

# Public access to chemistry and toxicity data for 760,000 substances via the EPA CompTox Chemistry Dashboard Antony Williams, Chris Grulke, Jeremy Dunne, Nancy Baker, Richard Judson and Jeff Edwards

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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 webbased 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)

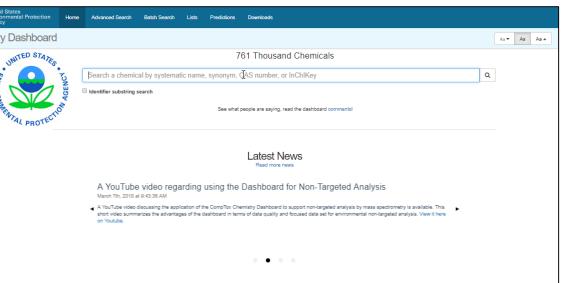
The dashboard is an integration hub for ~70 public resources helping the user to navigate to other data and information for a particular chemical on other websites, including Google Scholar and PubMed. A batch search also allows users to search using inputs of thousands of chemical names or CAS Registry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

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



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 CompTox Chemistry Dashboard



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

# **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.

#### **Dashboard Entry Page**

| SEPA United States<br>Environmental Protection Home Advanced Search E                                | tich Search Lists Predictions Downloads  | Search All Data Q |
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| Chemistry Dashboard  | Submit Comment Share  Copy   | / • Aa • Aa •     |
| Malathion<br>121-75-5   DTXSID4020791<br>@ Searched by Approved Name: Found 1 result for 'malathion' |  |                   |
| Q IM B ±- Q-   |  |                   |
|  | Wikipedia  |                   |
|  | Malathion is an organophosphate insecticide which acts as an acetylcholinesterase inhibitor. In the USSR, it was known as<br>carbophos, in New Zealand and Australia as maldison and in South Africa as mercaptothionRead more |                   |
| H <sub>3</sub> C O   | Intrinsic Properties   |                   |
| S CH3  | Structural Identifiers   |                   |
| o s=p-o  | Linked Substances  |                   |
| CH <sub>2</sub> H <sub>2</sub> C   | Presence in Lists  |                   |
|  | Record Information   |                   |
|  | Quality Control Notes  |                   |
| Executive Summary (Beta) Chemical Properties Env. Fate/Transport H                                   | tard ADME (Beta) Exposure Bioassays Similar Compounds Related Substances Synonyms Literature   | Links Comments    |

#### **Chemical Record Page: Malathion**

including IRIS,

18

The Hazard tab integrates

toxicity data sourced from

and multiple databases

from around the world.

different databases

PPRTV

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|                        |                      | +          | 7                   | RfC       | Acute       | acute                       | 0.2       | mg/m3            | -               | inhalation        | -        | ATSDR Final  | RAIS            |      |
|                        |                      | +          | 7                   | RfD       | Subchronic  | subchronic                  | 0.02      | mg/kg-day        |                 | oral              | -        | ATSDR Final  | RAIS            | ١.   |
|                        |                      | +          | 7                   | RfD       | Short-term  | short-term                  | 0.02      | mg/kg-day        | -               | oral              |          | ATSDR Final  | RAIS            |      |
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The Hazard Tab: Human and Eco Tox

