

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

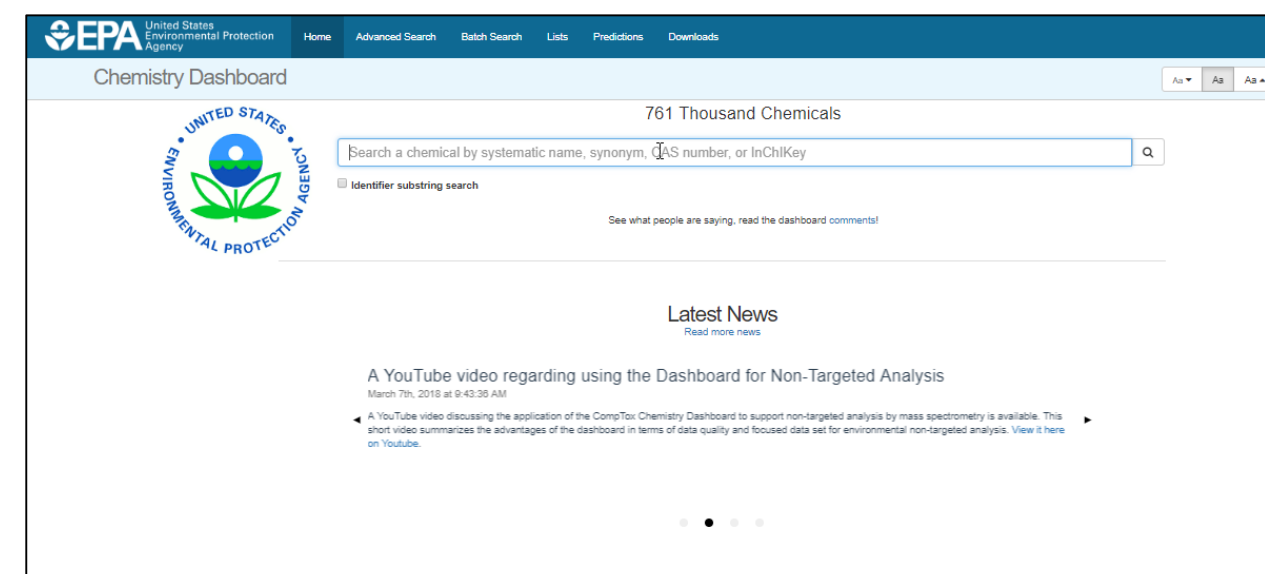
Problem: There are many freely available data available online to support computational toxicology in environmental science, but an easy way to access available data across multiple sites is lacking.

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

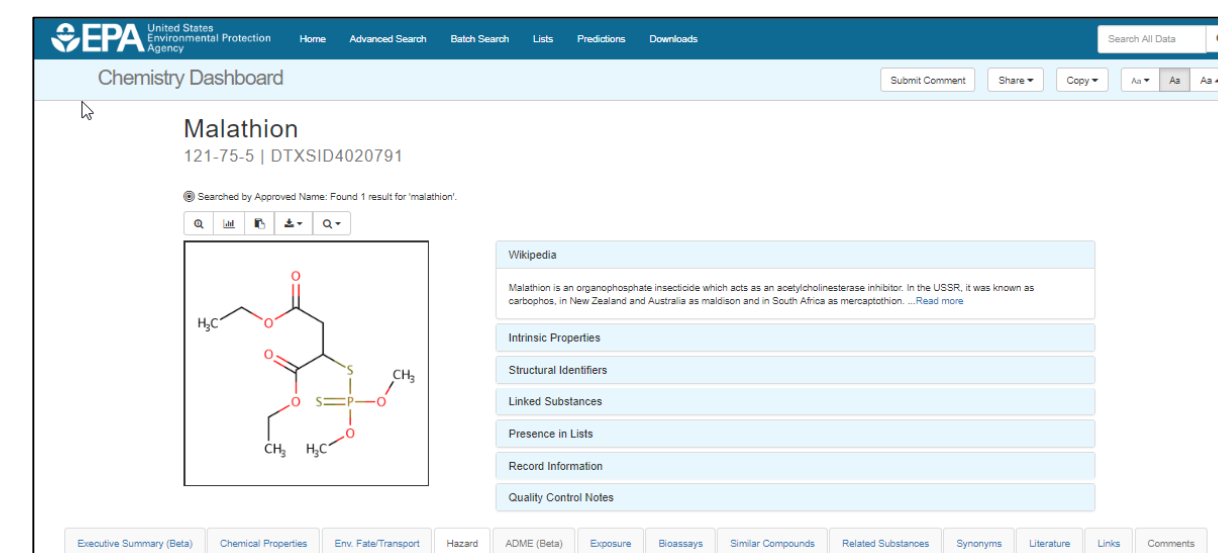
The EPA Comptox Chemistry Dashboard is a web-based application providing access to a set of data resources provided by the National Center of Computational Toxicology. Diverse data types include bioassay screening results, physicochemical and toxicological endpoints (both experimental and predicted), 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

