NJRisk PROJECT

For Implementing an Integrated Computational Tool to Support Prioritization of Chemicals of Emerging Concern

FINAL REPORT

April 1, 2014 to June 30, 2015)

Submitted to Robert Mueller
New Jersey Department of Environmental Protection

by Panos G. Georgopoulos (Principal Investigator)

Environmental and Occupational Health Sciences Institute
December 31, 2015

Table of Contents

1 Summary Overview....1
1.1 Rationale....1
1.2 Methods....2
1.3 Installation of METIS....17
2 STRUCTURE AND COMPONENTS OF NJrisk....19
3 Current Progress....20
3.1 Establishment of software requirements....20
3.2 Adaptation and customization of modules from METIS and PRoTEGE....20
4 Results of Exploratory Case Studies for 40 Chemicals....25
PRoTEGE Ranking for 1,2,3–Trichlorobenzene....26
METIS Results for 1,2,3–Trichlorobenzene....28
NJrisk Preliminary Results for 1,2,3–Trichlorobenzene....29
PRoTEGE Results for 2,4,5-Trichlorophenoxyacetic acid....30
METIS Results for 2,4,5-Trichlorophenoxyacetic acid....32
NJrisk Preliminary Results for 2,4,5-Trichlorophenoxyacetic acid....33
PRoTEGE Results for 2,4-D....34
METIS Results for 2,4-D....36
NJrisk Preliminary Results for 2,4-D....37
PRoTEGE Results for Aldicarb....38
METIS Results for Aldicarb....40
NJrisk Preliminary Results for Aldicarb....41
PRoTEGE Results for Aroclor_1254....42
METIS Results for Aroclor_1254....44
NJrisk Preliminary Results for Aroclor_1254....45
PRoTEGE Results for Arsenic (and As compounds)....46
METIS Results for Arsenic (and As compounds)....48
NJrisk Preliminary Results for Arsenic (and As compounds)....49
PRoTEGE Results for Atrazine....50
METIS Results for Atrazine....52
NJrisk Preliminary Results for Atrazine....53
PRoTEGE Ranking for Bisphenol-A....54
METIS Results for Bisphenol-A....56
NJrisk Preliminary Results for Bisphenol-A....57
PRoTEGE Ranking for C10-13 Chloroalkanes....58
METIS Results for C10-13 Chloroalkanes....60
NJrisk Preliminary Results for C10-13 Chloroalkanes....61
PRoTEGE Results for Cadmium....62
METIS Results for Cadmium....64
NJrisk Preliminary Results for Cadmium....65
PRoTEGE Ranking for Carbaryl....66
METIS Results for Carbaryl....68
NJrisk Preliminary Results for Carbaryl....69
PRoTEGE Results for DDT....70
METIS Results for DDT....72

NJrisk Preliminary Results for DDT 73
PRoTEGE Results for decaBDE 74
METIS Results for decaBDE 76
NJrisk Preliminary Results for decaBDE 77
PRoTEGE Results for DEHP, Di(2-ethylhexyl)phthalate 78
METIS Results for DEHP, Di(2-ethylhexyl)phthalate 80
NJrisk Preliminary Results for DEHP, Di(2-ethylhexyl)phthalate 81
PRoTEGE Results for Diethyl Phthalate 82
METIS Results for Diethyl Phthalate 84
NJrisk Preliminary Results for Diethyl Phthalate 85
PRoTEGE Results for Di-n-butylphthalate 86
METIS Results for Di-n-butylphthalate 88
NJrisk Preliminary Results for Di-n-butylphthalate 89
PRoTEGE Results for Ethane 1,1,2,2-tetrachloro- 90
METIS Results for Ethane 1,1,2,2-tetrachloro- 92
NJrisk Preliminary Results for Ethane 1,1,2,2-tetrachloro- 93
PRoTEGE Results for Perchlorethylene 94
METIS Results for Perchlorethylene 96
NJrisk Preliminary Results for Perchlorethylene 97
PRoTEGE Results for Ethylene Thiourea 98
METIS Results for Ethylene Thiourea 100
NJrisk Preliminary Results for Ethylene Thiourea 101
PRoTEGE Ranking for Ethylparaben 102
METIS Results for Ethylparaben 104
NJrisk Preliminary Results for Ethylparaben 105
PRoTEGE Results for Formaldehyde 106
METIS Results for Formaldehyde 108
NJrisk Preliminary Results for Formaldehyde 109
PRoTEGE Results for gamma-Hexachlorocyclohexane 110
METIS Results for gamma-Hexachlorocyclohexane 112
NJrisk Preliminary Results for gamma-Hexachlorocyclohexane 113
PRoTEGE Ranking for Lead 114
METIS Results for Lead 116
NJrisk Preliminary Results for Lead 117
PRoTEGE Results for Malathion 118
METIS Results for Malathion 120
NJrisk Preliminary Results for Malathion 121
PRoTEGE Results for Manganese 122
METIS Results for Manganese 124
NJrisk Preliminary Results for Manganese 125
PRoTEGE Results for Methoxychlor 126
METIS Results for Methoxychlor 128
NJrisk Preliminary Results for Methoxychlor 129
PRoTEGE Results for Methyl Mercury 130
METIS Results for Methyl Mercury 132
NJrisk Preliminary Results for Methyl Mercury 133
PRoTEGE Ranking for n-Hexane 134

METIS Results for n-Hexane 136
NJrisk Preliminary Results for n-Hexane 137
PRoTEGE Results for octaBDE 138
METIS Results for octaBDE 140
NJrisk Preliminary Results for octaBDE 141
PRoTEGE Results for Parathion 142
METIS Results for Parathion 144
NJrisk Preliminary Results for Parathion 145
PRoTEGE Results for Pentachlorophenol 146
METIS Results for Pentachlorophenol 148
NJrisk Preliminary Results for Pentachlorophenol 149
PRoTEGE Results for pentaBDE 150
METIS Results for pentaBDE 152
NJrisk Preliminary Results for pentaBDE 153
PRoTEGE Results for Permethrin 154
METIS Results for Permethrin 156
NJrisk Preliminary Results for Permethrin 157
PRoTEGE Ranking for PFOS 158
METIS Results for PFOS 160
NJrisk Preliminary Results for PFOS 161
PRoTEGE Results for Phenol, (1,1-dimethylethyl)-4-methoxy- 162
METIS Results for Phenol, (1,1-dimethylethyl)-4-methoxy- 164
NJrisk Preliminary Results for Phenol, (1,1-dimethylethyl)-4-methoxy- 165
PRoTEGE Ranking for Trifluralin 166
METIS Results for Trifluralin 168
NJrisk Preliminary Results for Trifluralin 169
PRoTEGE Ranking for Tris (1,3-dichloro-2-propyl) phosphate 170
METIS Results for Tris (1,3-dichloro-2-propyl) phosphate 172
NJrisk Preliminary Results for Tris (1,3-dichloro-2-propyl) phosphate 173
PRoTEGE Ranking for Tris (2-chloroethyl) phosphate 174
METIS Results for Tris (2-chloroethyl) phosphate 176
NJrisk Preliminary Results for Tris (2-chloroethyl) phosphate 177
PRoTEGE Ranking for Vinclozolin 178
METIS Results for Vinclozolin 180
NJrisk Preliminary Results for Vinclozolin 181
PRoTEGE Results for Vinyl Chloride 182
METIS Results for Vinyl Chloride 184
NJrisk Preliminary Results for Vinyl Chloride 185

References 186

1 Summary Overview

The objective of the NJrisk project is to develop, text, and deploy an integrated tiered system coupling computational platforms to support prioritization of Chemicals of Current and of Emerging Concern.

A nine-month Pilot Study was conducted from July 2013 to March 2014, in order to complete the necessary groundwork for the subsequent implementation. The full study, which began in April 2014, uses two operational computational platforms for hazard and for exposure ranking, respectively METIS (Metanomics Information System), developed by DuPont, and PRoTEGE (Prioritization and Ranking of Toxic Exposures with GIS Extension), developed by the Computational Chemodynamics Laboratory of EOHSI. This effort also takes advantage of, and incorporates in the development of the new system, current and anticipated outcomes of ongoing efforts by Federal Agencies, such as the USEPA [see, e.g., 1,2,3 and Figure 1]. The goal is to implement an integrated software platform or "tool" (NJrisk) that will allow many types of users to assess both hazard and exposure potentials of chemicals that are found (or could be introduced) in the New Jersey environment and/or biota, and to prioritize these chemicals for regulatory action based on tiered risk analysis.

1.1 Rationale

All regulatory agencies, nationally and internationally, face current challenges in their efforts to address concerns regarding the rapid introduction of many "new" chemicals or the use of "old" chemicals in new products, resulting to "new types of exposures" for human populations and ecosystems. A variety of approaches are being developed to support these efforts; our present effort directly addresses a critical State and National need.

A major attribute of the integrated NJrisk system currently under development is that, in addition to addressing chemicals of "current regulatory concern," it will also facilitate characterization of contaminants of "emerging concern." In general the term "emerging contaminants" refers to hazardous materials or mixtures that may have:

a. a perceived or real threat to human health, public safety or the environment;
b. no published or evolving health standards or guidelines;
c. insufficient or limited available toxicological information that is evolving or being re-evaluated; or
d. significant new sources, pathways, or detection limits.

Some major classes of Chemicals of Emerging Concern (CECs) include pharmaceutical and personal care products (PPCPs); engineered nanomaterials (ENMs) such as silver nanoparticles and carbon nanotubes; plasticizers, flame retardants, protective coatings; home cleaning products; and food additives.

In the pilot phase of this project, METIS and PRoTEGE were employed to conduct a study involving hazard and exposure characterization applications for a broadly representative set of 15 chemicals of current and emerging concern, corresponding to various combinations of production volume, chemical properties, environmental distribution, usages, exposure pathways, etc. These case studies were analyzed and evaluated in order to identify optimal ways for linking and merging appropriate METIS and PRoTEGE components and corresponding data retrieval and calculation procedures, and to establish initial software requirements and specifications for NJrisk that will be completed through the current and subsequent implementation phases. The

initial phase of the full study (from April 1, 2014 to June 30, 2015) expanded the list of the 15 "pilot" substances to include the following 40 chemicals:

	Chemical	**CAS#**
1.	1,2,3–Trichlorobenzene	87-61-6
2.	2,4,5-Trichlorophenoxyacetic acid	93-76-5
3.	2,4-D	94-75-7
4.	Aldicarb	116-06-3
5.	Aroclor_1254	11097-69-1
6.	Arsenic	7440-38-2
7.	Atrazine	1912-24-9
8.	Bisphenol-A	80-05-7
9.	C10-13 Chloroalkanes	85535-84-8
10.	Cadmium	7440-43-9
11.	Carbaryl	63-25-2
12.	DDT	50-29-3
13.	decaBDE	1163-19-5
14.	DEHP, Di(2-ethylhexyl)phthalate	117-81-7
15.	Diethyl Phthalate	84-66-2
16.	Di-n-butylphtalate	84-74-2
17.	Ethane, 1,1,2,2-tetrachloro-	79-34-5
18.	Perchlorethylene	127-18-4
19.	Ethylene thiourea	96-45-7
20.	Ethylparaben	120-47-8
21.	Formaldehyde	50-00-0
22.	gamma-Hexachlorocyclohexane	58-89-9
23.	Lead	7439-92-1
24.	Malathion	121-75-5
25.	Manganese	7439-96-5
26.	Methoxychlor	72-43-5
27.	Methyl Mercury	22967-92-6
28.	n-Hexane	110-54-3
29.	octaBDE	32536-52-0
30.	Parathion	56-38-2
31.	Pentachlorophenol	87-86-5
32.	pentaBDE	32534-81-9
33.	Permethrin	52645-53-1
34.	PFOS	1763-23-1
35.	Phenol, (1,1-dimethylethyl)-4-methoxy-	25013-16-5
36.	Trifluralin	1582-09-8
37.	Tris (1,3-dichloro-2-propyl) phosphate	13674-87-8
38.	Tris (2-chloroethyl) phosphate	115-96-8
39.	Vinclozolin	50471-44-8
40.	Vinyl Chloride	75-01-4

1.2 Methods

The ongoing research and development effort addresses Tiers 1, 2 and 3 of the Chemicals of Emerging Concern evaluation process depicted in Figure 1. Starting components are the initial screening of substances of concern (Tier 1) and the preliminary hazard and exposure assessment

(Tier 2). These two steps provide a sound specific basis for extending the analysis into a Risk Assessment (Tier 3).

As stated earlier, the current effort utilizes components from two operational state-of-the-art platforms for hazard and for exposure characterization and ranking:

- METIS (Metanomics Information System), developed by DuPont, and
- PRoTEGE (Prioritization and Ranking of Toxic Exposures with GIS extension), developed by the Computational Chemodynamics Laboratory of EOHSI.

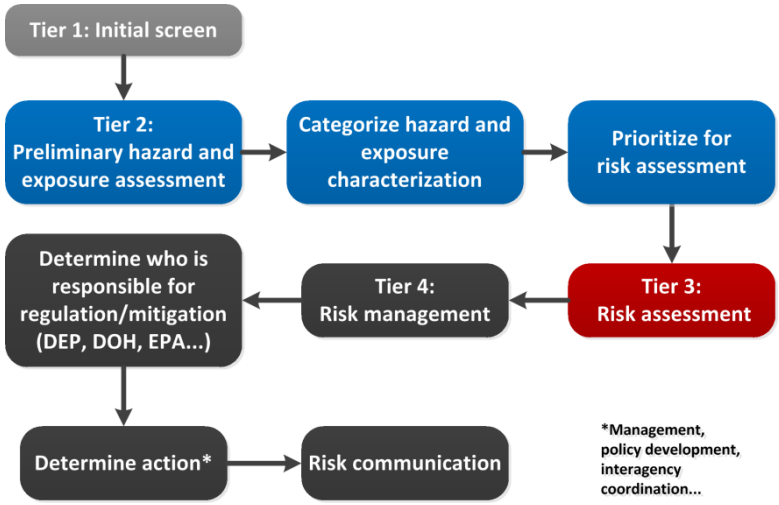
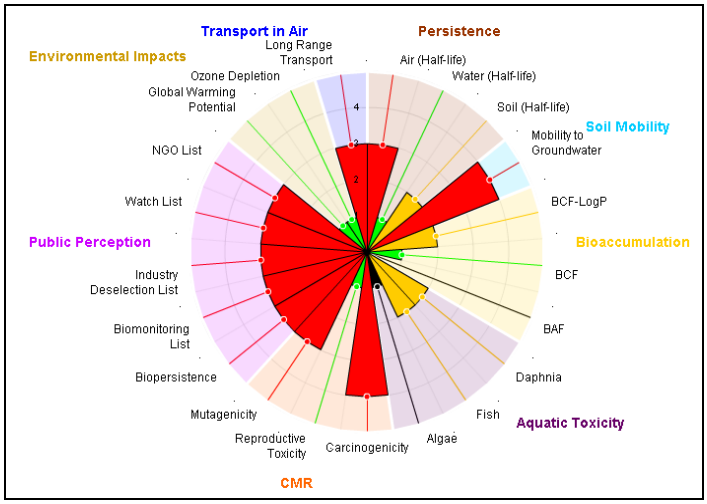


Figure 1. . Overview of the Chemicals of Emerging Concern (CEC) evaluation process; adapted from NJ DEP SAB CEC Subcommittee [5]

METIS [4] is a chemical informatics platform that provides a screening level view of potential environmental fate and effects, human health concerns, and societal perception issues associated with a chemical of concern. As an example, Figure 2 depicts "METIS attributes" that have been retrieved in a systematic manner from a variety of databases for a representative chemical. Typically these attributes are:

- Environmental Persistence – indicates the predicted half-life in each environmental compartment,



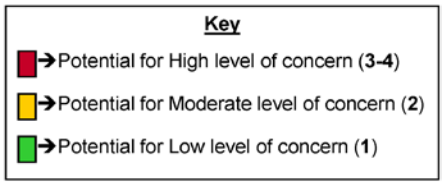


Figure 2. . Hazard-related attributes of chemicals retrieved and plotted by the Metanomics Information System (METIS)

- Soil Mobility – the potential for a chemical to migrate from soil into groundwater,
- Bioaccumulation – uses measured or estimated values to indicate the potential for a chemical to sorb to lipids,
- Aquatic Toxicity – the measured or estimated toxicity to aquatic organisms,
- CMR – indicates whether the compound is classified as known or suspected animal and/or human Carcinogen, Mutagen or Reproductive toxin,
- Public Perception – indicates that the chemical is present on a variety of regulatory, industrial and/or non-governmental lists that may influence how the public views a particular chemical,
- Environmental Impact – indicates the potential for the chemical to affect global warming and ozone depletion as compared to reference compounds,
- Long Range Transport (Air) – the potential for the chemical to travel long distances from its point of entry into the environment,
- Environmental Partitioning (Fugacity) – steady-state partitioning of a chemical in the environment (Air, Water, Soil, Sediment) based on different emission scenarios.