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| IRIS                         |                | PMID          | Year     | Title<br>Pesticide residues in drinking water and associated r |                  | ithors<br>ekonen; Argaw; Simanesew; Ho | ubrakan: Sanaay      | Journal                  |  | Rev       |
|                              |                | 21112834      | -        | Effects of chronic dietary exposure to a low-dose of I         |                  | ckenberger; Jarić; Hackenberg          |                      | Acta biologica Hungar    | rica   |           |
|                              |                |               | -        | Exposure to pesticides residues from consumption o             |                  | llico; D'Urso; Chiappara               |                      |                          | aminants. Part A, Chemistry,                               |           |
|                              |                | 19496443      | 2009     | A probabilistic risk assessment for deployed military          | personnel Sch    | hleier; Davis; Barber; Macedo; I       | Peterson             | Journal of medical ent   | tomology   |           |
|                              |                | 19228383      | 2009     | Determination of no-observed effect level (NOEL)-bio           | omarker eq Val   | loke; Bouchard                         |                      | Environmental health     | : a global access science sou                              | ır        |
|                              |                | 20021041      | 2006     | Stimulatory effects of malathion on the key enzymes            | activities o Par | nahi; Vosough-Ghanbari; Pourr          | ourmohammadi;        | Toxicology mechanism     | ns and methods   |           |
|                              |                | 16297537      | 2005     | Toxicity assessment of pesticides to Pseudokirchneri           | ella subca Yeł   | h; Chen                                |                      | Journal of hazardous     | materials  |           |
|                              |                | 12657741      | 2003     | A toxicokinetic model of malathion and its metabolite          | s as a tool Bo   | uchard; Gosselin; Brunet; Sami         | uel; Dumoulin; Ca    | Toxicological sciences   | s : an official journal of the So                          | c         |
|                              |                | 11859430      | 2002     | Assessment of organophosphorous pesticide exposu               | ures in the Fer  | nske; Kedan; Lu; Fisker-Anders         | en; Curl             | Journal of exposure a    | nalysis and environmental ep                               | й         |

#### The Literature Tab: PubMed integration

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Innovative Research for a Sustainable Future

This presentation does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.





