



Cheminformatics Analysis Modules

NAMs Training Workshop

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Purpose of the Cheminformatics Modules

- PoCs are research software builds to **prove approaches** before moving into production software environments
- Assemble data, develop data model(s), **test** user interface **approaches**, work with test user base to **garner feedback**
- PoCs are internal access data refreshes and application updates can be more frequent

Accessing the Cheminformatics Analysis Modules

- <https://www.epa.gov/comptox-tools/cheminformatics>

Cheminformatics Modules
version: DEV, build: 2023-03-09 06:08:29 UTC

HAZARD ALERTS PREDICT 1.0 PREDICT 2.0 SEARCH STANDARDIZE TOXPRINTS

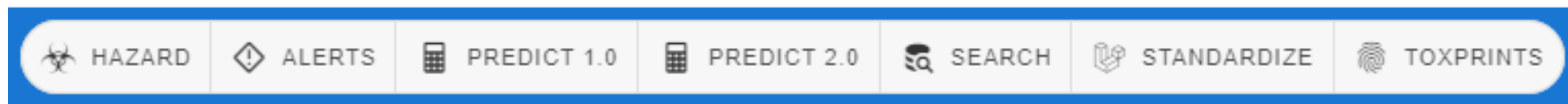
Full

Chemicals: 3
Toxicity: **VH** - Very High **H** - High **M** - Medium **L** - Low **I** - Inconclusive **N/A** - Not Applicable Authority: **Authoritative** Screening QSAR Model

CAS Name	Human Health Effects															Ecotoxicity		Fate		
	Acute Mammalian Toxicity			Carcinogenicity	Genotoxicity/Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity		Systemic Toxicity		Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
	Oral	Inhalation	Dermal						Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure								
626-38-0 ^{GBT} 2-Pentanyl acetate	L	I	L	I	L	L	I	H			M	M	H	M	H	L	L	M	L	M
625-16-1 2-Methylbutan-2-...	L				L	L		H								M			L	

Purpose of the Cheminformatics Modules

- The Cheminformatics Modules includes:
 - Hazard Comparison
 - Batch QSAR Predictions
 - Structure/Substructure/Similarity Search
 - ToxPrints



- These modules allow for user testing and feedback and provide inspiration for implementation into production systems

Initiated in Cheminformatics Modules

- Structure/substructure/similarity search module

The screenshot displays the Cheminformatics Modules web interface. At the top, a blue navigation bar contains the title "Cheminformatics Modules" and version information "version: DEV, build: 2023-03-09 06:08:29 UTC". To the right of the navigation bar are several menu items: HAZARD, ALERTS, PREDICT 1.0, PREDICT 2.0, SEARCH, STANDARDIZE, and TOXPRINTS, along with a user profile icon.

Below the navigation bar is a search bar with the placeholder text "Search by Name, CAS, SMILES, DTXSID, DTXCID, InChI or InChIKey". To the right of the search bar is a "Fuzzy" checkbox. Below the search bar is a toolbar with various icons for file operations and editing.

The main workspace is divided into two sections. On the left is a chemical structure editor showing a benzene ring with two cyano groups (C≡N) and two chlorine atoms (Cl). On the right is a search settings panel. The "Similarity" radio button is selected. The "Min similarity" is set to 0.82, and the "Similarity-type" is set to "Tanimoto". There are several checkboxes for search criteria: Stereo, Chiral, Isotopes, Charged, Multicomponent, Radicals, Salts, Polymers, and Sgroups. There are also input fields for "Elements must be included" and "Elements must be excluded", both containing "e.g. C,F,H". At the bottom of the settings panel are dropdown menus for "Minimum toxicity" and "Minimum authority".

Reimplemented in the Dashboard

- A subset of functionality was moved to the Dashboard

The screenshot displays the CompTox Chemicals Dashboard v2.4.1 interface. The main content area shows the chemical structure of Chlorothalonil, a hexachlorocyclohexadiene derivative with two cyano groups. The search bar at the top left contains the text "Chlorothalonil". To the right of the search bar, there is a "Fuzzy" checkbox and a "Search Type" dropdown menu. Below the search bar, there are two tabs: "Substructure" and "Similarity". The "Substructure" tab is active, showing fields for "Elements must be included:" and "Elements must be excluded:", both containing the text "e.g. C,F,H". There is also a checkbox for "Toxval Data Only" and a "Search" button. The dashboard includes a navigation menu at the top with "Home", "Search", "Lists", "About", and "Tools". The footer of the dashboard displays the chemical name "Chlorothalonil", the CAS number "1897-45-6", and the DTXSID "DTXSID0020319".