METIS has been built on open-source software that provides access to an aggregated database and estimation tool set. METIS retrieves and assembles information from over 1,400 publicly available databases (see Table 1 for a representative set of these databases). These data resources may contain, but are not limited to, physical and chemical properties, hazard, toxicological, environmental and regulatory information. The input for METIS is simply the chemical name, CAS #, or chemical structure. METIS retrieves information and assembles it together into a comprehensible view in seconds to minutes versus weeks to months that could be required, in some cases, by conventional searches.

Table 1. Selected databases accessed by METIS (hosted locally)

Database	Expanded Name
BCF	Bio-concentration Factors Gold standard database (Cefic LRI, EURAS)
CDAT – CDR	Chemical Data Access Tool -Chemical Data Reporting
CCRIS	Chemical Carcinogenesis Research Information System
DIPPR	Design Institute for Physical Properties
ECOTOX	ECOTOXicology database
HSDB	Hazardous Substances Data Bank
MITI	Ministry of International Trade and Industry (Existing and New Chemical Substances List)
PBDB	
PHYSPROP	Physical Properties Database
PubChem	--
SRC BCF	SRC Bioconcentration Factor
ToxMiner	--

PRoTEGE [6,7] is an analysis and modeling platform that facilitates exposure calculations at multiple tiers, utilizing available data on:

- chemical production volumes,
- intrinsic properties that affect the environmental dynamics of the chemical (e.g. volatility, solubility, etc.),
- intrinsic properties (such as lipophilicity) that affect the biological dynamics (absorption, distribution, metabolism, elimination) of the chemical, and subsequent uptake/bioaccumulation by humans and wildlife,
- chemical transportation modes and amounts,
- chemical usage in industrial, agricultural, etc. applications,
- environmental release/disposal amounts and spatiotemporal pattern,
- chemical uses in consumer products and in foodstuffs,
- environmental concentrations of chemicals in multiple media (including food and beverages),
- age- and gender-specific population distributions of physiological and behavioral attributes.

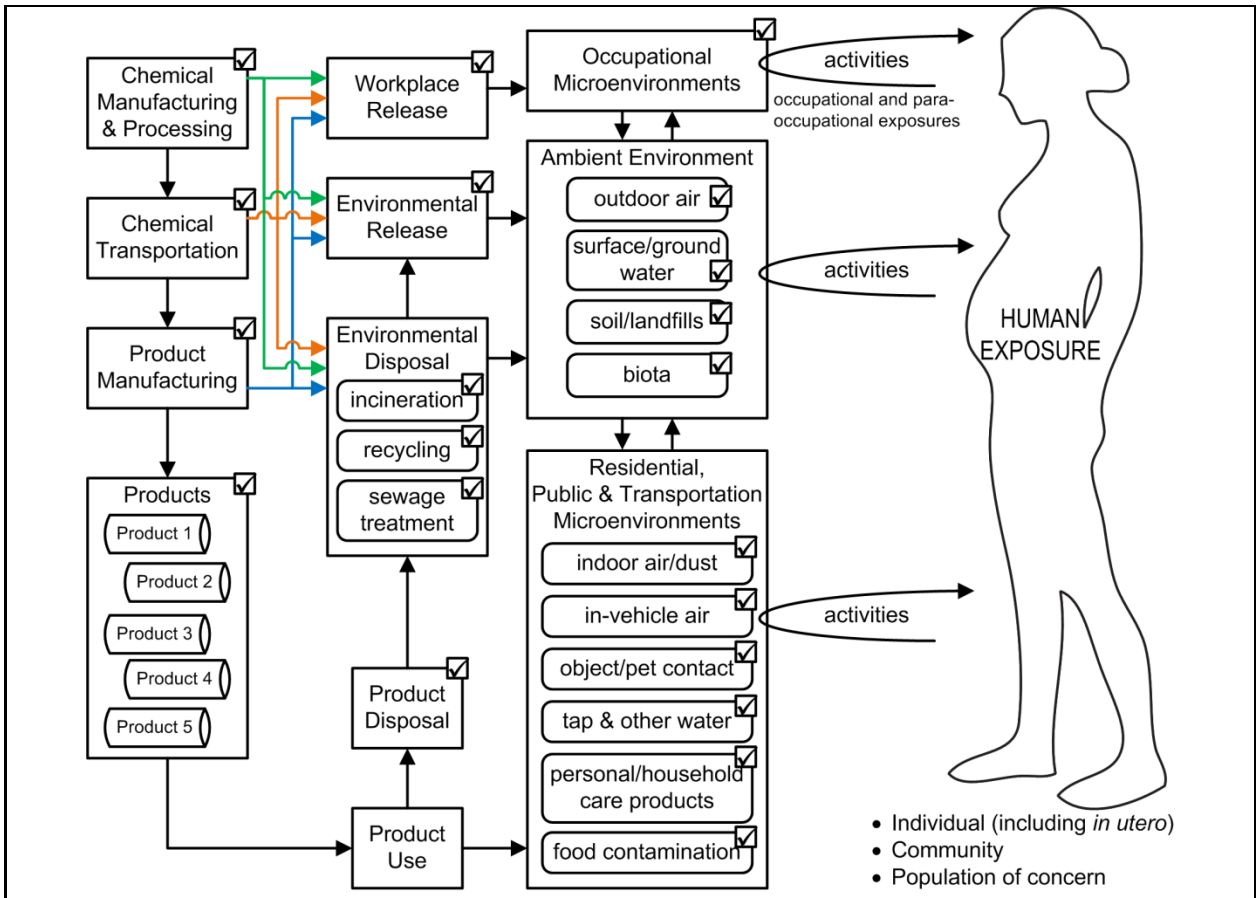


Figure 3. A schematic depiction of the conceptual framework of PRoTEGE (Prioritization and Ranking of Toxic Exposures with GIS Extension) [6,7]; this system uses a Life Cycle Assessment (LCA) approach to assess potential human exposures to chemicals that could take place during manufacturing, transportation, or using products containing these chemicals as well as following their environmental disposal.

PRoTEGE derives from and complements the Modeling ENvironment for TOtal Risk studies (MENTOR) [2,8-10], which supports detailed person-oriented ("bottom-up") source-to-dose

exposure modeling for mixtures of multiple multimedia contaminants. MENTOR allows a study to focus on specific locations and subpopulations, but is both data and resource intensive. The simplified "top-down" population-oriented approach of PRoTEGE provides tiered estimates of exposures experienced by populations of concern, allowing calculations at the national, state or county level.

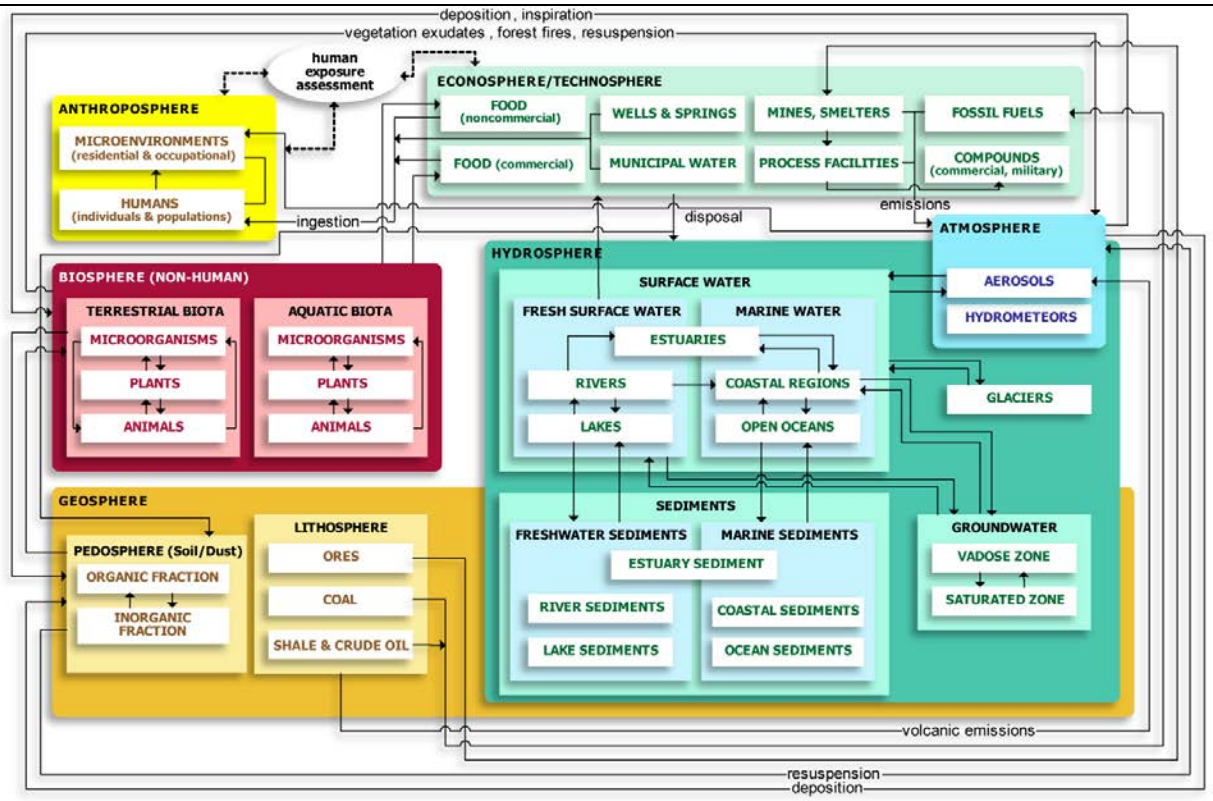
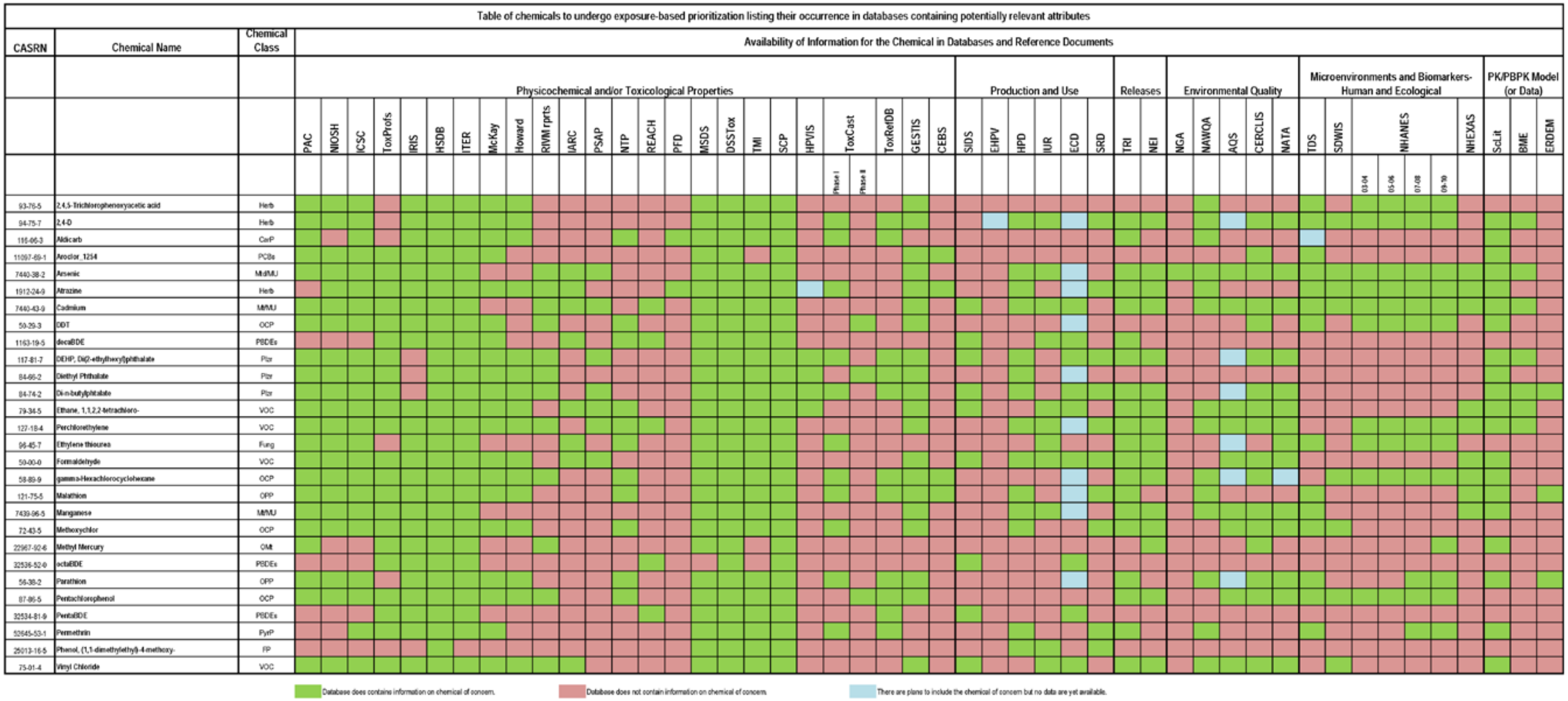


Figure 4. Multimedia/multipathway/multiroute exposure assessment in MENTOR (Modeling Environment for Total Risk studies) [2,8,9]; simplified modules of MENTOR focusing on human exposures have been developed for incorporation in PRoTEGE (Prioritization and Ranking of Toxic Exposures with GIS Extension) to support chemical ranking and screening when limited data are available. Additional PRoTEGE modules focusing on ecological exposures will be developed as part of the integrated NJrisk system.

