

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.

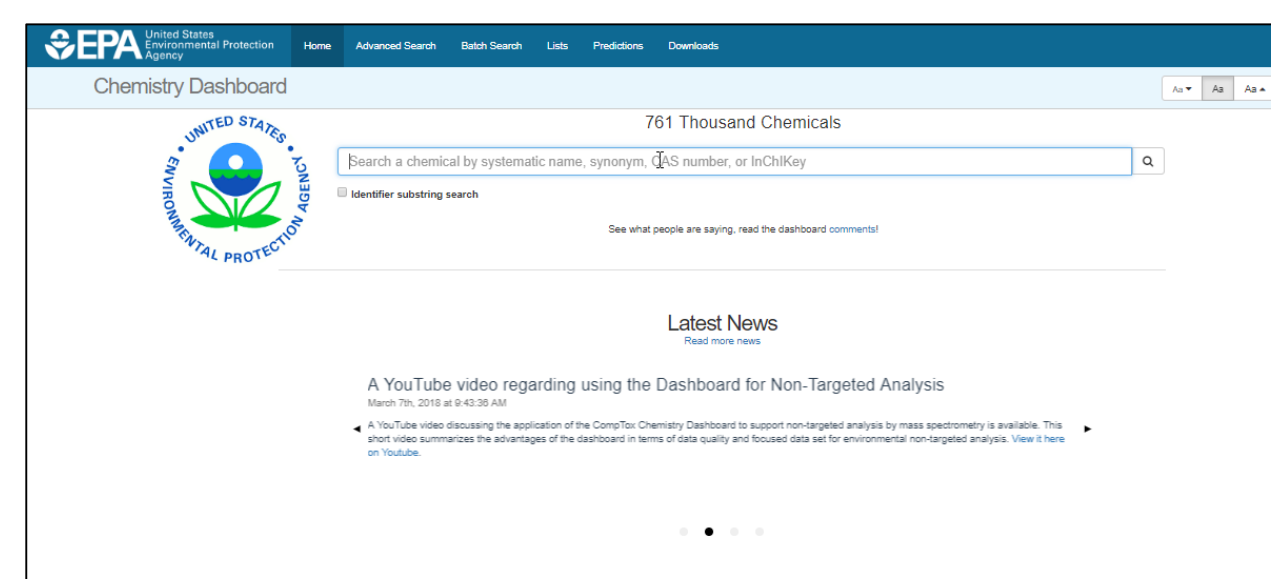
Goals: To deliver online access via a simple to use web-based interface supporting diverse types of data associated with environmental chemistry, and specifically computational toxicology. To make the data available for ~760,000 chemical substances available as downloadable data for reuse and repurposing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

Abstract

The EPA Comptox Chemistry Dashboard (<https://comptox.epa.gov>) is a web-based application providing access to a set of data 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.

