044594		4,4'-Propane-1,1'-diyl(diphenol)	1576-13-2	Level 2: Expert curate...	0	7	26	228.115030

Data displayed for each record returned in the Search Results include DTXSID, structure, Preferred Name, and CAS. Additional valuable data for suspect screening and non-targeted analysis are the number of data sources, number of PubChem data sources, and the product occurrence count (CPCat Count) of each chemical returned in the results. It has been documented that ordering the number of data sources from high to low, the most likely chemicals observed in a sample rise to the top of the search results list (McEachran *et al*, 2016). Results can be downloaded, sorted, and investigated one a time. Additional data displayed as the ToxCast symbol on the left hand side indicates whether or not ToxCast data is available for the record. Hovering on the label will display the overall percentage of active assays out of the total for that chemical (Bisphenol A says "14% Active Calls: 174 Active Assays/1220 Total").

Batch Searching

An additional manner in which to search the Dashboard is through Batch Searching, where a user can enter lists of many chemicals at a time and return results.

Batch Search

Please enter one identifier per line ✕

Select Input Type(s)

- Chemical Name
- CAS-RN
- InChIKey
- DSSTox Substance ID
- Exact Molecular Formula ?

Enter Identifiers to Search

Display All Chemicals
Download Chemical Data

A user can search based on a list of CAS Numbers, Chemical Names, InChIKeys, DSSTox Substance Identifiers (DTXIDs) or molecular formulae. Mixed searches, for example a mixture of names and CAS Numbers, is possible by selecting the input type and pasting a list of identifiers into the entry box. The user then selects whether they wish to display the chemicals hit list or whether to download the chemical data (see below for details). Of particular interest to suspect screening and non-targeted analysis is the ability to search many molecular formula(e) at once. Having identified a potential chemical formula of an unknown chemical compound, a user can enter the formula into the box on the right after checking the “Molecular Formula” box. This query searches the Dashboard for each formula entered and returns 1-10 results per formula (identified by the user) rank-ordered by the number of data sources. Results can be displayed or downloaded. When downloading results, the user selects data to be included in the download file (below). This enables the user to return the most likely candidate chemicals for a long list of unknown chemicals with associated identifiers, structures, and chemical properties.

Batch Search

Please enter one identifier per line ✕

Select Input Type(s)

Chemical Name

CAS-RN

InChIKey

DSSTox Substance ID

Exact Molecular Formula ?

Include top ▼

hits in download

Enter Identifiers to Search

C15H10F6O2
 C14H14O2
 C18H20O2
 C14H11C12NO2
 C7H4C1NO2
 C10H13NO2
 C18H25NO
 C32H41NO2
 C8H9NO2

Display All Chemicals
Download Chemical Data

Select Output Format

Download as... ▼

Customize Results

Select All

Chemical Identifiers

Chemical Name

DTXSID

CAS-RN

InChIKey

IUPAC Name

Metadata

Curation Level Details

Data Sources

Assay Hit Count

NHANES/Predicted Exposure

Include ToxVal Data Availability

Structures

Mol File

SMILES

InChI String

Presence In Lists

CHEMINV: EPA Chemical Inventory for ToxCast (20170203)

DNT Screening Library

EPA Toxcast Screening Library

Tox21 Screening Library

Intrinsic And Predicted Properties

Molecular Formula

Average Mass

Monoisotopic Mass

OPERA Model Predictions

TEST Model Predictions

Download

Of further interest to the mass spectrometry community is the creation and inclusion of “MS-Ready” structures in the Dashboard. In this manner, an analyst attempting to identify unknowns searches the formula generated from spectra against de-salted, neutral, single component chemicals (“MS-Ready”). As one MS-Ready structure may map to several substances, the download of this file can rapidly expand to large files.

Data Downloads

Various types of data contained within the database can be downloaded via the Downloads Page listed in the website footer or via [this URL](#).

Downloads

[DSSTox Identifier to PubChem Identifier Mapping File](#) Posted: 11/14/2016
The DSSTox to PubChem Identifiers mapping file is in TXT format and includes the PubChem SID, PubChem CID and DSSTox substance identifier (DTXSID).

[DSSTox identifiers mapped to CAS Numbers and Names File](#) Posted: 11/14/2016
The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

[DSSTox MS Ready Mapping File](#) Posted: 11/14/2016
The CompTox Chemistry Dashboard can be used by mass spectrometrists for the purpose of structure identification. A normal formula search would search the exact formula associated with any chemical, whether it include solvents of hydration, salts or multiple components. However, mass spectrometry detects ionized chemical structures and molecular formulae searches should be based on desalted, and desolvated structures with stereochemistry removed. We refer to these as "MS ready structures" and the MS-ready mappings are delivered as Excel Spreadsheets containing the Preferred Name, CAS-RN, DTXSID, Formula, Formula of the MS-ready structure and associated masses, SMILES and InChI Strings/Keys.

Future Work

Future versions of the CompTox Dashboard will include addition of the following functionality:

- Structure, substructure and similarity searching
- Additional visualization widgets for displaying search results
- Real-time prediction of properties
- Categorization of chemicals using various forms of tagging and ontology-based classifications