The PRoTEGE approach takes advantage of, and integrates, both available measurements and model estimates to understand and quantify exposures of populations potentially at risk. Specifically, by utilizing over 50 available "information bases" (including various traditional databases and metadatabases, literature surveys, etc. as well as original studies reported in the literature – see Table 2a and 2b) of environmental releases, chemical production and usage, multimedia environmental concentrations, and age- and gender-specific population distributions of major physiological and behavioral patterns, the estimates of PRoTEGE provide a reasonably realistic assessment of exposures that could be experienced by the general population or by subpopulations of concern.

This page is intentionally left blank

Table 2a. Representative databases and other information sources currently employed by PRoTEGE for developing exposure rankings of Chemicals of Emerging and Current Concern



IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

Table 2b. Databases and other information sources appearing in Table 2a

Data Source Abbreviation	Expanded Name
PAC	Protective Action Criteria
NIOSH	National Institute for Occupational Safety and Health
ICSC	International Chemical Safety Cards
ToxProfs	Toxicological Profiles
IRIS	Integrated Risk Information System
HSDB	Hazardous Substance Databank
ITER	International Toxicity Estimates for Risk
McKay	Mackay's "Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals"
Howard	Howard's "Handbook of Environmental Fate and Exposure Data for Organic Chemicals"
RIVM rprts	RIVM National Institute for Public Health and the Environment reports
IARC	International Agency for Research on Cancer
PSAP	Priority Substances Assessment Program
NTP	National Toxicology Program database search
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
PFD	Pesticide Fate Database
MSDS	Material Safety Data Sheets
DSSTox	Distributed Structure-Searchable Toxicity
TMI	The Merck Index
SCP	Scorecard Chemical Profiles
HPVIS	High Production Volume Information System
ToxCast	Toxicity Forecaster
ToxRefDB	Toxicity Reference Database
GESTIS	GESTIS - Information system on hazardous substances of the German Social Accident Insurance
CEBS	Chemical Effects in Biological Systems
SIDS	Screening Information Data Set
EHPV	Expended High Production Volume
HPD	Household Products Database
IUR	Inventory Update Reporting
ECD	Existing Chemicals Database
SRD	Source Ranking Database
TRI	Toxics Release Inventory Program
NEI	National Emission Inventory
NGA	National Geochemical Atlas
NAWQA	National Water-Quality Assessment Program
AQS	Air Quality System
CERCLIS	Comprehensive Environmental Response, Compensation, and Liability Information System
NATA	National-Scale Air Toxics Assessments
TDS	Total Diet Study
SDWIS	Safe Drinking Water Information System
NHANES	National Health and Nutrition Examination Survey
NHEXAS	National Human Exposure Assessment Survey
ScLit	Scientific Literature
BME	Biomonitoring Equivalents
ERDEM	Exposure Related Dose Estimating Model

PRoTEGE incorporates various modeling methods that are available for developing screening estimates of exposure-relevant environmental concentrations of chemicals, including fugacity calculations [11,12], intake fractions [13,14], biomonitoring equivalents [15], etc.

When data are not available for a specific chemical, various assumptions need to be made; in these cases the estimates of PRoTEGE reflect plausible scenarios of chemical production, distribution, usage, disposal, etc.

Exposure metrics calculated by PRoTEGE provide semi-quantitative and quantitative (depending on the information that is available and the level/tier of analysis performed) measures of potential exposures to the chemical of concern. These metrics are based on a combination of available information on releases and concentrations, on types and degree of exposures reported in the literature, and expert judgment on various facets of the exposures. The four population-based metrics used for exposure ranking are: *pervasiveness*, *persistence*, *severity*, and *efficacy*.

- *Pervasiveness* reflects how widespread the exposures are (or could be) within the population of concern.
    - Quantitative factors that are considered in ranking pervasiveness include: fraction of administrative unit (e.g. counties or municipalities) where emissions or usage of the chemical are reported; production amounts for the chemical; extent of usage of the chemical in consumer products; percentage of ambient concentrations above a threshold, etc.
    - Semi-quantitative factors include information from the literature on whether exposures are wide-spread (e.g. based on the major release types), localized (e.g. based on transport scales), or limited to specific geographic areas (e.g. urban areas, farmland, coastal fishing regions, etc.).
- *Persistence* reflects the temporal frequency and/or duration of exposures experienced by the general population.
    - Factors that are considered in ranking persistence include: temporal patterns of emissions and releases, pattern of potential contact with the chemical through food consumption or usage of consumer products, environmental half-lives, chemical reactivity, etc.
    - Semi-quantitative factors include information on whether exposures are episodic, cyclical, or generally uniform over a long period of time.
- *Severity* reflects the potential for high levels of exposures.
    - Quantitative factors that are considered in ranking severity include: peak release rates, levels of peak concentrations, acute effects occurring at or near reported ambient or microenvironmental levels of the chemicals, etc.
    - Semi-quantitative factors include additional information on frequency of localized high releases, special behavior patterns that could lead to potentially high exposures, etc.
- *Efficacy* reflects the potential of the contact with the chemical to result in intake by humans (or other organisms of concern) and resulting in biologically relevant uptake.
    - Quantitative factors include biological partition coefficients, while semi-quantitative factors include information on the form of the chemical exposures (e.g. food matrix).

The above four exposure metrics of PRoTEGE are assigned integer values on a scale of 1 to 5 for each chemical considered, corresponding to “very low,” “low,” “moderate,” “high,” and “very high” exposure estimates, respectively. These rankings are calculated individually for the three major exposure routes: inhalation, ingestion, and dermal absorption; additionally, the rankings are averaged for the three routes to obtain an “aggregate ranking.”

Table 3. PRoTEGE "Tier 1" exposure rankings for the 40 selected chemicals

Chemical	Ranking Based on Inhalation Route				Ranking Based on Ingestion Route				Ranking Based on Dermal Route				Ranking Based on Aggregate Exposure				Ranking Based on Dominant Exposure Route for Each Metric			
	Pervasiveness	Persistence	Severity	Efficacy	Pervasiveness	Persistence	Severity	Efficacy	Pervasiveness	Persistence	Severity	Efficacy	Pervasiveness	Persistence	Severity	Efficacy	Pervasiveness	Persistence	Severity	Efficacy
1,2,3–Trichlorobenzene	1	1	1	2	2	2	1	2	1	1	1	2	1.33	1.33	1.00	2.00	2	2	1	2
2,4,5-Trichlorophenoxyacetic acid	1	1	1	1	2	2	2	2	1	1	1	2	1.33	1.33	1.33	1.67	2	2	2	2
2,4-D	1	1	1	1	2	2	2	2	1	1	1	2	1.33	1.33	1.33	1.67	2	2	2	2
Aldicarb	1	1	1	1	2	2	2	2	1	1	1	1	1.33	1.33	1.33	1.33	2	2	2	2
Aroclor 1254	1	1	1	1	2	2	1	2	1	1	1	2	1.33	1.33	1.00	1.67	2	2	1	2
Arsenic	1	1	1	2	4	4	2	3	2	2	2	1	2.33	2.33	1.67	2.00	4	4	2	3
Atrazine	1	1	1	1	2	2	2	2	1	1	1	2	1.33	1.33	1.33	1.67	2	2	2	2
Bisphenol-A	1	1	1	1	2	2	2	2	1	1	1	1	1.33	1.33	1.33	1.33	2	2	2	2
C10-13 Chloroalkanes	1	1	1	1	2	2	1	2	1	1	1	2	1.33	1.33	1.00	1.67	2	2	1	2
Cadmium	1	1	1	2	3	3	2	3	2	2	2	1	2.00	2.00	1.67	2.00	3	3	2	3
Carbaryl	1	1	1	2	4	4	2	3	1	2	2	1	2.00	2.33	1.67	2.00	4	4	2	3
DDT	1	1	1	1	2	2	2	2	1	1	1	1	1.33	1.33	1.33	1.33	2	2	2	2
decaBDE	1	1	1	1	3	3	1	2	1	1	1	1	1.67	1.67	1.00	1.33	3	3	1	2
DEHP, Di(2-ethylhexyl)phthalate	1	1	1	1	3	3	1	2	2	2	1	1	2.00	2.00	1.00	1.33	3	3	1	2
Diethyl Phthalate	1	1	1	1	3	3	1	2	2	2	1	1	2.00	2.00	1.00	1.33	3	3	1	2
Di-n-butylphtalate	1	1	1	1	3	3	1	2	2	2	1	1	2.00	2.00	1.00	1.33	3	3	1	2
Ethane, 1,1,2,2-tetrachloro-	2	2	1	3	1	1	1	2	1	1	1	3	1.33	1.33	1.00	2.67	2	2	1	3
Perchlorethylene	3	2	2	4	1	1	1	2	2	2	1	4	2.00	1.67	1.33	3.33	3	2	2	4
Ethylene thiourea	2	2	1	2	2	2	2	2	2	2	1	1	2.00	2.00	1.33	1.67	2	2	2	2
Ethylparaben	1	1	1	2	3	2	2	3	3	3	2	3	2.33	2.00	1.67	2.67	3	3	2	3
Formaldehyde	5	3	3	3	1	1	1	2	2	2	1	4	2.67	2.00	1.67	3.00	5	3	3	4
gamma-Hexachlorocyclohexane	1	1	1	1	2	2	2	2	1	1	1	1	1.33	1.33	1.33	1.33	2	2	2	2
Lead	2	2	2	3	3	1	2	4	1	1	1	1	2.00	1.33	1.67	2.67	3	2	2	4
Malathion	1	1	1	1	2	2	2	2	1	1	1	2	1.33	1.33	1.33	1.67	2	2	2	2
Manganese	2	2	2	2	4	4	3	3	2	2	1	2	2.67	2.67	2.00	2.33	4	4	3	3
Methoxychlor	1	1	1	1	2	2	2	2	1	1	1	1	1.33	1.33	1.33	1.33	2	2	2	2
Methyl Mercury	1	1	1	1	4	3	3	3	1	1	1	1	2.00	1.67	1.67	1.67	4	3	3	3
n-Hexane	5	3	2	3	1	1	1	2	3	2	2	4	3.00	2.00	1.67	3.00	5	3	2	4
octaBDE	1	1	1	1	3	3	1	2	1	1	1	1	1.67	1.67	1.00	1.33	3	3	1	2
Parathion	1	1	1	1	2	2	2	2	1	1	1	2	1.33	1.33	1.33	1.67	2	2	2	2
Pentachlorophenol	2	2	2	2	1	1	1	1	1	1	1	1	1.33	1.33	1.33	1.33	2	2	2	2
pentaBDE	1	1	1	1	3	3	1	2	1	1	1	1	1.67	1.67	1.00	1.33	3	3	1	2
Permethrin	1	1	1	1	2	2	2	2	1	1	1	1	1.33	1.33	1.33	1.33	2	2	2	2
PFOS	1	1	1	1	2	2	2	2	2	2	1	2	1.67	1.67	1.33	1.67	2	2	2	2
Phenol, (1,1-dimethylethyl)-4-methoxy-	1	1	1	2	4	3	2	3	3	3	2	3	2.67	2.33	1.67	2.67	4	3	2	3
Trifluralin	1	1	1	1	2	2	2	2	1	1	1	2	1.33	1.33	1.33	1.67	2	2	2	2
Tris (1,3-dichloro-2-propyl) phosphate	3	2	1	1	3	2	2	2	1	1	1	2	2.33	1.67	1.33	1.67	3	2	2	2
Tris (2-chloroethyl) phosphate	3	2	1	1	3	3	2	2	1	1	1	2	2.33	2.00	1.33	1.67	3	3	2	2
Vinclozolin	1	1	1	1	2	2	2	2	1	1	1	2	1.33	1.33	1.33	1.67	2	2	2	2
Vinyl Chloride	3	2	2	4	1	1	1	1	1	1	1	3	1.67	1.33	1.33	2.67	3	2	2	4

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Table 4. PRoTEGE "Tier 2" raw data for the 40 selected chemicals