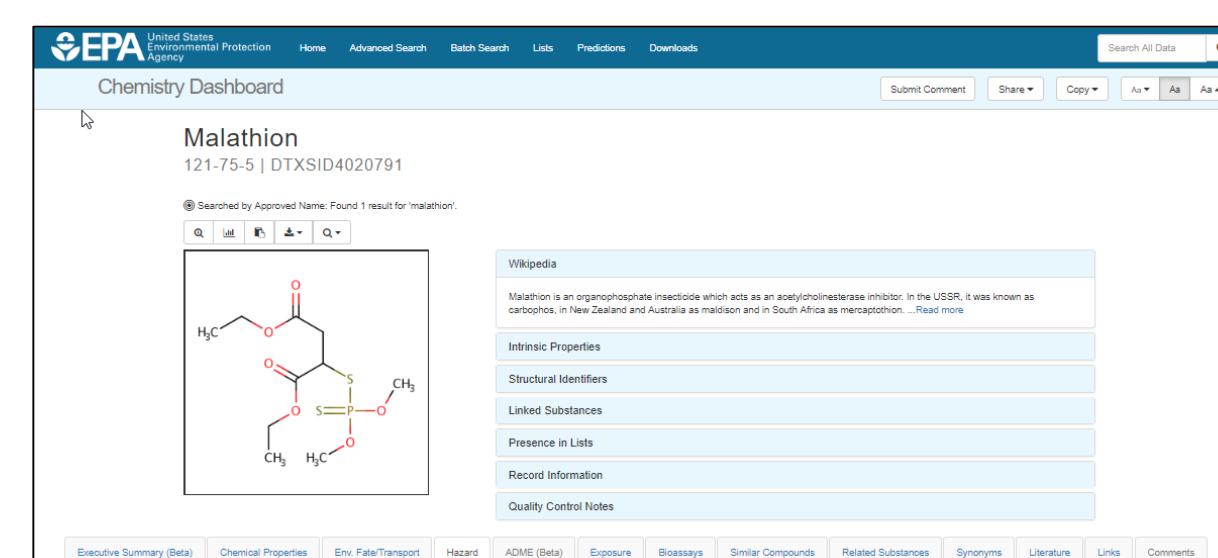
The CompTox Chemistry Dashboard



Dashboard Entry Page

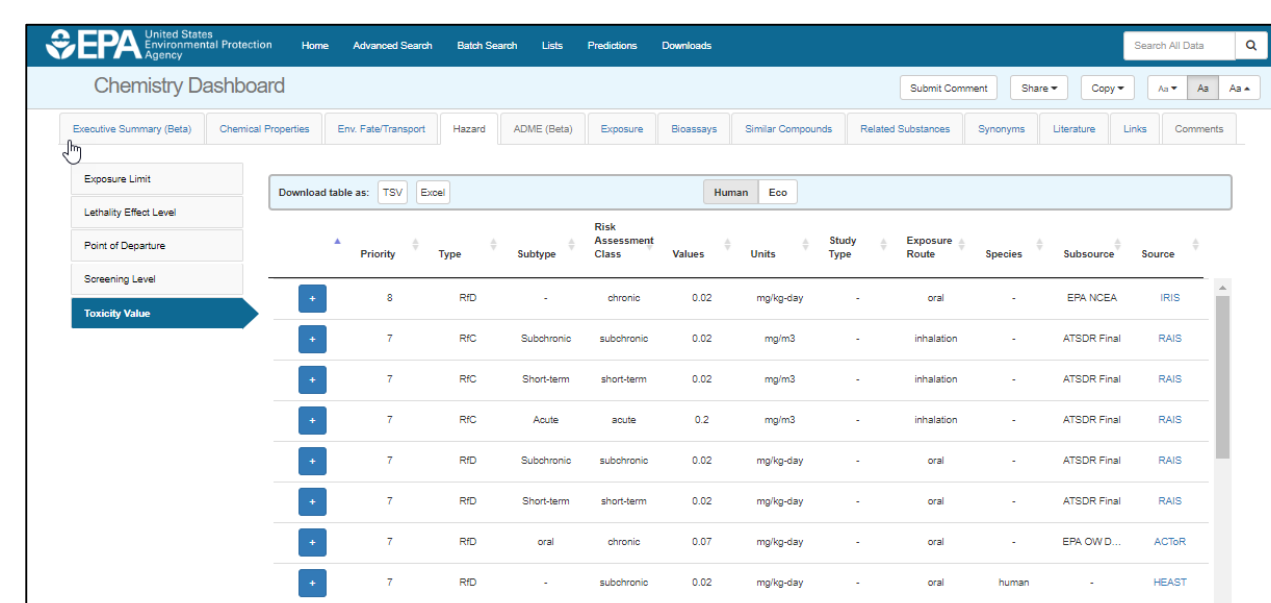
The home page is a simple text entry box allowing a type-ahead search for systematic, trade and trivial names, CAS Registry Numbers and InChIs.