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| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimuu</li> <li>Minimuu</li> <li>IVIVE P</li> <li>Quantitative I</li> <li>Minimuu</li> <li>IVIVE P</li> <li>Quantitative I</li> <li>Minimuu</li> <li>Minimuu</li> <li>Lowest</li> <li>CYP2C19</li> <li>Cancer Inform</li> <li>No cant</li> <li>No cant</li> <li>Carcino</li> <li>ToxNet HS0</li> <li>Carcino</li> <li>ToxNet HS0</li> <li>No geni</li> <li>Reproductive</li> <li>111 Rep</li> <li>Chronic Toxic</li> </ul>   | alues available 🛃<br>RTV values<br>SL values available 🖾<br>Im RfD: 0.020 mg/kg-day (chror<br>m RfC: 0.020 mg/kg-day (chror<br>POD not calculated<br>Hazard Values<br>Im oral POD: 0.013 mg/kg-day (<br>Im inhalation POD: 1.0e+2 mg/m<br>I Observed Bioactivity Equivalen<br>, CYP2C18, CYP286, CYP1A2<br>mation<br>Incer slope factor<br>alation unit risk value<br>ogenicity data available: IARC: O<br>IDB carcinognicity warning Univer-<br>totoxicity findings reported<br>e Toxicology<br>productive toxicity PODs available<br>cology   | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (acute, ACTOR, inhalati<br>nt Level: Cyp3a2 , Cyp2c8v<br>2 , ONECUT1<br>Group 3, Not classifiable as<br>ersity of Maryland carcinoge<br>ble  | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | И          | screening I<br>screening I<br>screening I<br>screening I   | level (residential Soil) (mg<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k  | y/kg-day)<br>y/kg-day)<br>kg-day)                     | reening  | THQ=1           THQ=0.1           THQ=1           THQ=1           THQ=0.1   | ·<br>·<br>·  | 1300<br>130<br>16000<br>1600  | -   |
| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimuu</li> <li>Minimuu</li> <li>IVIVE P</li> <li>Quantitative I</li> <li>Minimuu</li> <li>Minimuu</li> <li>Minimuu</li> <li>Minimuu</li> <li>Minimuu</li> <li>Lowest</li> <li>CYP2C19</li> <li>Cancer Inform</li> <li>No cance</li> <li>No geni</li> <li>Reproductive</li> <li>111 Rep</li> <li>Chronic Toxic</li> <li>599 Christian</li> <li>Subchronic T</li> </ul>   | alues available [2]<br>RTV values<br>SL values available [2]<br>Im RfC: 0.020 mg/kg-day (chror<br>mRfC: 0.020 mg/kg-day (chror<br>POD not calculated<br>Hazard Values<br>Im oral POD: 0.013 mg/kg-day (<br>Im inhalation POD: 1.0e+2 mg/m<br>t Observed Bioactivity Equivalen<br>, CYP2C18, CYP286, CYP1A2<br>mation<br>Noer slope factor<br>alation unit risk value<br>logenicity data available: IARC: 0<br>IDB carcinognicity warning Univer-<br>totoxicity findings reported<br>e Toxicology<br>productive toxicity PODs available<br>[2]<br>Toxicology   | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (acute, ACTOR, inhalati<br>nt Level: Cyp3a2 , Cyp2c6v<br>2 , ONECUT1<br>Group 3, Not classifiable as<br>ersity of Maryland carcinogo<br>ble C  | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | и          | screening I<br>screening I<br>screening I<br>screening I   | level (residential Soil) (mg<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k<br>level (tap water) (ug/L)<br>level (tap water) (ug/L)  | y/kg-day)<br>y/kg-day)<br>kg-day)                     | reening  | THQ=1<br>THQ=0.1<br>THQ=1<br>THQ=1<br>THQ=1<br>THQ=1  | ·<br>·<br>·<br>·<br>·  | 1300<br>130<br>18000<br>1800<br>390   |     |
| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimur</li> <li>Minimur</li> <li>I/V/V F</li> <li>Quantitative F</li> <li>Minimur</li> <li>I/V/V F</li> <li>Quantitative F</li> <li>Minimur</li> <li>Minimur</li> <li>Lowest<br/>CYP2C19,</li> <li>Cancer Inform</li> <li>No cance</li> <li>No inha</li> <li>Carcino<br/>Tox/Net HSI</li> <li>No genutive</li> <li>Chronic Toxic</li> <li>\$ 599 Chritication</li> <li>Subchronic T</li> <li>\$ 24 Subchronic T</li> </ul>   | alues available<br>RTV values<br>RTV values<br>SL values available<br>m RfD: 0.020 mg/kg-day (chror<br>m RfC: 0.020 mg/m3 (subchron<br>POD not calculated<br>Hazard Values<br>im inhalation POD: 1.0e+2 mg/m<br>t Observed Bioactivity Equivalen<br>, CYP2C18, CYP2B6, CYP1A2<br>mation<br>toor slope factor<br>alation unit risk value<br>ogenicity data available: IARC: CI<br>DB carcinognicity warning Unive<br>totoxicity findings reported<br>a Toxicology<br>productive toxicity PODs available<br>Toxicology<br>cohronic toxicity PODs available [20]   | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (acute, ACTOR, inhalati<br>nt Level: Cyp3a2 , Cyp2c6v<br>2 , ONECUT1<br>Group 3, Not classifiable as<br>ersity of Maryland carcinogo<br>ble C  | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | И          | screening I<br>screening I<br>screening I<br>screening I<br>screening I  | level (residential Soil) (mg/k<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k<br>level (tap water) (ug/L)<br>level (tap water) (ug/L)<br>g/kg-day)   | y/kg-day)<br>y/kg-day)<br>kg-day)                     | reening  | THQ=1<br>THQ=0.1<br>THQ=1<br>THQ=1<br>THQ=1<br>THQ=1  | ·<br>·<br>·<br>·<br>·<br>·<br>·<br>·   | 1300<br>130<br>18000<br>1800<br>390<br>39                                   | -   |
| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimur</li> <li>Minimur</li> <li>I/V/VE P</li> <li>Quantitative F</li> <li>Minimur</li> <li>I/V/VE P</li> <li>Quantitative F</li> <li>Minimur</li> <li>Minimur</li> <li>Lowest<br/>CYP2C19,</li> <li>Cancer Inform</li> <li>No cance</li> <li>No can</li></ul>     | alues available<br>RTV values<br>RTV values<br>SL values available<br>m RfD: 0.020 mg/kg-day (chror<br>m RfC: 0.020 mg/m3 (subchron<br>POD not calculated<br>Hazard Values<br>im inhalation POD: 1.0e+2 mg/m<br>t Observed Bioactivity Equivalen<br>, CYP2C18, CYP2B6, CYP1A2<br>mation<br>toor slope factor<br>alation unit risk value<br>ogenicity data available: IARC: CI<br>DB carcinognicity warning Unive<br>totoxicity findings reported<br>a Toxicology<br>productive toxicity PODs available<br>Toxicology<br>cohronic toxicity PODs available [20]   | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (aoute, ACTOR, inhalation<br>tt Level: Cyp3a2, Cyp2c8v<br>2, ONECUT1<br>Group 3, Not classifiable as<br>ersity of Maryland carcinogo<br>ble  | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | и          | screening I<br>screening I<br>screening I<br>screening I<br>screening I<br>GIABS (mg/k                             | level (residential Soil) (mg/k<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k<br>level (tap water) (ug/L)<br>level (tap water) (ug/L)<br>g/kg-day)   | y/kg-day)<br>y/kg-day)<br>kg-day)                     | reening  | THQ=1<br>THQ=0.1<br>THQ=1<br>THQ=1<br>THQ=1<br>THQ=1  | ۰<br>۰<br>۰<br>۰<br>۰<br>۰   | 1300<br>130<br>16000<br>1800<br>390<br>39<br>1                              |     |
| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimur</li> <li>Minimur</li> <li>I/V/V F</li> <li>Quantitative F</li> <li>Minimur</li> <li>I/V/V F</li> <li>Quantitative F</li> <li>Minimur</li> <li>Minimur</li> <li>Minimur</li> <li>Lowest</li> <li>CYP2C19</li> <li>Cancer Inform</li> <li>No cance</li> <li>No inha</li> <li>Carcino</li> <li>Tox/Net HSI</li> <li>No genutian</li> <li>Reproductive</li> <li>111 Rep</li> <li>Chronic Toxic</li> <li>599 Christian</li> <li>Subchronic T</li> <li>24 Subcitien</li> <li>No devitien</li> <li>No devitien</li> <li>No devitien</li> <li>Acute Toxicol</li> </ul>  | alues available [2]<br>RTV values<br>RTV values available [2]<br>Im RfD: 0.020 mg/kg-day (chror<br>m RfC: 0.020 mg/m3 (subchron<br>POD not calculated<br>Hazard Values<br>Im oral POD: 0.013 mg/kg-day (<br>Im inhalation POD: 1.0e+2 mg/m<br>1: Observed Bioactivity Equivalen<br>1: Observed Bioactivity Equivalent<br>1: Observed Bioactivity Equivalent<br>1: Observed Bioactivity PODs available<br>1: Observed Bioactivity PODs available [2]<br>Foxicology<br>revoluctive toxicity PODs available [2]<br>Foxicology<br>revoluctive toxicity PODs available [2]<br>Foxicology<br>revoluctive toxicity PODs available [2]<br>1: Observed Bioactivity Gata available [2]                        | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (aoute, ACTOR, inhalation<br>tt Level: Cyp3a2, Cyp2c8v<br>2, ONECUT1<br>Group 3, Not classifiable as<br>ensity of Maryland carcinogon<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>control to the second seco | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | и          | screening I<br>screening I<br>screening I<br>screening I<br>screening I<br>GIABS (mg/k<br>risk-based               | level (residential Soil) (mg/k<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k<br>level (tap water) (ug/L)<br>level (tap water) (ug/L)<br>g/kg-day)<br>g-day)                               | y/kg-day)<br>y/kg-day)<br>kg-day)                     | reening  | THQ=1           THQ=0.1           THQ=1           THQ=0.1           THQ=0.1           THQ=0.1           THQ=1           THQ=1.1           THQ=0.1           THQ=1.1           THQ=0.1           THQ=1.1           THQ=0.1           THQ=0.1           THQ=0.1   | ۰<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱ | 1300<br>130<br>18000<br>18000<br>380<br>38<br>1<br>0.1<br>0.1<br>0.1<br>0.1 |     |
| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimui</li> <li>Minimui</li> <li>IVIVE P</li> <li>Quantitative I</li> <li>Minimui</li> <li>IVIVE P</li> <li>Quantitative I</li> <li>Minimui</li> <li>Lowest<br/>CYP2C19,</li> <li>Cancer Inform</li> <li>No cancer Inform</li> <li>Subchronic Toxicol</li> <li>2944 Ac</li> <li>Subacute Tox</li> </ul>  | alues available<br>RTV values<br>RTV values<br>SL values available<br>SL values available<br>SL values available<br>SL values available<br>m RfC: 0.020 mg/m3 (subchron<br>POD not calculated<br>Hazard Values<br>Im oral POD: 0.013 mg/kg-day (<br>im inhalation POD: 1.0e+2 mg/m<br>: Observed Bioactivity Equivalen<br>; CYP2C18 ; CYP2B6 ; CYP1A2<br>mation<br>loser slope factor<br>alation unit risk value<br>ogenicity data available: IARC: O<br>iDB carcinognicity warning Univer<br>iotoxicity findings reported<br>a Toxicology<br>productive toxicity PODs available<br>cology<br>inonic toxicity PODs available<br>tal Toxicology<br>relopmental toxicity data available<br>would toxicity PODs available<br>cology<br>would toxicity PODs available<br>inter solution (inter solution)<br>inter solution (inter solution)<br>i | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (aoute, ACTOR, inhalation<br>tt Level: Cyp3a2, Cyp2c8v<br>2, ONECUT1<br>Group 3, Not classifiable as<br>ensity of Maryland carcinogon<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>control to the second seco | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | И          | screening I<br>screening I<br>screening I<br>screening I<br>screening I<br>GIABS (mg/k<br>risk-based               | level (residential Soil) (mg/k<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k<br>level (tap water) (ug/L)<br>level (tap water) (ug/L)<br>g/kg-day)<br>g-day)<br>SSL (mg/m3)<br>SSL (mg/m3) | y/kg-day)<br>y/kg-day)<br>kg-day)                     | reening  | THQ=1           THQ=0.1           THQ=0.1           THQ=1           THQ=0.1           THQ=0.1           THQ=0.1           THQ=1           THQ=1.1           THQ=0.1           THQ=1.1           THQ=1.1           THQ=1.1   | ۰<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱ | 1300<br>130<br>16000<br>1800<br>390<br>39<br>1<br>0.1<br>0.1                |     |
| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimui</li> <li>Minimui</li> <li>IVIVE F</li> <li>Quantitative F</li> <li>Cancer Inform</li> <li>No cante</li> <li>No inha</li> <li>Carcino</li> <li>ToxNet HSC</li> <li>No inha</li> <li>Carcino</li> <li>ToxNet HSC</li> <li>No genut</li> <li>Reproductive</li> <li>Chronic Toxice</li> <li>599 Ch</li> <li>Subchronic T</li> <li>24 Subte</li> <li>Development</li> <li>No deval</li> <li>Acute Toxicol</li> <li>2944 Ac</li> <li>Subacute Tox</li> <li>No subte</li> <li>Neurotoxicolo</li> </ul>   | alues available [2]<br>RTV values<br>RTV values available [2]<br>Im RfD: 0.020 mg/kg-day (chror<br>mRfD: 0.020 mg/kg-day (chror<br>POD not calculated<br>Hazard Values<br>Im oral POD: 0.013 mg/kg-day (<br>Im inhalation POD: 1.0e+2 mg/m<br>I Observed Bioactivity Equivalen<br>, CYP2C18, CYP2B6, CYP1A2<br>mation<br>IICO Bioactivity Equivalent<br>, CYP2C18, CYP2B6, CYP1A2<br>Int risk value<br>ogenicity data available: IARC: 0<br>IDB carcinognicity warning Univer-<br>totoxicity findings reported<br>e Toxicology<br>productive toxicity PODs available<br>icology<br>ronic toxicity PODs available [2]<br>Toxicology<br>telopmental toxicity data available<br>values toxicity PODs available [2]<br>values toxicity PODs available [2]<br>values toxicity PODs available [2]<br>values toxicity data available.  | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (aoute, ACTOR, inhalation<br>tt Level: Cyp3a2, Cyp2c8v<br>2, ONECUT1<br>Group 3, Not classifiable as<br>ensity of Maryland carcinogon<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>control to the second seco | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | И          | screening I<br>screening I<br>screening I<br>screening I<br>screening I<br>GIABS (mg/k<br>risk-based<br>risk-based | level (residential Soil) (mg/k<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k<br>level (tap water) (ug/L)<br>level (tap water) (ug/L)<br>g/kg-day)<br>g-day)<br>SSL (mg/m3)<br>SSL (mg/m3) | y/kg-day)<br>y/kg-day)<br>kg-day)                     | reening  | THQ=1           THQ=0.1           THQ=0.1           THQ=1           THQ=0.1           THQ=0.1           THQ=0.1           THQ=1           THQ=1.1           THQ=0.1           THQ=1.1           THQ=1.1           THQ=1.1   | ۰<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱ | 1300<br>130<br>18000<br>18000<br>380<br>38<br>1<br>0.1<br>0.1<br>0.1<br>0.1 |     |
| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimuu</li> <li>Minimuu</li> <li>Minimuu</li> <li>IVIVE P</li> <li>Quantitative H</li> <li>Minimuu</li> <li>IVIVE P</li> <li>Quantitative H</li> <li>Minimuu</li> <li>Lowest<br/>CYP2C19</li> <li>Cancer Inform</li> <li>No cant</li> <li>So ho inha</li> <li>Carcino</li> <li>ToxNet HSC</li> <li>No gent</li> <li>Reproductive</li> <li>111 Rep</li> <li>Chronic Toxic</li> <li>599 Christ</li> <li>Subchronic T</li> <li>24 Subc</li> <li>Development</li> <li>No devi</li> <li>Acute Toxicol</li> <li>2944 Acute Toxicol</li> <li>2944 Acute Toxicol</li> <li>2944 Acute Toxicol</li> <li>Subacute Toxicol</li> <li>No subc</li> <li>No neuri</li> <li>Endocrine Sy</li> <li>No sign</li> </ul>  | alues available [2]<br>RTV values<br>SL values available [2]<br>Im RfD: 0.020 mg/kg-day (chror<br>mRfC: 0.020 mg/kg-day (chror<br>POD not calculated<br>Hazard Values<br>Im oral POD: 0.013 mg/kg-day (<br>Im inhalation POD: 1.0e+2 mg/m<br>I Observed Bioactivity Equivalen<br>, CYP2C18, CYP286, CYP1A2<br>mation<br>Icor slope factor<br>alation unit risk value<br>ogenicity data available: IARC: 0<br>IDB carcinognicity warning Univer-<br>totoxicity findings reported<br>e Toxicology<br>productive toxicity PODs available<br>cology<br>ronic toxicity PODs available [2]<br>Toxicology<br>wchronic toxicity PODs available [2]<br>tal Toxicology<br>velopmental toxicity data available<br>isology<br>volue toxicity PODs available [2]<br>xicology<br>vacute toxicity data available.