Chemical	Estimated Intake through the Inhalation Route					Estimated Intake through the Ingestion Route					Estimated Total Intake				
	10th %tile	median	90th %tile	95th %tile	% > 0.1 µmol/day	10th %tile	median	90th %tile	95th %tile	% > 0.1 µmol/day	10th %tile	median	90th %tile	95th %tile	% > 0.1 µmol/day
1,2,3–Trichlorobenzene	0	0	0	0	0	0	4.49E-06	2.95E-05	4.21E-05	0	0	4.49E-06	3.02E-05	4.43E-05	0
2,4,5-Trichlorophenoxyacetic acid	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2,4-D	0	0	1.29E-04	6.57E-04	0	0	0	2.77E-04	5.78E-04	0	0	0	4.41E-04	1.52E-03	0
Aldicarb	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aroclor_1254	0	0	0	0	0	0	6.32E-07	2.25E-06	3.07E-06	0	0	6.32E-07	2.29E-06	3.22E-06	0
Arsenic	1.63E-04	4.30E-04	1.58E-03	1.85E-03	0	2.65E-03	1.72E-02	3.64E-01	6.89E-01	2.01E+01	2.73E-03	1.76E-02	3.86E-01	7.40E-01	2.05E+01
Atrazine	0	0	2.50E-06	4.95E-06	0	1.56E-05	1.06E-04	7.74E-04	1.30E-03	0	1.50E-05	1.06E-04	8.08E-04	1.39E-03	0
Bisphenol-A	1.19E-05	2.58E-05	5.54E-05	6.88E-05	0	7.53E-07	2.36E-06	7.88E-04	6.79E-03	0	1.25E-05	2.81E-05	1.11E-03	8.55E-03	0
C10-13 Chloroalkanes	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Cadmium	1.06E-05	6.66E-05	1.98E-04	2.47E-04	0	1.44E-02	3.58E-02	7.64E-02	9.65E-02	4.49E+00	1.41E-02	3.59E-02	7.77E-02	9.98E-02	4.98E+00
Carbaryl	0	0	1.95E-04	4.48E-04	0	0	0	7.27E-03	1.48E-02	9.47E-01	0	0	7.86E-03	1.67E-02	
DDT	3.66E-07	1.34E-06	1.04E-05	2.32E-05	0	0	0	3.84E-05	1.00E-04	0	3.57E-07	1.34E-06	5.25E-05	1.40E-04	0
decaBDE	0	0	4.07E-09	9.47E-09	0	0	1.52E-06	8.64E-06	1.98E-05	0	0	1.52E-06	9.09E-06	2.07E-05	0
DEHP, Di(2-ethylhexyl)phthalate	8.68E-04	1.92E-03	5.38E-03	6.70E-03	0	1.27E-01	3.37E-01	9.25E-01	1.32E+00	9.41E+01	1.25E-01	3.39E-01	9.51E-01	1.40E+00	9.37E+01
Diethyl Phthalate	1.42E-02	3.35E-02	7.15E-02	8.81E-02	3.13E+00	1.56E-02	5.39E-02	9.70E-02	1.13E-01	8.78E+00	2.90E-02	8.74E-02	1.70E-01	2.07E-01	4.08E+01
Di-n-butylphtalate	4.13E-03	8.50E-03	1.59E-02	1.90E-02	2.19E-01	7.65E-02	2.48E-01	1.01E+00	1.63E+00	8.44E+01	7.86E-02	2.57E-01	1.05E+00	1.77E+00	8.53E+01
Ethane, 1,1,2,2-tetrachloro-	5.67E-03	1.48E-02	3.82E-02	6.10E-02	9.84E-01	0	0	0	0	0	5.59E-03	1.48E-02	3.92E-02	6.40E-02	1.90E+00
Perchlorethylene	8.48E-03	5.29E-02	2.99E-01	4.47E-01	3.46E+01	0	0	1.51E-03	4.11E-03	4.47E-01	8.21E-03	5.29E-02	3.09E-01	4.77E-01	3.47E+01
Ethylene thiourea	0	0	2.02E-08	1.65E-07	0	0	0	0	2.24E-03	8.26E-01	0	0	2.42E-08	2.76E-03	1.64E+00
Ethylparaben	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Formaldehyde	6.98E-01	5.50E+00	1.52E+01	1.99E+01	9.97E+01	0	0	0	0	0	6.83E-01	5.50E+00	1.54E+01	2.08E+01	9.94E+01
gamma-Hexachlorocyclohexane	3.74E-07	9.44E-07	3.48E-06	4.12E-06	0	0	0	6.49E-05	1.41E-04	0	3.66E-07	9.44E-07	7.21E-05	1.60E-04	0
Lead	1.92E-04	1.19E-03	2.63E-02	4.69E-02	6.30E-01	2.17E-04	4.55E-03	1.79E-02	2.50E-02	9.58E-01	3.85E-04	5.74E-03	4.61E-02	7.52E-02	2.75E+00
Malathion	0	0	0	0	0	1.48E-04	1.54E-03	5.84E-03	8.18E-03	3.59E-01	1.33E-04	1.54E-03	5.97E-03	8.53E-03	7.04E-01
Manganese	1.29E-03	4.51E-03	2.00E-02	2.88E-02	8.71E-01	8.68E+00	2.12E+01	4.37E+01	5.30E+01	0	8.50E+00	2.12E+01	4.43E+01	5.44E+01	9.99E+01
Methoxychlor	7.10E-06	8.63E-06	1.06E-05	1.07E-05	0	0	0	0	1.11E-05	0	7.08E-06	8.63E-06	1.06E-05	2.36E-05	0
Methyl Mercury	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
n-Hexane	1.69E-01	3.67E-01	7.99E-01	1.02E+00	9.80E+01	0	0	0	0	0	1.67E-01	3.67E-01	8.12E-01	1.06E+00	9.75E+01
octaBDE	9.43E-10	6.29E-09	2.36E-08	3.38E-08	0	0	0	1.88E-07	3.64E-07	0	8.52E-10	6.29E-09	2.22E-07	4.26E-07	0
Parathion	0	0	0	0	0	0	0	2.06E-04	2.97E-04	0	0	0	2.11E-04	3.13E-04	0
Pentachlorophenol	7.51E-04	1.08E-03	1.51E-03	1.69E-03	0	0	0	0	0	0	7.40E-04	1.08E-03	1.52E-03	1.70E-03	0
pentaBDE	1.09E-07	2.75E-07	6.97E-07	9.02E-07	0	1.46E-07	2.04E-06	7.45E-06	1.17E-05	0	2.41E-07	2.32E-06	8.39E-06	1.37E-05	0
Permethrin	0	0	0	0	0	0	0	6.10E-04	1.96E-03	9.98E-01	0	0	6.57E-04	2.46E-03	1.95E+00
PFOS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Phenol, (1,1-dimethylethyl)-4-methoxy-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Trifluralin	0	0	2.53E-05	5.30E-05	0	0	0	0	0	0	0	0	2.65E-05	6.10E-05	0
Tris (1,3-dichloro-2-propyl) phosphate	0	0	1.15E+00	2.54E+00	2.23E+01	8.44E-05	2.52E-04	3.25E-04	3.37E-04	0	8.37E-05	2.52E-04	1.20E+00	2.76E+00	2.25E+01
Tris (2-chloroethyl) phosphate	3.30E-02	2.85E-01	1.01E+01	1.85E+01	7.38E+01	8.27E-05	2.53E-04	3.36E-04	3.67E-04	5.63E-01	3.08E-02	2.85E-01	1.07E+01	1.92E+01	7.36E+01
Vinclozolin	0	0	0	0	0	0	0	0	1.48E-04	9.11E-01	0	0	0	2.16E-04	1.82E+00
Vinyl Chloride	3.45E-03	1.48E-02	4.14E-02	5.81E-02	1.83E+00	0	0	0	3.00E-04	5.05E-01	3.33E-03	1.48E-02	4.23E-02	6.12E-02	2.56E+00

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Table 5. PRoTEGE "Tier 2" exposure rankings for the 40 selected chemicals

Chemical	Ranking Based on Inhalation Route					Ranking Based on Ingestion Route					Ranking Based on Aggregate Exposure					Ranking Based on Dominant Exposure Route for Each Metric				
	10th %tile	median	90th %tile	95th %tile	% > 0.1 µmol/day	10th %tile	median	90th %tile	95th %tile	% > 0.1 µmol/day	10th %tile	median	90th %tile	95th %tile	% > 0.1 µmol/day	10th %tile	median	90th %tile	95th %tile	% > 0.1 µmol/day
1,2,3–Trichlorobenzene	0	0	0	0	0	0	2	1	1	0	0	2	2	1	0	0	4	4	5	0
2,4,5-Trichlorophenoxyacetic acid	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2,4-D	0	0	2	3	0	0	0	2	3	0	0	0	2	2	0	0	0	4	4	0
Aldicarb	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aroclor 1254	0	0	0	0	0	0	1	1	1	0	0	1	1	1	0	0	5	5	5	0
Arsenic	2	2	3	3	0	3	4	5	5	5	3	4	5	5	3	3	2	2	2	2
Atrazine	0	0	1	2	0	1	2	3	3	0	2	2	2	2	0	4	4	4	4	0
Bisphenol-A	2	2	2	2	0	1	1	3	3	0	2	2	3	3	0	4	4	4	3	0
C10-13 Chloroalkanes	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Cadmium	2	2	3	2	0	4	5	5	5	4	4	4	4	4	3	2	2	2	2	3
Carbaryl	0	0	3	3	0	0	0	3	4	3	0	0	3	3	2	0	0	3	3	4
DDT	1	1	2	2	0	0	0	2	2	0	1	1	2	2	0	5	5	4	4	0
decaBDE	0	0	1	1	0	0	1	1	1	0	0	1	1	1	0	0	5	5	5	0
DEHP, Di(2-ethylhexyl)phthalate	3	3	3	3	0	5	5	5	5	5	5	5	5	5	5	1	1	1	1	1
Diethyl Phthalate	5	4	4	4	3	5	5	5	5	5	4	4	4	4	4	2	2	2	2	2
Di-n-butylphtalate	4	4	4	4	1	5	5	5	5	5	5	5	5	5	5	1	1	1	1	1
Ethane, 1,1,2,2-tetrachloro-	4	4	4	4	2	0	0	0	0	0	3	3	3	4	2	3	3	3	2	4
Perchlorethylene	4	5	5	5	4	0	0	3	3	1	4	4	4	4	4	2	2	2	2	2
Ethylene thiourea	0	0	1	1	0	0	0	0	3	2	0	0	1	3	1	0	0	5	3	5
Ethylparaben	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Formaldehyde	5	5	5	5	5	0	0	0	0	0	5	5	5	5	5	1	1	1	1	1
gamma-Hexachlorocyclohexane	1	1	2	1	0	0	0	2	2	0	1	1	2	2	0	5	5	4	4	0
Lead	3	3	4	4	1	3	3	4	4	3	2	3	4	4	3	4	3	3	3	4
Malathion	0	0	0	0	0	2	3	3	3	1	2	3	3	3	1	4	3	3	3	5
Manganese	3	3	4	4	2	5	5	5	5	0	5	5	5	5	5	1	1	1	1	5
Methoxychlor	2	2	2	2	0	0	0	0	1	0	2	2	1	1	0	5	4	5	5	0
Methyl Mercury	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
n-Hexane	5	5	5	5	5	0	0	0	0	0	5	5	5	5	5	1	1	1	1	1
octaBDE	1	1	1	1	0	0	0	1	1	0	1	1	1	1	0	5	5	5	5	0
Parathion	0	0	0	0	0	0	0	2	2	0	0	0	2	2	0	0	0	4	4	0
Pentachlorophenol	3	3	3	3	0	0	0	0	0	0	3	3	3	2	0	4	4	3	4	0
pentaBDE	1	1	1	1	0	1	1	1	1	0	1	2	1	1	0	5	5	5	5	0
Permethrin	0	0	0	0	0	0	0	3	3	3	0	0	2	2	2	0	0	4	4	3
PFOS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Phenol, (1,1-dimethylethyl)-4-methoxy-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Trifluralin	0	0	2	2	0	0	0	0	0	0	0	0	1	1	0	0	0	5	5	0
Tris (1,3-dichloro-2-propyl) phosphate	0	0	5	5	3	2	2	2	2	0	2	2	5	5	4	4	4	1	1	2
Tris (2-chloroethyl) phosphate	5	5	5	5	4	2	2	2	3	1	4	5	5	5	4	2	1	1	1	1
Vinclozolin	0	0	0	0	0	0	0	0	2	2	0	0	0	2	1	0	0	0	4	5
Vinyl Chloride	4	4	4	4	2	0	0	0	2	1	3	3	3	4	3	3	3	2	2	3

1.2.1 Hazard, Exposure and Risk Characterization

The next paragraphs summarize the project implementation steps followed in the exploratory case studies for 40 representative chemicals; in the current project phases these steps are being optimized, coded, and incorporated in the integrated computational system.

The conceptual approach being "automated" in the current project phase is schematically presented in Figure 5.

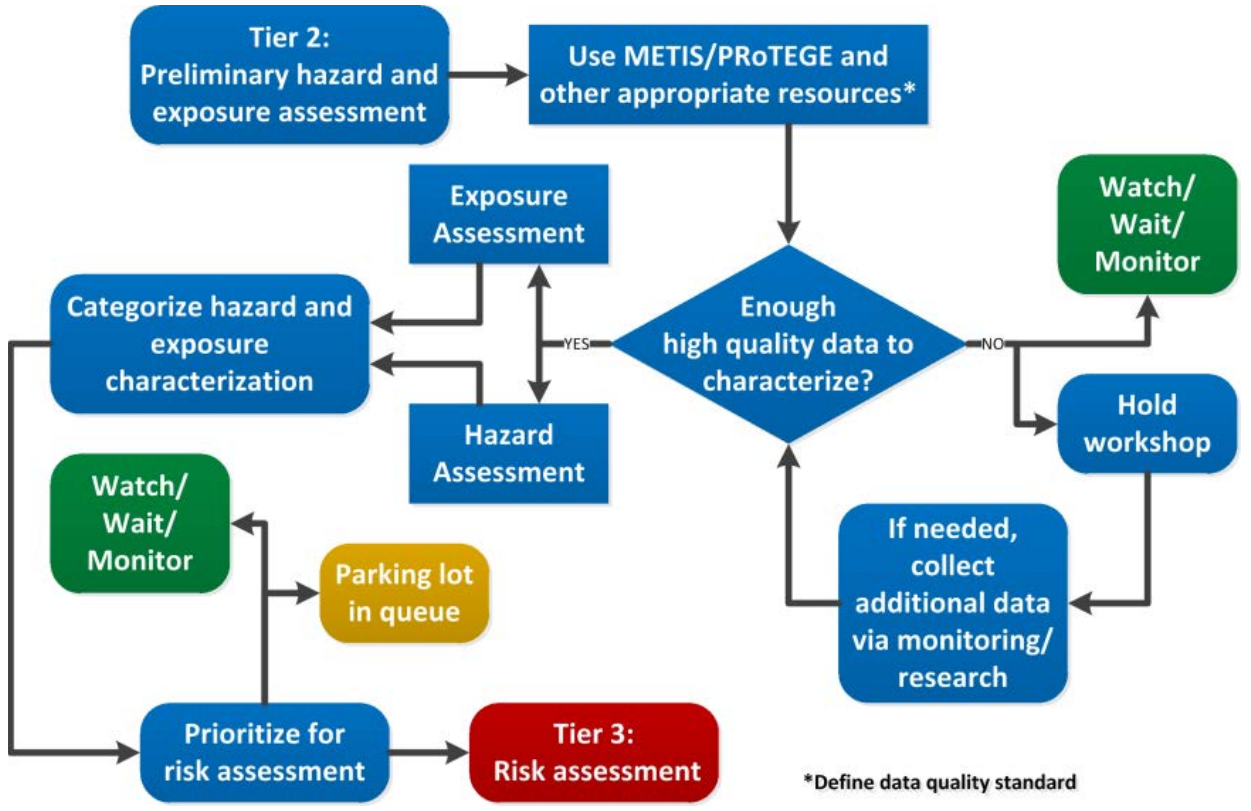


Figure 5. Tier 2 approach for preliminary hazard and exposure assessment employing PRoTEGE and METIS; adapted from NJ DEP SAB CEC Subcommittee [5]

1.2.1.1 Hazard characterization and categorization

Hazard characterization and categorization employs information retrieved using METIS, following the criteria described in:

- EPA - TSCA Work Plan Chemicals: Methods Document [16],
- EPA - Design for the Environment Program Alternatives Assessment Criteria for Hazard Evaluation [17].

For hazards related to human health, evidence relevant to mammalian toxicity are considered, specifically:

- acute systemic toxicity,
- carcinogenicity, mutagenicity, reproductive/developmental toxicity (including endocrine disruption),
- neurobehavioral toxicity,
- repeated dose target organ toxicity,
- chemical respiratory sensitization.

These human health hazards are categorized as very high, high, moderate, low and very low, correspondingly, when there is:

- strong weight of evidence for mammalian toxicity (high hazard),

- uncertainty about or moderate weight of evidence or no data for mammalian toxicity (moderate hazard),
- weak weight of evidence for mammalian toxicity (low hazard).

Though the current focus is primarily on human health hazards, exposures and risks, exploratory work has also commenced for the consideration of ecological risks (that will be fully incorporated in the integrated NJrisk system in subsequent project phases).

For hazards related to ecological impact, evidence related to acute and/or chronic aquatic toxicity will be considered, specifically:

- fish toxicity,
- crustacean toxicity,
- algal toxicity.

Ecological hazards will be categorized as high, moderate and low when there is:

- strong weight of evidence for environmental (aquatic) toxicity (high hazard),
- uncertainty about or moderate weight of evidence or no data for environmental (aquatic) toxicity (moderate hazard),
- weak weight of evidence for environmental (aquatic) toxicity (low hazard).