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



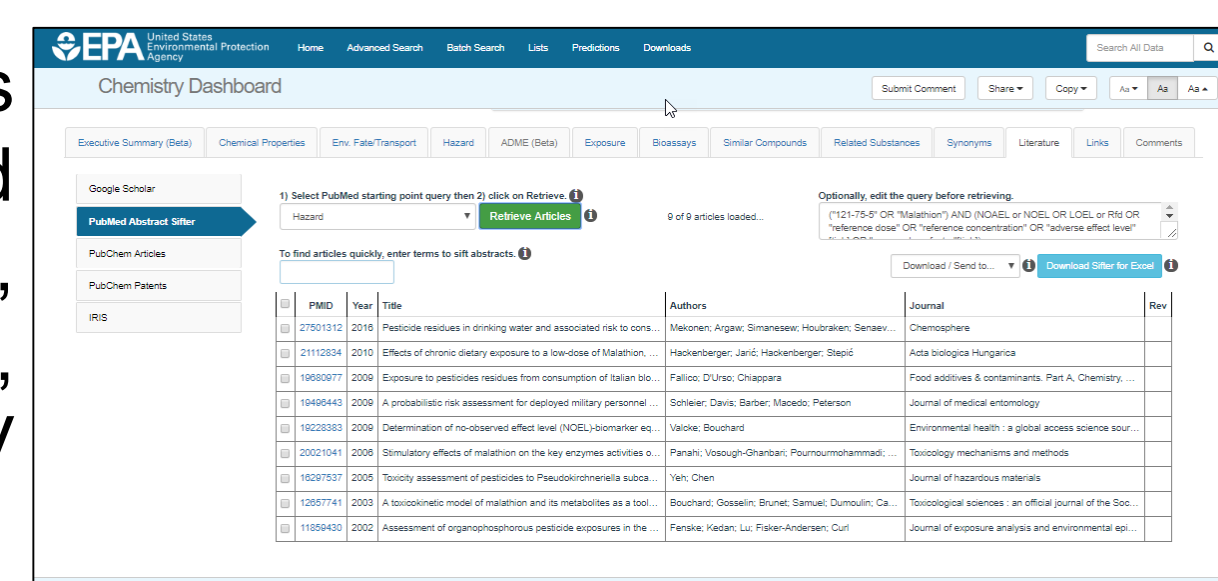
Chemical Record Page: Malathion

The Hazard tab integrates toxicity data sourced from 18 different databases including IRIS, PPRTV and multiple databases from around the world.



The Hazard Tab: Human and Eco Tox

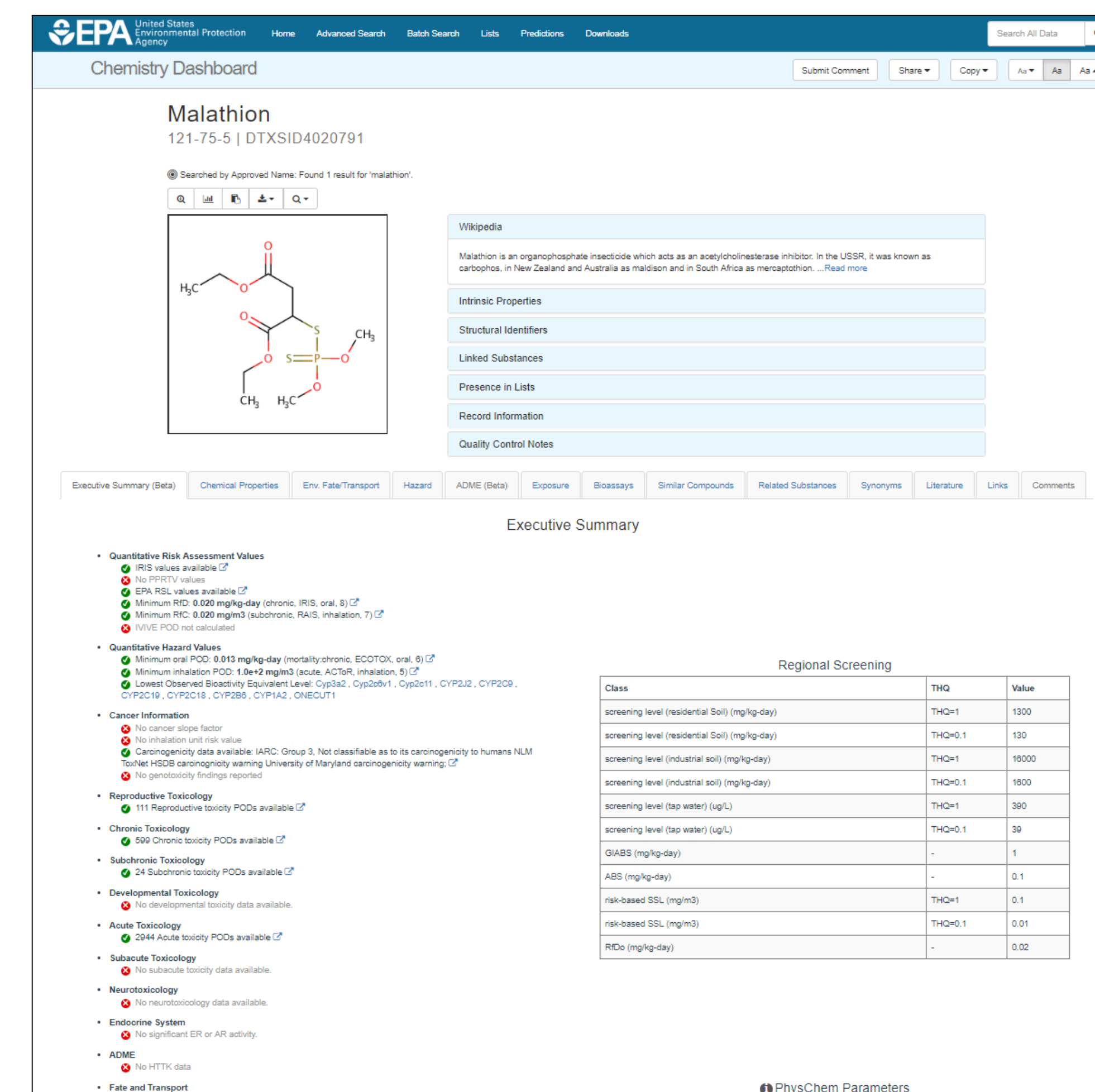
The literature tab provides integration to both PubMed (with ~28 million citations), searching of Google Scholar, display of IRIS and PPRTV reports embedded in the app.



