

Public access to chemistry and toxicity data for 760,000 substances via the EPA CompTox Chemistry Dashboard

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Problem Definition and Goals

Problem: There are many freely available data available online to support computational toxicology in environmental science, but an easy way to access available data across multiple sites is lacking.

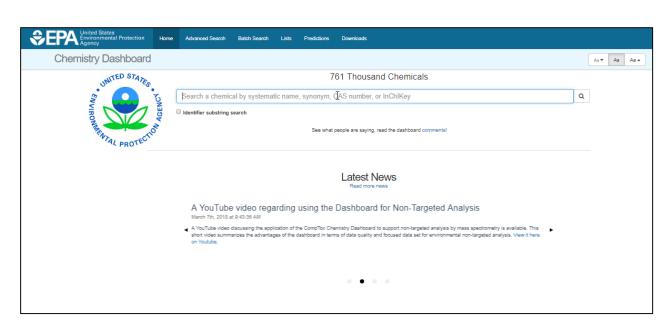
Goals: To deliver online access via a simple to use web-based interface supporting diverse types of data associated with environmental chemistry, and specifically computational toxicology. To make the data available for ~760,000 chemical substances available as downloadable data for reuse and repurposing in other databases.

Abstract

Chemistry Dashboard Comptox The web-based (https://comptox.epa.gov) application providing access to set resources provided by the National Center of Computational Toxicology. Diverse data types include bioassay screening results, physicochemical and toxicological endpoints (both experimental and predicted), and consumer product and functional use data (from the CPDat database)

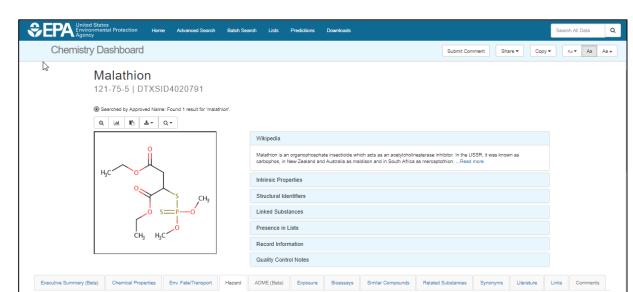
The dashboard is an integration hub for ~70 public resources helping the user to navigate to other data and information for a particular chemical on other websites, including Google Scholar and PubMed. A batch search also allows users to search using inputs of thousands of chemical names or CAS Registry Numbers and download details regarding the availability of bioassay, exposure and toxicity data.

The CompTox Chemistry Dashboard



Dashboard Entry Page

Where possible, links are provided to related Wikipedia articles. A summary report containing record data can be provided as a PDF file.



Registry

page is a

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Chemical Record Page: Malathion

The Hazard tab integrates

toxicity data sourced from

IRIS,

multiple databases

databases

PPRTV

different

from around the world.

SEPA United States Fredictions Downloads Agency Agen													ata
Chemistry Dashboa	ard								Submit Comm	nent Share	Copy▼	Aa▼	Aa Aa
Executive Summary (Beta) Chemical	Properties	Env. Fate/Transport	Hazard	ADME (Beta)	Exposure	Bioassays	Similar Compour	nds Relate	ed Substances	Synonyms	Literature L	inks Con	nments
_													
Exposure Limit	Download ta	ble as: TSV Exce	el		Human Eco								
Lethality Effect Level Point of Departure			Гуре [‡]	Subtype	Risk Assessment Class	Values	Units	Study Type	Exposure Route	Species	Subsource	Source	<u>*</u>
Screening Level	+	8	RfD	-	chronic	0.02	mg/kg-day	-	oral	-	EPA NCEA	IRIS	<u>^</u>
Toxicity Value	+	7	RfC	Subchronic	subchronic	0.02	mg/m3		inhalation	-	ATSDR Final	RAIS	ш
	+	7	RfC	Short-term	short-term	0.02	mg/m3	-	inhalation	-	ATSDR Final	RAIS	н
	+	7	RfC	Acute	acute	0.2	mg/m3	-	inhalation	-	ATSDR Final	RAIS	н
	+	7	RfD	Subchronic	subchronic	0.02	mg/kg-day	-	oral	-	ATSDR Final	RAIS	
	+	7	RfD	Short-term	short-term	0.02	mg/kg-day	-	oral	-	ATSDR Final	RAIS	
	+	7	RfD	oral	chronic	0.07	mg/kg-day	-	oral	-	EPA OW D	ACToR	
	+	7	RfD	-	subchronic	0.02	mg/kg-day	-	oral	human	-	HEAST	