One special issue with respect to hazard characterization involves chemicals that impact the endocrine system. The integrated framework will evaluate endocrine activity rather than simply characterizing hazards in terms of "endocrine disruption." Endocrine activity can be defined as a change in endocrine homeostasis caused by a chemical or other stressor from human activities (e.g., application of pesticides, the discharge of industrial chemicals to air, land, or water, or the use of synthetic chemicals in consumer products.). Data to be considered will include:

- *in vitro* data such as hormone receptor binding assays or ex vivo assays,
- *in vivo* data from studies of intact animals or wildlife (including aquatic organisms),
- ethically conducted human studies,
- *in vivo* short term exposures or altered (e.g., ovariectomized) animal models,
- structural similarity to known endocrine active substances using SAR tools such as AIM, QSAR, etc.

Each chemical of concern will be evaluated for evidence of presence of endocrine activity:

- If data show evidence of endocrine activity then the chemical is designated as *potentially endocrine active*, while noting caveats and limitations.
- If there are no data available to evaluate this endpoint, endocrine activity is unknown and would be marked to indicate the *absence of information*.
- If data conclude no evidence of activity (no binding, perturbation, or evidence of endocrine-related adverse effects) then the chemical will be designated as having *no evidence of endocrine activity*, noting caveats and limitations.

1.2.1.2 Exposure characterization and categorization

Exposure characterization and categorization employs PRoTEGE to quantify and rank (potential) exposures as very high, high, moderate, low, and very low:

- **Very High and High Exposures** are associated with presence of the chemical of (current or emerging) concern in:
  - New Jersey environmental media and biota at significant concentration levels or as significant levels of biomarker measurements (where, in both cases, significance is determined for each chemical in relation to threshold levels associated with hazardous effects of the chemical),
  - food, children's toys, cosmetics/personal care products, consumer products, etc.
- **Moderate Exposures** are associated with presence of the chemical of concern in New Jersey environmental media and biota at concentrations less than the levels considered significant above but that may be steadily increasing due to continuing use of the chemical in products or due to ongoing activity of emission sources.
- **Low and Very Exposures** are associated with presence of the chemical of concern in New Jersey environmental media and biota at low detectable concentrations or in new consumer products that have minor but potential increasing market penetration.

1.2.1.3 Risk characterization and categorization

Risk characterization and categorization ("tiered assessment") for each chemical of current or emerging concern employs the hazard and exposure rankings developed in the steps above. (These characterizations will ultimately include both human [mammalian] and ecological risk assessments and will determine whether or not a CEC candidate could be a significant risk that merits consideration on the New Jersey CEC prioritization list. The system will ultimately offer various options to the user, for both analysis and visualization.) One basic option for initial prioritization of chemicals for risk assessment is the calculation of a simple "prioritization score" that is defined as:

$$\boxed{\textit{Prioritization Score} = \textit{Hazard Category} \times \left(1 + \textit{Exposure Category}\right)}$$

In the initial prioritization process, a value of 1, 2, 3, 4 and 5, respectively, is assigned to the very low, low, moderate, high, and very high categories of hazard and of exposure. In this process any value of the initial prioritization score higher than "12" results in a recommendation for further analysis. So a "very high" designation (assigning a value of "5") in any hazard or any exposure category by itself assures that the chemical is ranked for further prioritization in the framework.

Values of the initial prioritization score in the range of 8-12 are considered as identifying a "medium priority" chemical. Values of this score that are "20" or higher identify "very high priority" chemicals for further analysis. Figure 6 provides a visualization of this scoring via a "prioritization grid" for risk assessment. The initial prioritization scores, derived through the process described above, are depicted in the right hand side of the figure: the red cells correspond to very high priority chemicals, the orange cells correspond to high priority chemicals, the yellow cells correspond to moderate priority chemicals, and the light green and dark green cells correspond to low and very low priority chemicals, respectively. The risk assessment grids in the left hand side of Figure 6 present the more detailed procedures analyzing and assessing relevant data and other information that is "condensed" into the scores used in the 5x5 grid of the right hand side of Figure 6.

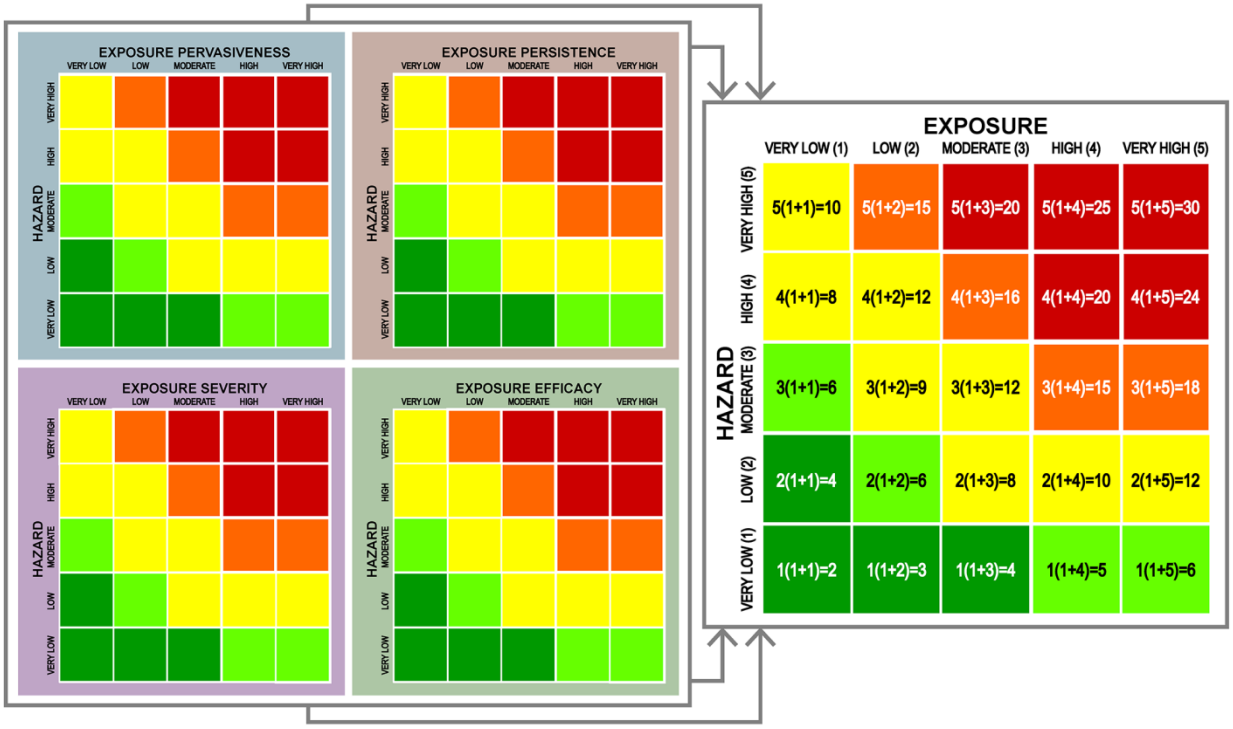


Figure 6. Prioritization grids for risk assessment. The left hand side represents metrics and scoring being developed using METIS and PRoTEGE in conjunction with available data and other information. The right hand side depicts a simple risk prioritization grid that uses "aggregated" information from the underlying processes to offer a user-friendly characterization and categorization of risk from chemicals of current and emerging concern.

1.3 Installation of METIS

In order to implement this project a "LAMP server" was set up at the Computational Chemodynamics Laboratory (CCL) for hosting METIS[1] and for the incorporation of PRoTEGE modules and expanded databases in the integrated NJrisk system. "LAMP" is an acronym for the following components of the server structure:

- Linux operating system
- Apache web server application, using Hypertext Transfer Protocol (HTTP)
- MySQL (My Structural Query Language) relational data management system
- PHP, Perl, and Python programming languages for dynamic web pages

The specific component versions of the present CCL LAMP server for METIS are:

[1] The installation of METIS on CCL's server took place under the expert guidance of Mario Chen, of Du Pont de Nemours & Co.

- Linux Fedora v15 (Lovelock)
- Apache Tomcat v6.0.37
- MySQL v5.5.20
- Perl v5.12
- Python v2.7.3
- Javascript v1.8

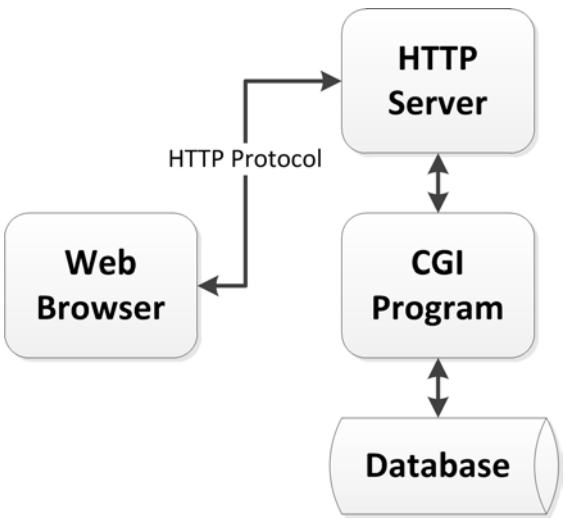


Figure 7. A general schematic for the interaction between a web browser and a LAMP server

The chain of events when accessing ("clicking on") a link in the METIS software is as follows:

- HTTP request is sent to the Apache Tomcat server with the user-specified data (e.g., chemical name, CAS number, etc.)
- The CGI program associated with the link is invoked
  - Every link in METIS is associated with a CGI program
  - All CGI programs are written in Perl
- The program opens a connection to MySQL and retrieves the user-specified data
- Then the program generates an HTML file, placing the retrieved data in the "place holders"
- The server provides this HTML file and the user is able to view the webpage from the web browser.

Apache Tomcat is being utilized as it is an open source web server that provides an environment for executing Java code. Common Gateway Interface (CGI) is enabled in Tomcat; it is required to produce dynamic web pages and it facilitates the exchange of information between the web server and a custom script (CGI script). The CGI scripts for METIS are written in Perl, although such scripts will also be written in Python, PHP, Java, C, etc. in the final implementation of NJrisk.

MySQL serves as the warehouse for the contents of METIS and is also utilized in the integrated NJrisk system. Currently, for METIS, the database contents are accessed through the Perl DBI (database-independent) interface.

2 STRUCTURE AND COMPONENTS OF NJrisk

The implementation and the completion of the Pilot case studies, employing both METIS and PRoTEGE, were used to identify and assess potential issues of consistency, compatibility, etc. in data formats and core elements, and to develop plans for implementing the linking and integration of the two software tool sets in a manner to best address analysis of the risk-relevant problems at hand while optimizing user accessibility of options and outcomes. Special effort is being put in designing a system that is flexible and easy to use so as to substantially facilitate tasks involved in the risk analysis and management processes. The full implementation utilizes specific software requirements [18] and data/workflow models to optimize usability by employing principles of "user-centered design" [19]. Figure 9 illustrates the structure and components of the in-progress integrated NJrisk system, which incorporates all the databases currently utilized in METIS and PRoTEGE *and will eventually also include other publicly-available Federal databases*, as they become available.

When completed the full integrated NJrisk system:

- will facilitate characterizing and assessing separately both hazard and exposure potentials of chemicals found in the ambient environment and/or biota as well as in various residential, occupational, and public microenvironments;
- will specifically provide tools for *rapid screening of human and ecological health risk potential*, by using the above characterizations of hazard and exposure potentials;
- will support prioritization of chemicals for regulatory action based on potential and actual human health risks relevant to both the general population and to specific subpopulations of concern and ecological health risks relevant to wildlife in aquatic, terrestrial, and air environments; and
- will be expandable, allowing the users to incorporate information and address issues related not only to human but also to ecological health risks.

As mentioned above, development and application of NJrisk is also taking advantage of and incorporating the outcomes of various ongoing initiatives by Federal (as well as international) agencies to assemble information on the physicochemical and toxicological profiles of chemicals. Such outcomes, resulting in integrated databases, are listed in Figure 9 under "Federal Database Network" (see, e.g. [1,20,21]). As an example, a database that was already linked with METIS and PRoTEGE as part of the Pilot Phase of the project, and is expected to continue to be one of the data sources for NJrisk, is USEPA's ACToR (Aggregated Computational Toxicology Resource) [1] (see Table 6). This is an evolving database that allows access to various types of data on environmental chemicals, such as information on chemical structure, *in vitro* bioassays and *in vivo* toxicology assays. Chemicals in ACToR are compiled from sources that include the U.S. Environmental Protection Agency (USEPA), Centers for Disease Control (CDC), U.S. Food and Drug Administration (FDA), National Institutes of Health (NIH), state agencies, corresponding government agencies in Canada, Europe and Japan, universities, the World Health Organization (WHO) and non-governmental organizations (NGOs).

The integrated NJrisk system is being formulated and tested so as to ensure that it will be able to address a variety of specific issues, situations, and chemicals that would be of particular concern for the State of New Jersey. However, when completed it will be applicable at the national (US) scale and at any location (state/county/municipality) within the contiguous US. *Special attention is being given to the development of the user interface in order to optimize its*

functionality and simplicity, ensuring that users with a wide variety of backgrounds will be able to learn its usage quickly and access efficiently the integrated NJrisk system.

Table 6. Selected databases accessed by ACToR (a project currently in progress for the USEPA)

Database	Expanded Name
ATSDR reports	Agency for Toxic Substances and Disease Registry Reports
ChEMBL	--
Danish EPA – Reports	
DSSTox	Distributed Structure-Searchable Toxicity
ECHA chemicals	--
Endocrine Disruptor Screening Program Database	--
Environment Canada Domestic Substances List	--
EPA SRS	EPA Substance Registry Services
EPISuite data	Experimental data used for EpiSuite modeling program
ExpoCastDB	--
IRIS	Integrated Risk Information System
IUCLID	International Uniform Chemical Information Database
NIOSH-IDLH	NIOSH - Immediately Dangerous To Life or Health Concentrations
NIOSH-NPG	NIOSH Pocket Guide to Chemical Hazards
OECD List of HPV Chemicals	--
ToxCastDB	Toxicity Forecaster database
TOXNET Toxicological data	--
ToxRefDB	Toxicity Reference Database
TSCA	Toxic Substances Control Act (TSCA) Chemical Substances Inventory
USDA PDP	USDA Pesticide Data Program

3 Current Progress

3.1 Establishment of software requirements

The findings of ongoing testing are currently being used to identify and assess potential issues of consistency, compatibility, etc. in data formats and core elements, and to establish protocols for implementing the linking and integration of the software components in a manner to best address analysis of the risk-relevant problems at hand, while optimizing user accessibility of options and outcomes. Special effort is being put in designing a system that is flexible and easy to use, so as to substantially facilitate tasks involved in the risk analysis and management processes. Ongoing effort involves establishing and refining specific software requirements [18] and developing complete data and workflow models for improved usability.

3.2 Adaptation and customization of modules from METIS and PRoTEGE

This task is systematically selecting, customizing, linking, testing, and merging components from the two operational state-of-the-art platforms (METIS and PRoTEGE) for hazard and for exposure characterization and ranking. Customization of METIS modules involves recoding that is necessary for removing various accessibility restrictions currently embedded in that system in order to allow its future use by a wider community.

The NJrisk website (Figure 9), deployed as a “testing platform” for CCL and NJDEP researchers, is accessible via password protected login. It is built on a content management system (CMS) platform using PHP and CSS3 coding and draws information from a MySQL database. This website includes an introductory information page and access to the alpha version of NJrisk, where one can search for a chemical by name or CAS number and pull up a visualization for its

hazard profile (Figure 10). There is also a comment form for NJDEP researchers to provide feedback. The current version of the NJrisk testing platform is essentially a customized version of METIS and its output does not yet include the PRoTEGE "risk grid" or "exposure rose" that will be incorporated in the near future.