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, physicochemical and environmental fate and transport properties.



Executive Summary

- Quantitative Risk Assessment Values**
 - IRIS values available ☑
 - PPRTV values available ☑
 - EPA RSL values available ☑
 - Minimum RfD: 0.020 mg/kg-day (chronic, IRIS, oral, 8) ☑
 - Minimum RfD: 0.020 mg/kg/day (subchronic, RAIS, inhalation, 7) ☑
 - WVVE POD not calculated
- Quantitative Hazard Values**
 - Minimum oral POD: 0.013 mg/kg-day (mortality chronic, ECOTOX, oral, 8) ☑
 - Minimum inhalation POD: 1.0e-2 mg/m3 (acute, ACTO, inhalation, 5) ☑
 - Lowest Observed Bioactivity Equivalent Level: Cys3a2, Cys3b1, Cys2a11, CYP2B1, CYP2C8, CYP2C19, CYP2C18, CYP2B6, CYP1A2, ONECUT1
- Cancer Information**
 - No general slope factor
 - No inhalation unit risk value
 - Carcinogenicity data available (ARC, Group 3, not classifiable as to its carcinogenicity to humans NLM Toxicol) (HCSB carcinogenicity warning University of Maryland carcinogenicity warning) ☑
 - No genotoxicity findings reported
- Reproductive Toxicology**
 - 111 Reproductive toxicity PODs available ☑
- Chronic Toxicology**
 - 209 Chronic toxicity PODs available ☑
- Subchronic Toxicology**
 - 24 Subchronic toxicity PODs available ☑
- Developmental Toxicology**
 - No developmental toxicity data available.
- Acute Toxicology**
 - 2044 Acute toxicity PODs available ☑
- Subacute Toxicology**
 - No subacute toxicity data available.
- Neurotoxicology**
 - No neurotoxicology data available.
- Endocrine System**
 - No significant ER or AR activity.
- ADME**
 - No HTTK data
- Fate and Transport**

Regional Screening

Class	THQ	Value
screening level (residential soil) (mg/kg-day)	THQ=1	1300
screening level (residential soil) (mg/kg-day)	THQ=0.1	130
screening level (industrial soil) (mg/kg-day)	THQ=1	10000
screening level (industrial soil) (mg/kg-day)	THQ=0.1	1000
screening level (tap water) (ug/L)	THQ=1	300
screening level (tap water) (ug/L)	THQ=0.1	30
GIABS (mg/kg-day)	-	1
ABS (mg/kg-day)	-	0.1
risk-based SSL (mg/m3)	-	0.1
risk-based SSL (mg/m3)	THQ=0.1	0.01
RfDs (mg/kg-day)	-	0.02

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.