<br>Nogy<br>Irrotoxicology data available.  | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (aoute, ACTOR, inhalation<br>tt Level: Cyp3a2, Cyp2c8v<br>2, ONECUT1<br>Group 3, Not classifiable as<br>ensity of Maryland carcinogon<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>control to the second seco | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | и          | screening I<br>screening I<br>screening I<br>screening I<br>screening I<br>GIABS (mg/k<br>risk-based<br>risk-based | level (residential Soil) (mg/k<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k<br>level (tap water) (ug/L)<br>level (tap water) (ug/L)<br>g/kg-day)<br>g-day)<br>SSL (mg/m3)<br>SSL (mg/m3) | y/kg-day)<br>y/kg-day)<br>kg-day)                     | reening  | THQ=1           THQ=0.1           THQ=0.1           THQ=1           THQ=0.1           THQ=0.1           THQ=0.1           THQ=1           THQ=1.1           THQ=0.1           THQ=1.1           THQ=1.1           THQ=1.1   | ۰<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱ | 1300<br>130<br>18000<br>18000<br>380<br>38<br>1<br>0.1<br>0.1<br>0.1<br>0.1 |     |
| <ul> <li>No PPF</li> <li>EPA RS</li> <li>Minimuu</li> <li>Minimuu</li> <li>IVIVE P</li> <li>Quantitative H</li> <li>Minimuu</li> <li>IVIVE P</li> <li>Quantitative H</li> <li>Minimuu</li> <li>Lowest<br/>CYP2C19,</li> <li>Cancer Inform</li> <li>No canter<br/>No canter</li> <li>No canter</li> <li>Subchronic To</li> <li>24 Subter</li> <li>Development</li> <li>No development</li> <li></li></ul> | alues available (2)<br>RTV values<br>SL values available (2)<br>Im RfD: 0.020 mg/kg-day (chror<br>mRfD: 0.020 mg/kg-day (chror<br>POD not calculated<br>Hazard Values<br>Im oral POD: 0.013 mg/kg-day (<br>Im inhalation POD: 1.0e+2 mg/m<br>I Observed Bioactivity Equivalen<br>, CYP2C18, CYP2B6, CYP1A2<br>mation<br>Icor slope factor<br>alation unit risk value<br>ogenicity data available: IARC: 0<br>IDB carcinognicity warning Univer-<br>totoxicity findings reported<br>e Toxicology<br>productive toxicity PODs available<br>(2)<br>Toxicology<br>victoronic toxicity PODs available (2)<br>Toxicology<br>victoronic toxicity PODs available (2)<br>tal Toxicology<br>victoronic toxicity PODs available (2)<br>victorony<br>victorology<br>victorony<br>victorology data available.<br>Nogy<br>Irrotoxicology data available.<br>Nogy<br>Irrotoxicology data available.<br>Nogy<br>Irrotoxicology data available.<br>Nogy<br>Irrotoxicology data available.<br>Nogy<br>Irrotoxicology data available.<br>Nogy  | nic, RAIS, inhalation, 7)<br>(mortality:chronic, ECOTO)<br>m3 (aoute, ACTOR, inhalation<br>tt Level: Cyp3a2, Cyp2c8v<br>2, ONECUT1<br>Group 3, Not classifiable as<br>ensity of Maryland carcinogon<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>ble<br>control to the second seco | on, 5) 🗗<br>1 , Cyp2c11 , CY<br>s to its carcinoge | nicity to humans NLN | и          | screening I<br>screening I<br>screening I<br>screening I<br>screening I<br>GIABS (mg/k<br>risk-based<br>risk-based | level (residential Soil) (mg/k<br>level (industrial soil) (mg/k<br>level (industrial soil) (mg/k<br>level (tap water) (ug/L)<br>level (tap water) (ug/L)<br>g/kg-day)<br>g-day)<br>SSL (mg/m3)<br>SSL (mg/m3) | y/kg-day)<br>y/kg-day)<br>kg-day)                     |          | THQ=1           THQ=0.1           THQ=1           THQ=1           THQ=0.1           THQ=1           THQ=1.1           THQ=0.1           .           .           THQ=1.1           THQ=0.1           .           .           .           THQ=1.1           THQ=1.1           THQ=1.1           THQ=1.1           THQ=1.1 | ۰<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱<br>۱ | 1300<br>130<br>18000<br>18000<br>380<br>38<br>1<br>0.1<br>0.1<br>0.1<br>0.1 |     |