In parallel, CCL researchers have been developing a local NJrisk module, that is currently undegoing online testing, which combines hazard and exposure ranking information visualized as a "hazard rose" and an "exposure rose" (for METIS hazard ranking values and PRoTEGE exposure ranking values, respectively) and a "risk grid" that shows a value based on calculation of exposure values from PRoTEGE with hazard values from METIS. This tool is also being developed on a CMS platform, making it fairly straightforward to merge all the modules of the NJrisk system.

3.2.1 How the local NJrisk module works

This module takes the following inputs:

- Chemical (name or CAS number, with and without dashes)
- ChartType (Human Exposure Rose, Human Hazard Rose or Risk Grid).

The search page is run by "inputparse.php" which calls "main.py" function, which writes the results to text files. These text files are accessed by pages which call makeCharts.js to make the exposure charts, hazard charts, and risk grids.

- Scripts include:
  - **irissearch.py** – Calculates values for exposure chart.
  - **makeCharts.js** - makes the human hazard and human exposure rose charts and human health risk grids; the coordinates for human health risk grids are calculated here.
  - **cmrsearch.py** (translated from Perl to Python) – gets data for human hazard rose chart.
  - **substancelist.txt** – CAS numbers of chemicals from IRIS. When searching for a chemical, that chemical is compared with this list. Returns result if the chemical is in this list (main.py finds the CAS number for the chemical and that CAS number is searched within this list).
  - **main.py** – Gets the chemical name from **inputparse.php**; Calls **irissearch.py** and **cmrsearch.py** functions and writes results to text files, **irisdata.txt** (info for the table that is added below the exposure chart), **cmrdata.txt** (info for Hazard chart and table below the chart) and **exposuredata.txt** (info for Exposure chart).

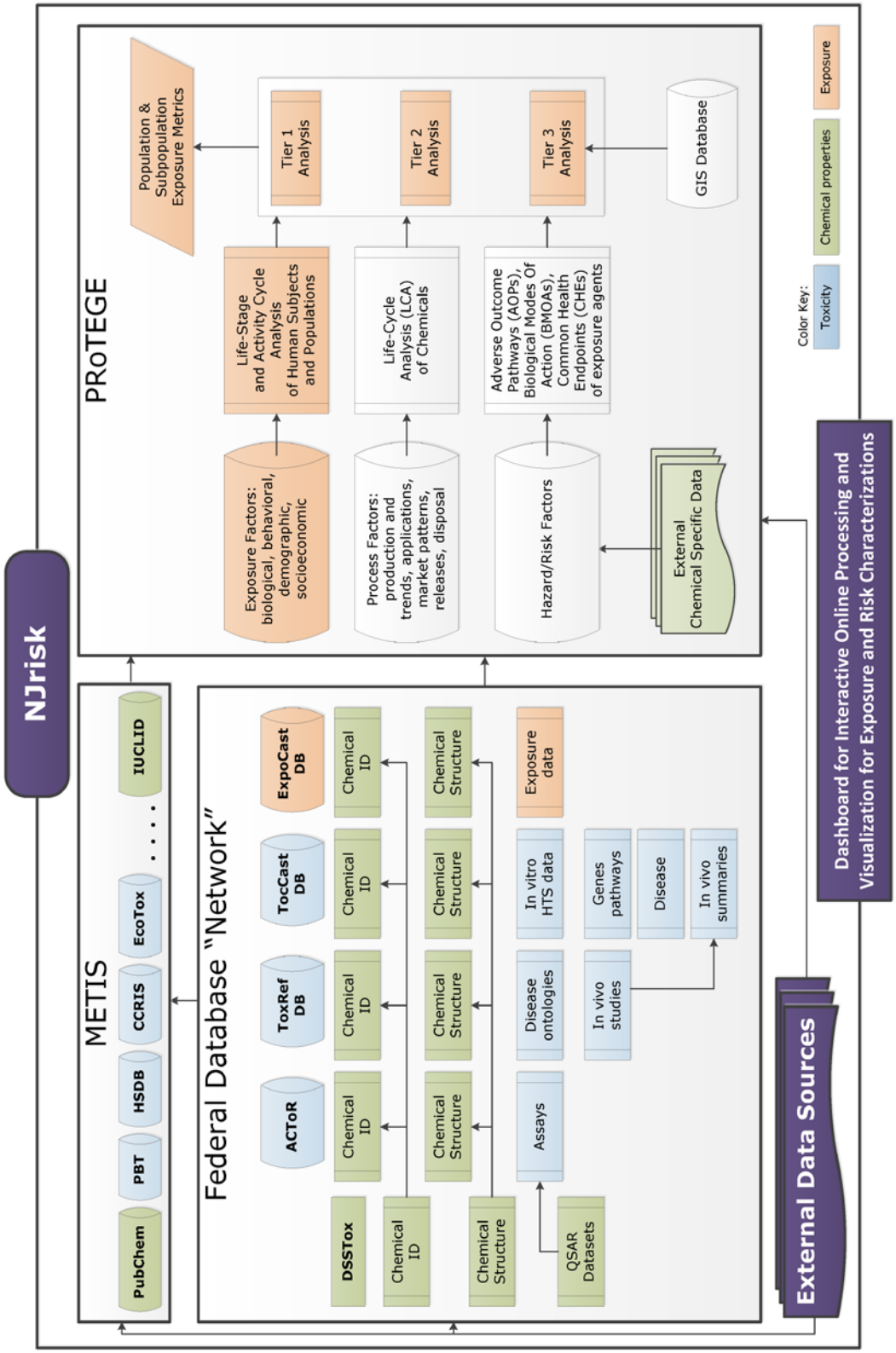


Figure 8. NJrisk – structure and components of an integrated system to allow easy user access to outcomes from PRoTEGE and METIS in conjunction with various extant databases that are available or under development at USEPA and other Federal agencies

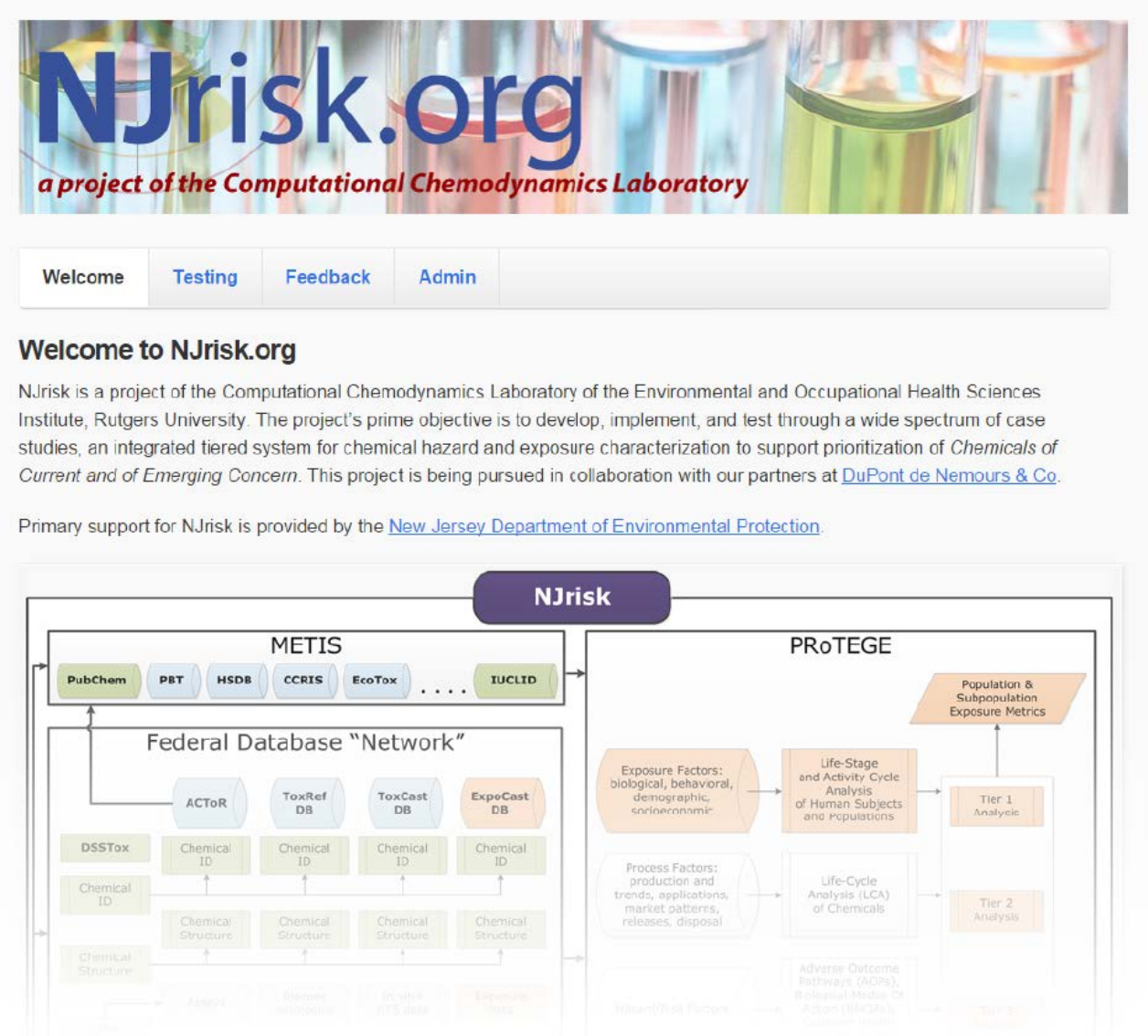
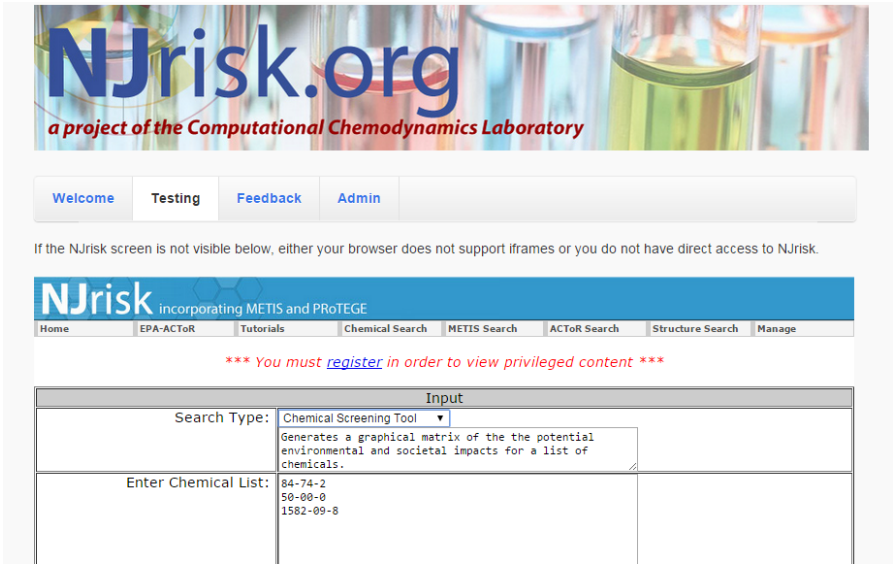


Figure 9. The njrisk.org website provides a testing platform for CCL and NJ DEP researchers



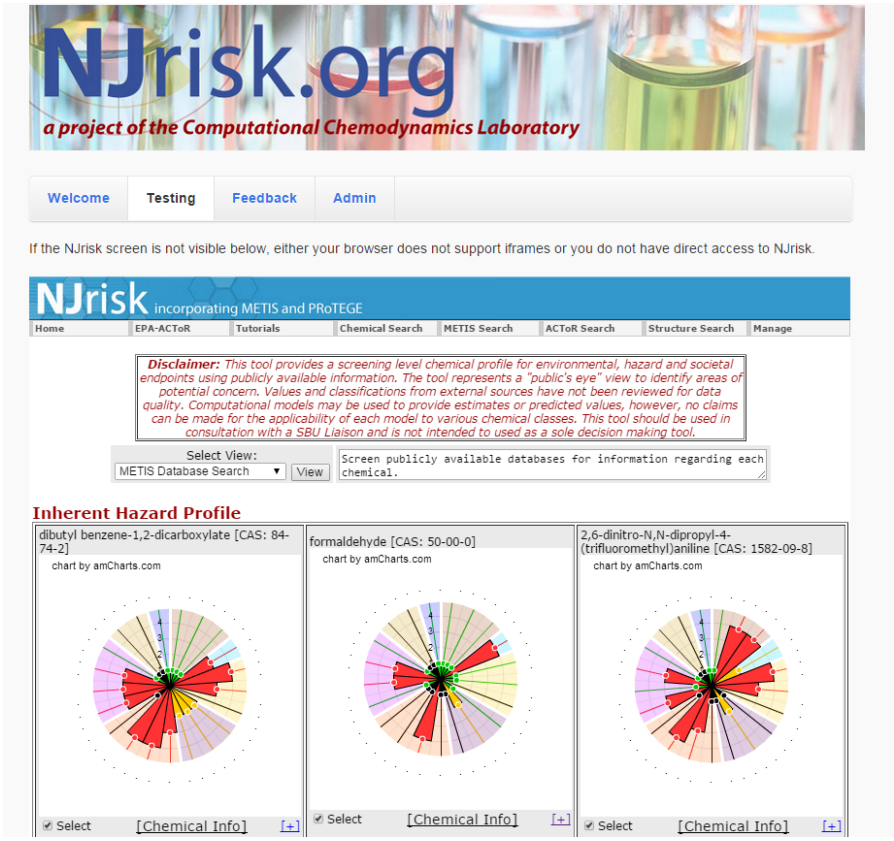


Figure 10. The "alpha" version of NJrisk allows the user to search for a chemical by name or CAS number and display a visualization for its hazard profile.