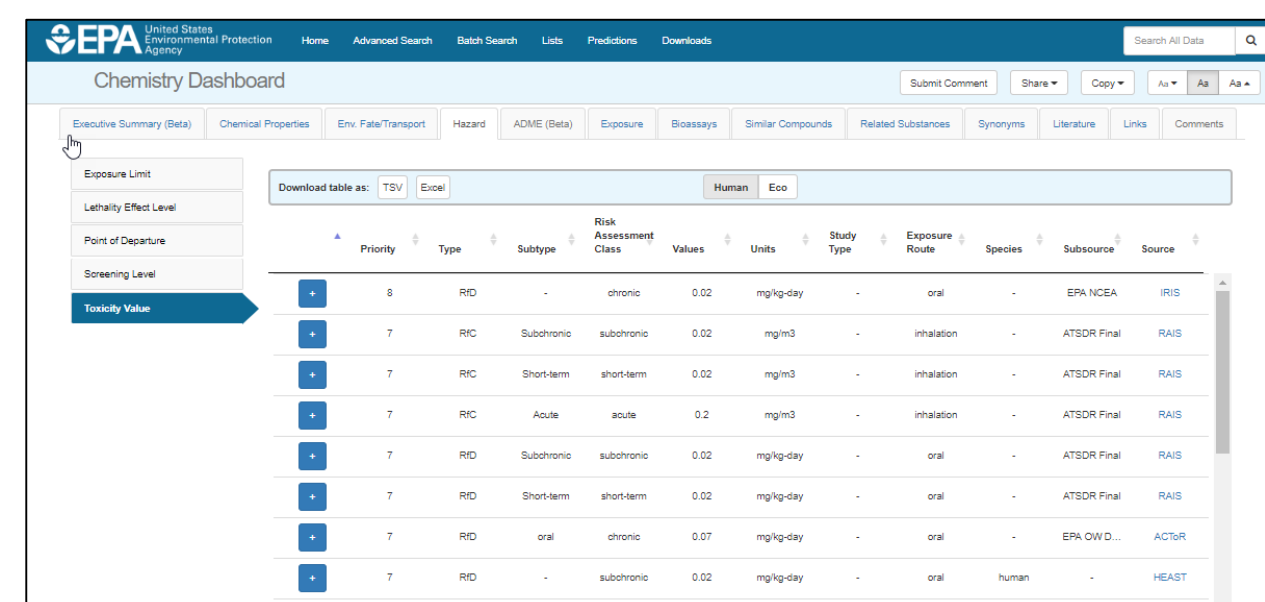


Dashboard Entry Page

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

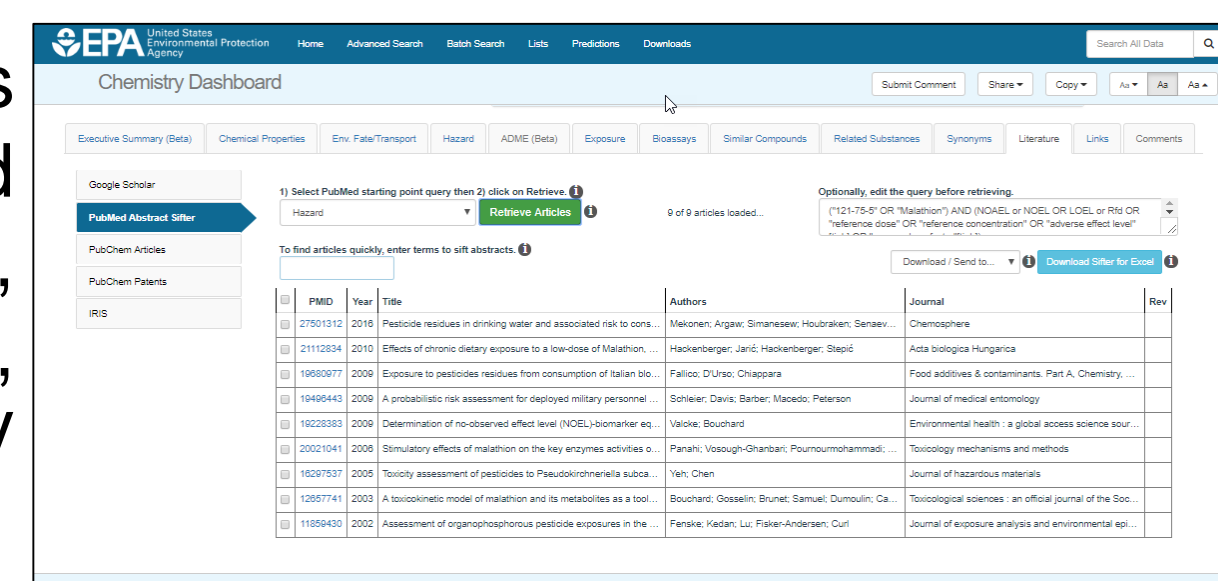


Chemical Record Page: Malathion



The Hazard Tab: Human and Eco Tox

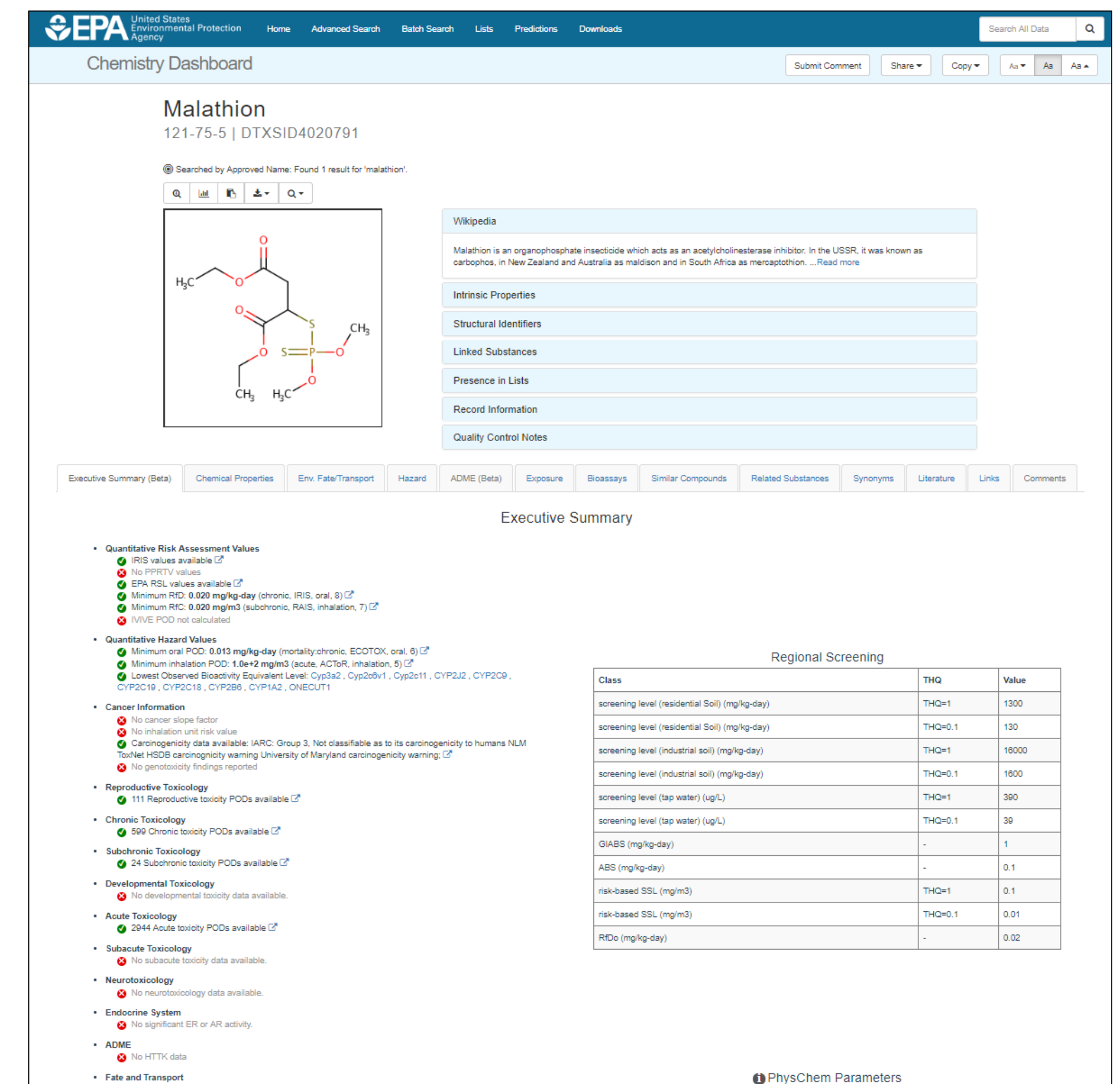
The literature tab provides integration to both PubMed (with ~28 million citations), searching of Google Scholar, display of IRIS and PPRTV reports embedded in the app.



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, physiochemical and environmental fate and transport properties.



Acknowledgements

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