The Hazard Tab: Human and Eco Tox

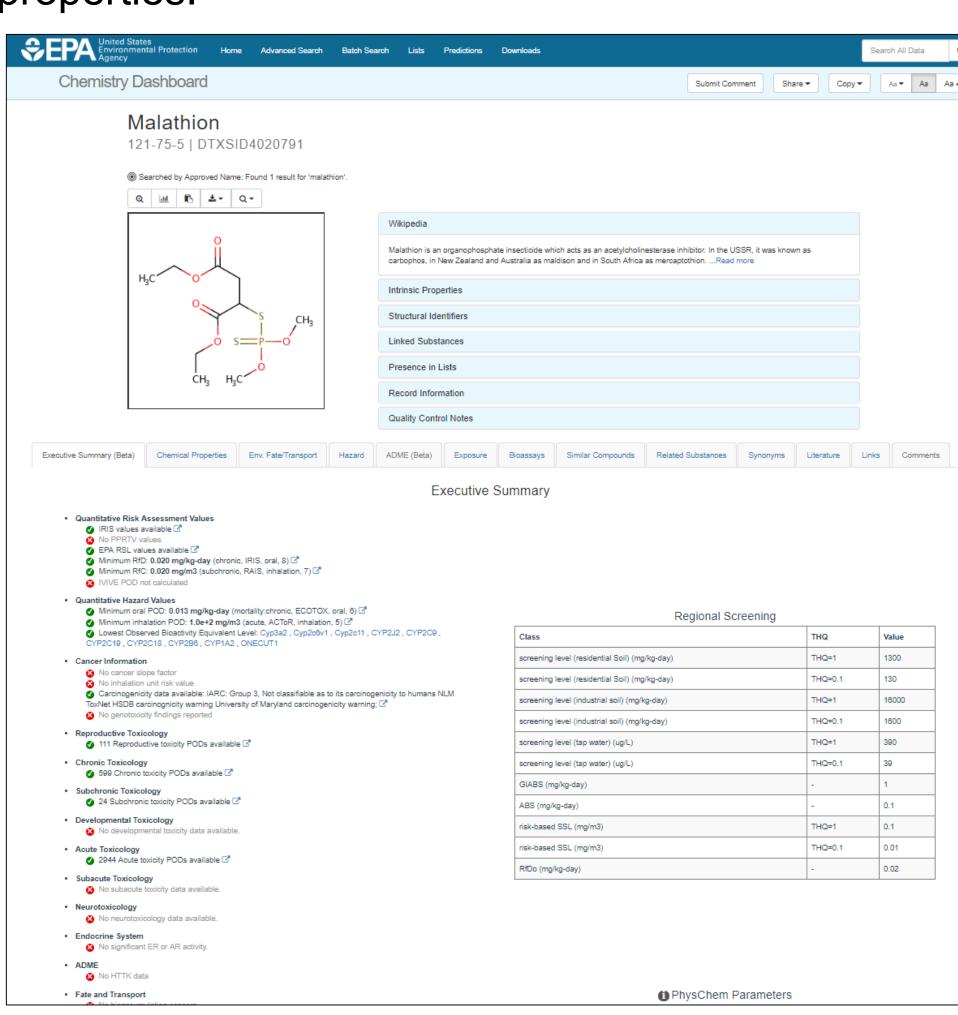
The literature tab provides integration to both PubMed (with ~28 million citations), searching of Google Scholar, display of IRIS and PPRTV reports embedded in the app.

Chemistry Da	ashboard								Subr	nit Comment	Share ▼	Copy ▼ Aa	a ▼ Aa	
							4							
Executive Summary (Beta)	Chemical Properties	Env. Fa	te/Transport	Hazard	ADME (Beta)	Exposure	Bioassays	Similar Compounds	Related Substar	oes Synony	ms Literatu	re Links	Comment	
Google Scholar	1) \$6	lost BubMod s	tarting point	wood thon 2)	click on Retrieve.				Optionally, edit the	augry before ret	riovina			
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IRIS			Pesticide residues in drinking water and associated risk to cons					Mekonen; Argaw; Simanesew; Houbraken; Senaev			Chemosphere			
	= 2	21112834 201	0 Effects of o	thronic dietary	exposure to a low-	-dose of Malathion	Hackenb	Hackenberger; Jarić; Hackenberger; Stepić			Acta biologica Hungarica			
	□ 1	19680977 200	9 Exposure t	Exposure to pesticides residues from consumption of Italian blo A probabilistic risk assessment for deployed military personnel				Fallico; D'Urso; Chiappara Schleier, Davis; Barber; Macedo; Peterson			Food additives & contaminants, Part A, Chemistry, Journal of medical entomology			
	□ 1	19496443 200	9 A probabili											
	□ 1	19228383 200	9 Determina	ion of no-obse	erved effect level (N	NOEL)-biomarker e	q Valcke; E	Valcke; Bouchard			Environmental health: a global access science sour			
	□ 2	20021041 200	6 Stimulator	effects of ma	alathion on the key	enzymes activities	o Panahi;	Panahi; Vosough-Ghanbari; Pournourmohammadi;			Toxicology mechanisms and methods			
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The Literature Tab: PubMed integration

Executive Summary of Toxicity Data

The toxicity data for a chemical is summarized in a single "Executive Summary" page listing quantitative risk assessment values, quantitative hazard values, physiochemical and environmental fate and transport properties.



Acknowledgements

The author acknowledges NCCT colleagues, especially the NCCT dashboard development team for all of their hard work. Also thanks to colleagues in NERL and NRMRL for their contributions regarding the CPDat product database and toxicity predictions.