4 Results of Exploratory Case Studies for 40 Chemicals

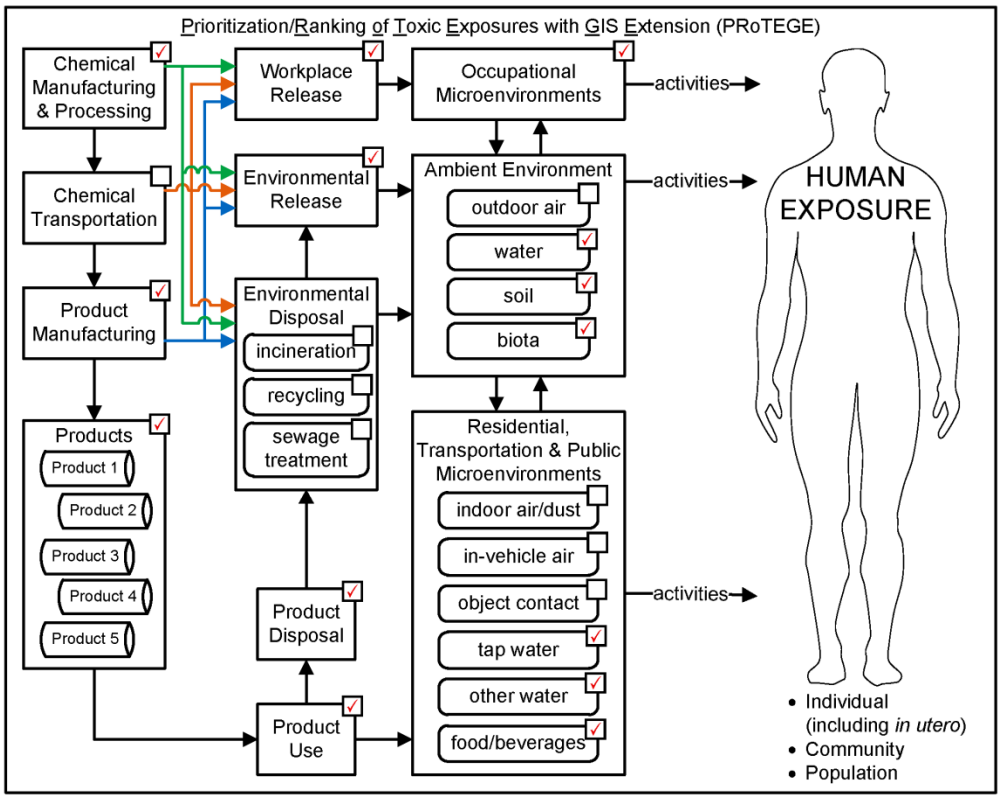
In the following pages:

- a "human hazard rose"
- a "human exposure rose" (for METIS hazard ranking values and PRoTEGE exposure ranking values, respectively) and
- a "human health risk grid" (showing a value based on calculation of exposure values from PRoTEGE with hazard values from METIS)

are presented for each of 40 current phase test-case chemicals, along with relevant information supporting the corresponding classifications and estimates.

IMPORTANT NOTE: The preliminary numerical and graphical estimates and rankings of hazard, exposure, and human health risks appearing on the following pages are being derived solely for the purpose of developing and testing the PRoTEGE and NJrisk systems and reflect work that is currently in progress and therefore incomplete. These preliminary estimates may, at this point, be using only a subset of the information sources available for completing calculations and should be expected to change, possibly substantially, in subsequent phases of the development of the PRoTEGE and NJrisk systems.

PRoTEGE Ranking for 1,2,3–Trichlorobenzene



Summary Physico-Chemical Information	
Name	1,2,3–Trichlorobenzene
Other Names	
Chemical Formula	$C_6H_3Cl_3$
Chemical Class	VOC
Identifier	CAS: 87-61-6
Chemical Forms	
Physical Properties	
Molecular weight:181.45 Solubility: Slightly soluble in ethanol; very soluble in ether and benzene Vapor pressure (25°C): 0.21 mm Hg	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits:
Toxicological Effects: Skin, eye and respiratory irritations
Exposure Limits: TEEL:5 mg/m³
Chemical Use: Transformer fluid, Chemical intermediate
Exposure Routes: Inhalation of ambient air, ingestion of food and drinking water, and dermal contact
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	NA			Data Source: Ground Water – HSDB, concluded from 78 wells in NJ; Food – HSDB [68]; Surface water – HSDB, high conc. collected in the vicinity of an industrial outfall in the Calacasieu River estuary, LA; Tap water – NCOD, 131 detected out of 136,462 analyses; Soil – HSDB; Biota – HSDB, medium (42% of fish in the 400 sites sampled in the US)	Air		
Ground water (ppb)		< LOD					
Food (µg/kg)	0.0175	0.05	0.11		Surface Water		
Indoor Air (ng/m³)	NA				Ground Water		
Surface water (ng/L)	0.1	2.3	12		Soil		
Tap water (µg/L)	0.03	1.141	15.00				
Soil (pg/g)		190	540		Chemical Production and Use		
Dust (µg/cm²)	NA				Production	< 500,000 lbs/yr	Data Source: IUR
Surfaces (µg/cm²)	NA						
Biota(ng/g)	0.1 -1	1.3	1.1-76				
Human Biomarkers				Data Source: All data from HSDB, and the studies are conducted in Canada; human milk study was done in 1992, in Canada, 54.1% of 497 samples > LOD			
Urine	NA						
Blood (ng/g)		1.17					
Adipose tissue (ng/g)		44					
Human milk (ng/g)		1.9	236				

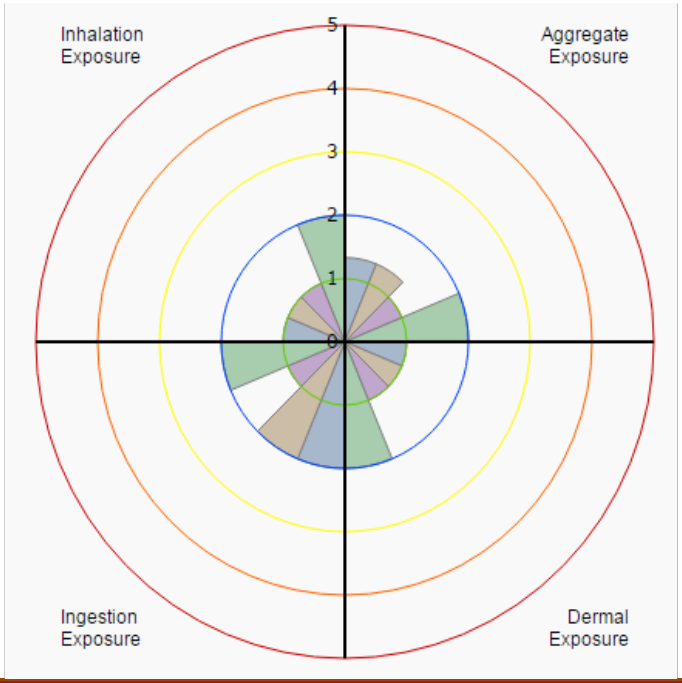
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		
	ICSC		●
	Tox Prof		
	IRIS		
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		●
	IARC		
	P□AP		●
	NTP		
	REACH		
	PFD		
	MSD		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		●
	To□Cast	Ph	
		Ph I	●
	□o□□□fDB		
	CEBS		
Prod□ction □nd Use	SIDS		
	EHPV		
	HPD		
	IUR		●
	ECD		
	□RD		
Releases	TRI		
	NEI		
Environmental Qual□ty	NGA		
	NAWQA		●
	AQS		
	CERCLIS		●
	NATA		
Mi□ro-environments and Biomarkers-Human and E□o□□□ical	TDS		
	SDW□S		
	NHA□ES	03-04	
		05-06	
		07-08	
		09-10	
	□HEXAS		
PK/PBPK Model (or Data)	ScLit		PKm (R) [19]
	BME		
	ERDEM		

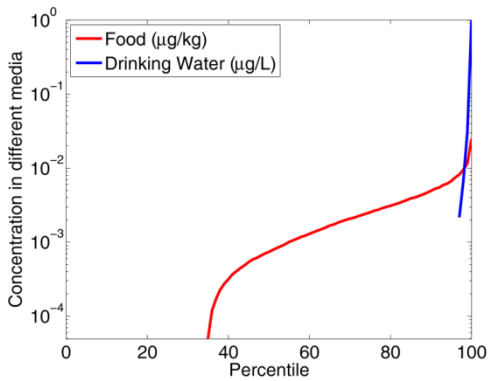
"Tier 1" Exposure Ranking for 1,2,3–Trichlorobenzene

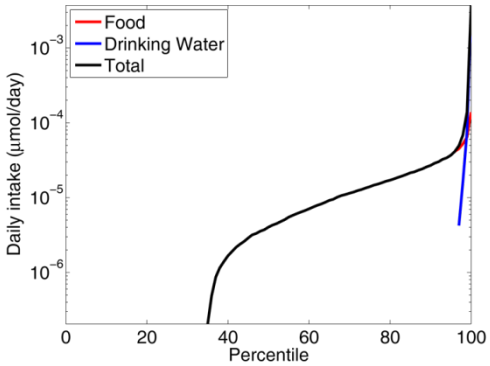
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	2
Ingestion	2	2	1	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1	2

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for 1,2,3–Trichlorobenzene





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	4.5E-06	NA	4.5E-06
90 % tile	0	2.95E-05	NA	3.02E-05
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

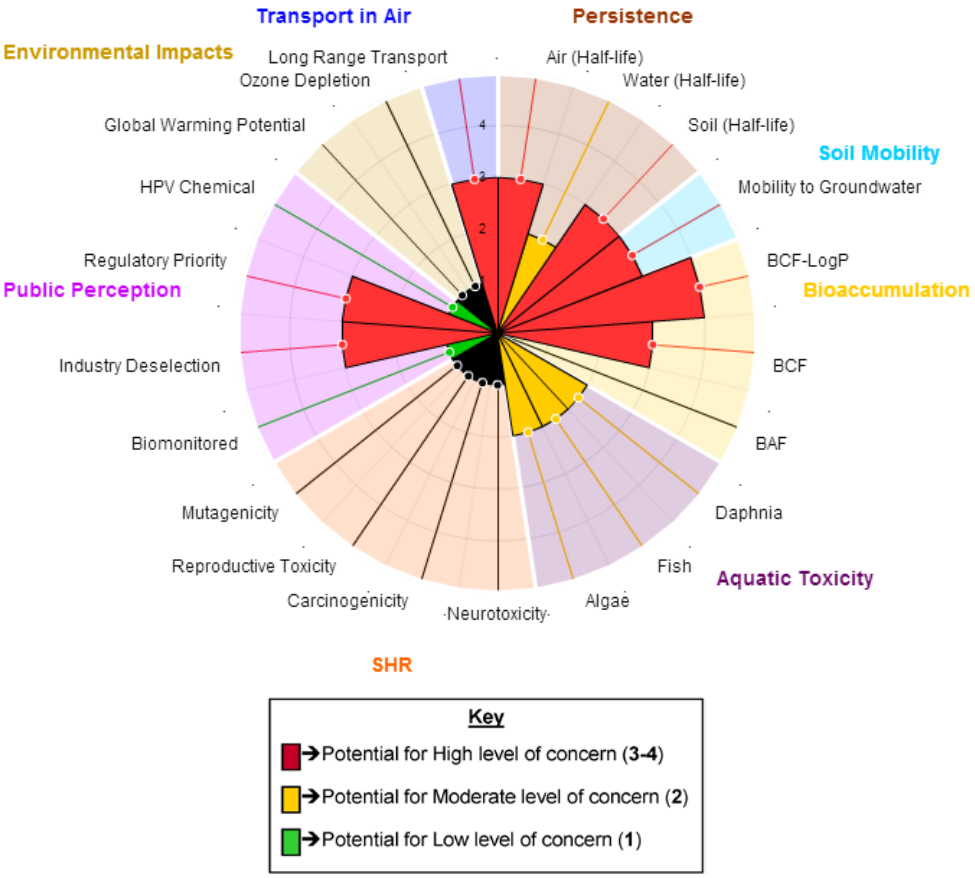
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for 1,2,3–Trichlorobenzene

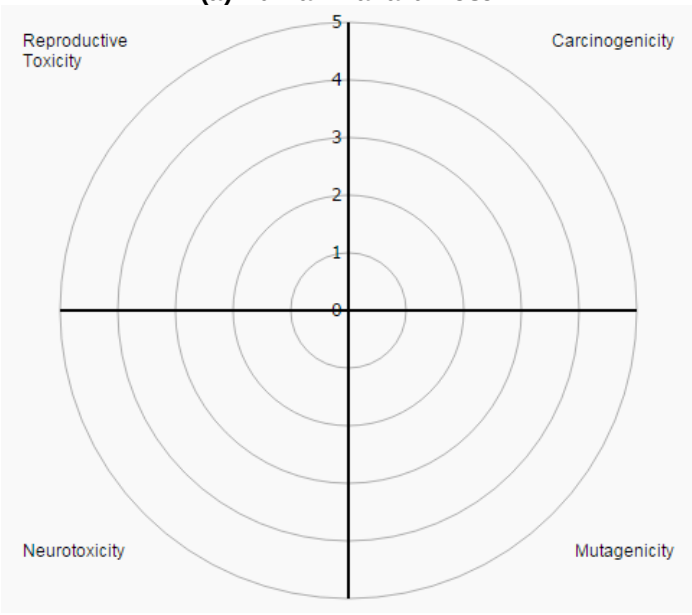
		CAS # 87-61-6
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 56.95 days)
	Water (Half-life)	Moderate persistence in Water (Estimated Half-life = 60 days)
	Soil (Half-life)	High persistence in Soil (Estimated Half-life = 120 days)
Soil Mobility	Mobility to Groundwater	High mobility to groundwater based on LogKoc = 3.141
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=4.05
	BCF	High bioconcentration potential based on Experimental LogBCF = 3.11
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) = 0.46 mg/L indicates a Moderate toxicity to Daphnia.
	Fish	A measured LC50 (96-hr) = 3.2 mg/L indicates a Moderate toxicity to Fish.
	Algae	A measured EC50 (72-hr) = 1.6 mg/L indicates a Moderate toxicity to Algae.
SHR	Neurotoxicity	
	Carcinogenicity	
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (SINLIST)
	Regulatory Priority	2 out of 10 lists (JDES_LST; JMON3)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 1382.05 km - A_TRNSPRT)



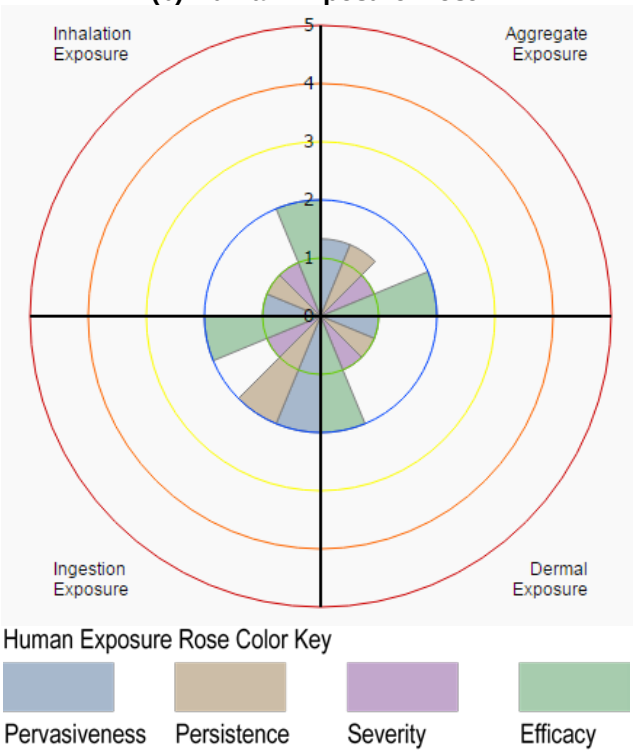
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for 1,2,3–Trichlorobenzene