Not all PoCs are Public: Work-In-Progress

- Safety Module

version: , build: HAZARD SAFETY ALERTS PREDICT 1.0 PREDICT 2.0 SEARCH STANDARDIZE TOXPRINTS

Search chemical by Name, CASRN or DTXSID Show Structure Full

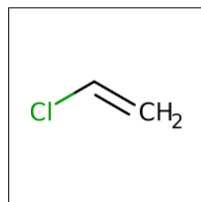
Chemical	Safety	Properties	Signal	Explosive	Flammable	Oxidizers	Compressed Gas	Corrosive	Acute Toxicity	Irritant	Health Hazard	Env. Hazard	NFPA 704	Fire Fighting	Accidental Release Measures	Handling and Storage	Stability and Reactivity	Transport Information	Regulatory Information	Other Safety Information	RQ Category	RQ in pounds (kilograms)
<small>AIGBT</small> 71-43-2 Benzene			Danger																		A	10 (4.54)
<small>AIGBT</small> 75-01-4 Vinyl chloride			Danger																			
<small>GBT</small> 25265-71-8 Dipropylene glycol																						
<small>AIGBT</small> 57-55-6 1,2-Propylene glycol																						
<small>GBTM</small> 111-46-6 Diethylene glycol			Danger																			
<small>AIGBT</small> 111-76-2 2-Butoxyethanol			Danger																			
<small>GBTM</small> 115-11-7 Isobutene			Danger																			
<small>GBTM</small> 141-32-2 Butyl acrylate			Danger																			
<small>GBT</small> 1322-13-0 Ethylhexyl acrylate																						

The Cheminformatics Modules is a set of prototype modules which are using a compilation of information sourced from many sites, databases and sources including U.S. Federal and state sources and international bodies that saves the user time by providing information in one location. The data are not reviewed by USEPA – the user must apply judgment in use of the information. The results do not indicate EPA's position on the use or regulation of these chemicals.

Not all PoCs are Public: Work-In-Progress

- Analytical Methods and Open Spectral Database

78 Results for "vinyl chloride"



(Preferred) Name: Vinyl chloride
DTXSID: [DTXSID8021434](#)
CASRN: 75-01-4
InChIKey: BZHJMEDXYGGRV-UHFFFAOYSA-N
Molecular Formula: C2H3Cl
Mass: 61.99233

[Download Results](#)

Display Single Point Spectra

Include MS-Ready methods

[All Results \(78\)](#) [Methods \(44\)](#) [Spectra \(28\)](#) [Fact Sheets \(6\)](#)

Methodology	Source	Method #	#	Information
GC	USEPA	EPA-TO-17	41	Determination of VOCs residues in air by GC.
GC/ELCD; GC/MS	NEMI	SMC-6200	66	Determination of Organohalides residues in water (ground, waste,
GC/ELCD; GC/PID	NEMI	EPA-502.2	60	Determination of VOCs residues in water (drinking, raw) by GC/EL
GC/FID	OSHA	OSHA-75	1	Determination of Vinyl chloride residues in air by GC/FID with a LC
GC/FID	OSHA	OSHA-4	1	Determination of Vinyl Chloride residues in air by GC/FID with a LC
GC/MS	USEPA	EPA-601	29	Determination of Halocarbons residues in municipal and industrial
GC/MS	USEPA	EPA-624.1	144	Determination of Purgeable organic pollutants residues in water (r
GC/MS	USEPA	EPA-1624B	33	Determination of VOCs residues in water (municipal waste, industr
GC/MS	USEPA	EPA-8260D	179	Determination of VOCs residues in various air sampling trapping n
GC/MS	USEPA	EPA-8261	106	Determination of VOCs residues in water, soil, sediment, sludge, o
GC/MS	Agilent	5994-3834	61	Determination of VOCs residues in water by GC/MS.
GC/MS	Agilent	5991-6539	48	Determination of VOCs residues in water by GC/MS with a LOD of
GC/MS	USGS	5-B12	102	Determination of VOCs residues in water by GC/MS.
GC/MS	USEPA	CTM-028	35	Determination of VOCs residues in stationary source emissions by
GC/MS	NEMI	USGS-0-3115-83	27	Determination of VOCs residues in water by GC/MS with a LOD of

Volatile Organic Compounds in Water by Purge and Trap Capillary Column Gas Chromatography with Photoionization and Electrolytic Conductivity Detectors in Series

Author: USEPA

Focus/Analyte: VOCs

Limitation: LOD of 0.01-2.2ppb

Synopsis: Determination of VOCs residues in water (drinking, raw) by GC/ELCD; GC/PID with a LOD of 0.01-2.2ppb.

[PDF Viewer](#)

[Substances \(60\).\(grid\)](#)

[Substances \(60\).\(table\)](#)

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METHOD 502.2 VOLATILE ORGANIC COMPOUNDS IN WATER BY PURGE AND TRAP CAPILLARY COLUMN GAS CHROMATOGRAPHY WITH PHOTOIONIZATION AND ELECTROLYTIC CONDUCTIVITY DETECTORS IN SERIES

Revision 2.1

Edited by J.W. Munch (1995)

Interested in a demo?

- Cheminformatics Modules:

<https://www.epa.gov/comptox-tools/cheminformatics>

- Contact for follow up demo: Antony Williams

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