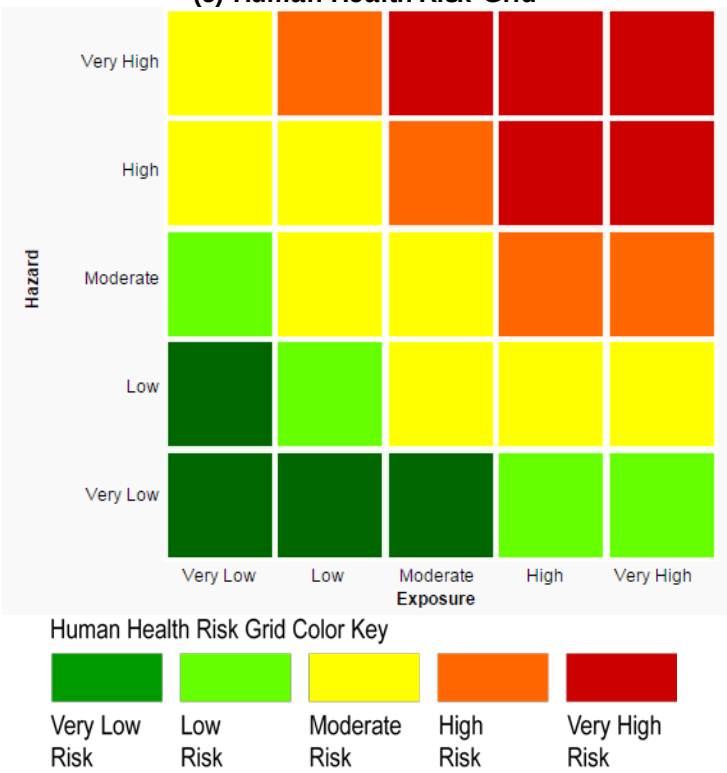
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



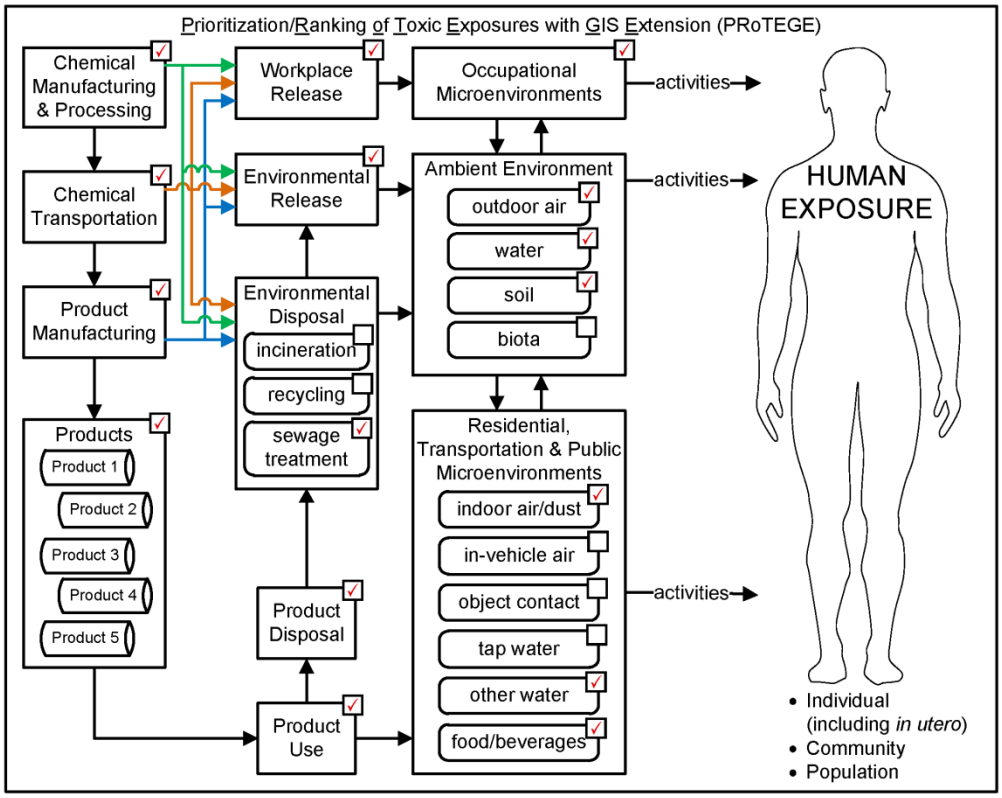
(a) Human Hazard
Estimated ranking of human hazard risk from 1,2,3–Trichlorobenzene, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of 1,2,3–Trichlorobenzene (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from 1,2,3–Trichlorobenzene, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for 2,4,5-Trichlorophenoxyacetic acid



Summary Physico-Chemical Information	
Name	2,4,5-Trichlorophenoxyacetic acid
Other Names	2,4,5-T
Chemical Formula	$Cl_3C_6H_2OCH_2COOH$
Chemical Class	Herb
Identifier	CAS: 93-76-5
Chemical Forms	
Physical Properties	
Molecular weight: 255.5 Boiling point: Decomposes Melting point: 153°C Solubility: (25°C): 0.03% Vapor pressure: 1 x 10^{-7} mmHg Specific gravity: 1.80	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD 0.01 mg/kg/day (IRIS)
Toxicological Effects: Possibly carcinogenic to humans (IARC); In animals: ataxia; skin irritation, acne-like rash; liver damage
Exposure Limits: OSHA PEL: TWA 10 mg/m³; NIOSH REL: TWA 10 mg/m³; HSDB (acceptable daily intake): 0.03 mg/kg; EPA drinking water guideline: 70 µg/L
Chemical Use: Herbicide
Exposure Routes: Inhalation, ingestion, skin and/or eye contact
Target Organs: Skin, liver, gastrointestinal tract

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air	NA			Data Source: Food - TDS('91 – '03), 1 out of 44 samples > LOD; Surface water – HSDB, 0.4% of surface water samples > LOD; Soil – HSDB, 0.2% sediment > LOD (9.1 ppb); Dust – HSDB; Biota - HSDB	Air		
Ground water (ppb)	NA						
Food (ppm)		0.004			Surface Water		
Indoor Air (ng/m³)	NA				Ground Water		
Surface water (µg/L)	<LOD – 0.4	3.0	12.9		Soil		
Tap water (µg/L)	NA						
Soil (ppb)	<LOD	9.1	100		Chemical Production and Use		
Dust (ng/g)		40			Production	Not produced in USA	HSDB
Surfaces (µg/cm²)	NA						
Biota (ppm)	<0.02	0.2- 1.8	30				
Human Biomarkers				Data Source: Urine – HSDB (Occupational study); 8.6% > LOD (NHANES)			
Urine (µg/mL)		3.5					
Blood	NA						
Other	NA						

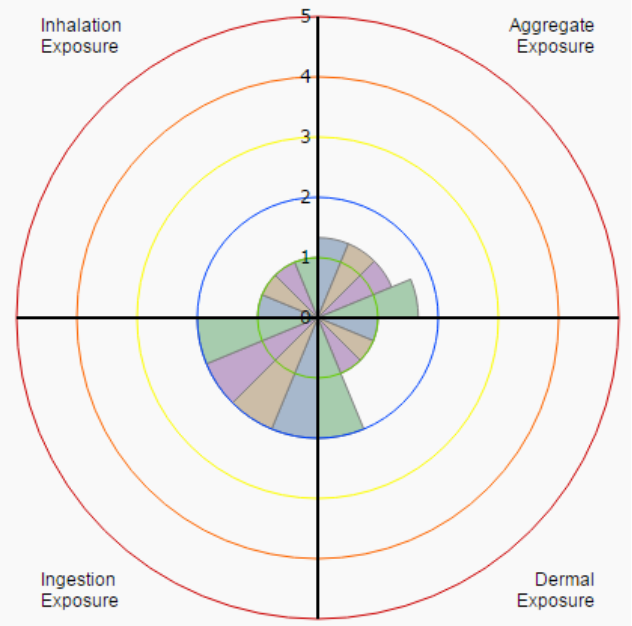
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		
	IUR		
	ECD		
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		●
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		
	NHANES	03-04	u
		05-06	(u)
		07-08	(u)
		09-10	(u)
	NHEXAS		
PK/PBPK Model (or Data)	ScLi		
	BME		
	ERDEM		

"Tier 1" Exposure Ranking for 2,4,5-Trichlorophenoxyacetic acid

Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for 2,4,5-Trichlorophenoxyacetic acid

insufficient data for analysis

insufficient data for analysis

	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0	0	NA	0
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

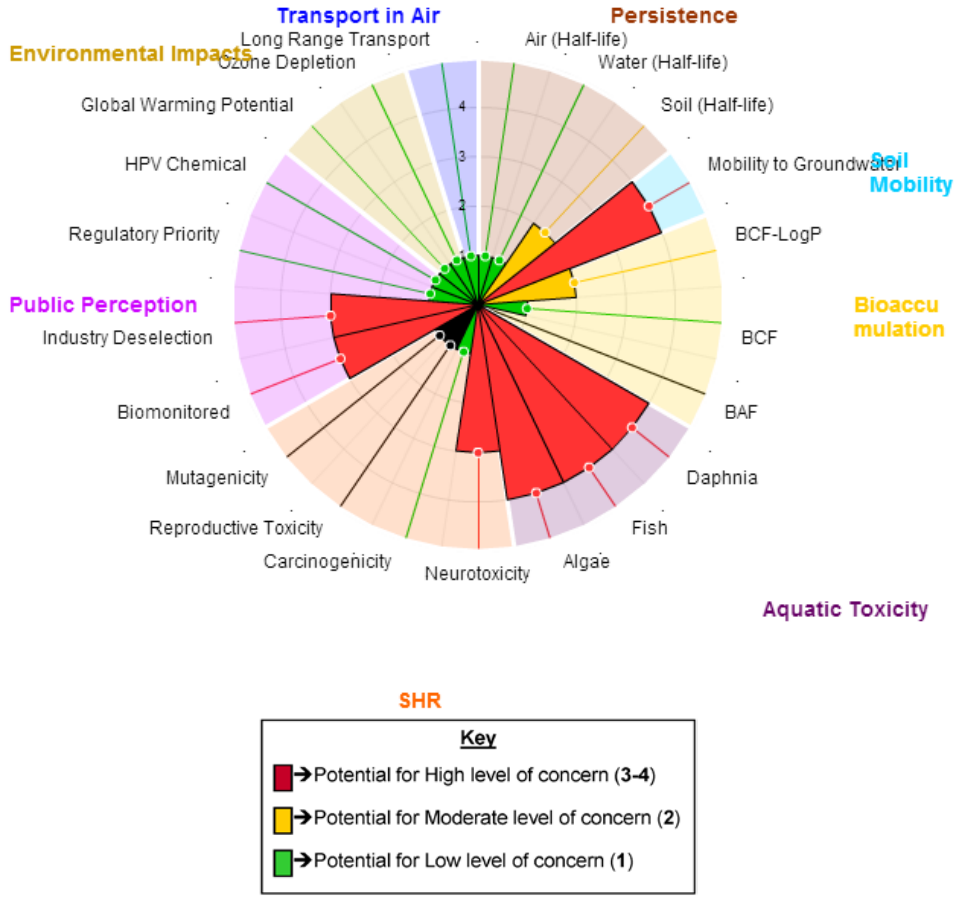
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for 2,4,5-Trichlorophenoxyacetic acid

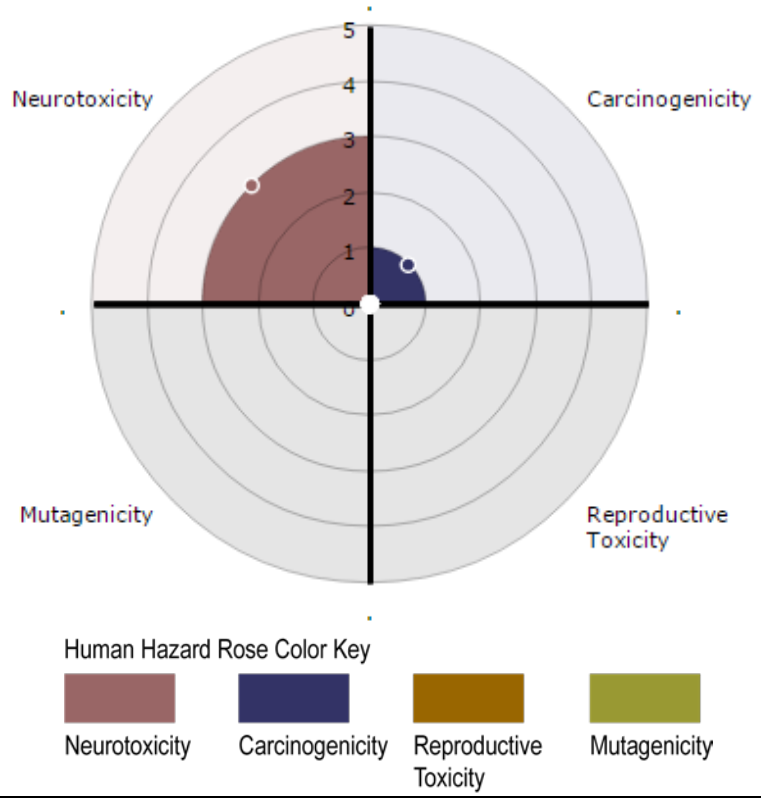
		CAS # 93-76-5
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 1.758 days)
	Water (Half-life)	Low persistence in Water (Estimated Half-life = 37.5 days)
	Soil (Half-life)	Moderate persistence in Soil (Estimated Half-life = 75 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 1.687
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=3.31
	BCF	Low bioconcentration potential based on Estimated LogBCF = 0.5
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 144.799 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 123.870 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	CLASS A4 - Not Classifiable as a Human Carcinogen [ACGIH]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	1 out of 6 lists (RC_PIC)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 37.3428 km - A_TRNSPRT)



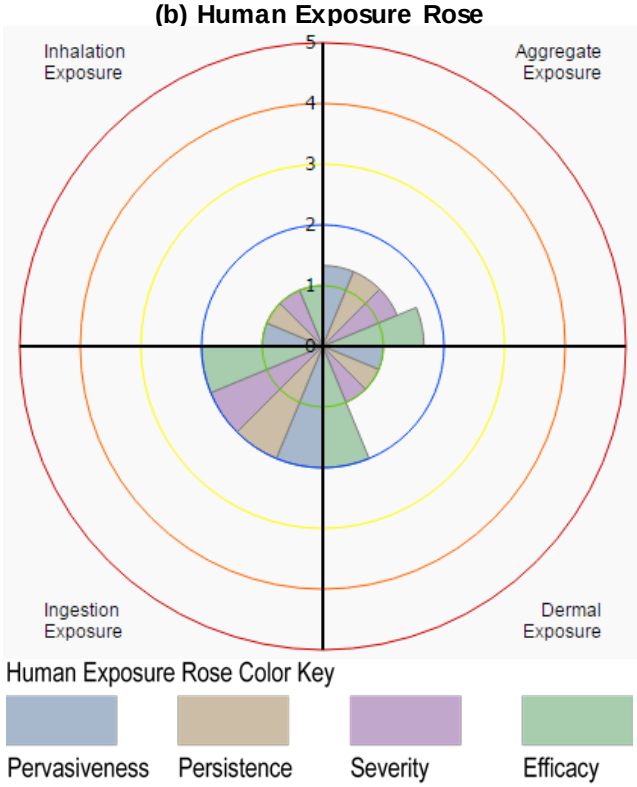
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for 2,4,5-Trichlorophenoxyacetic acid

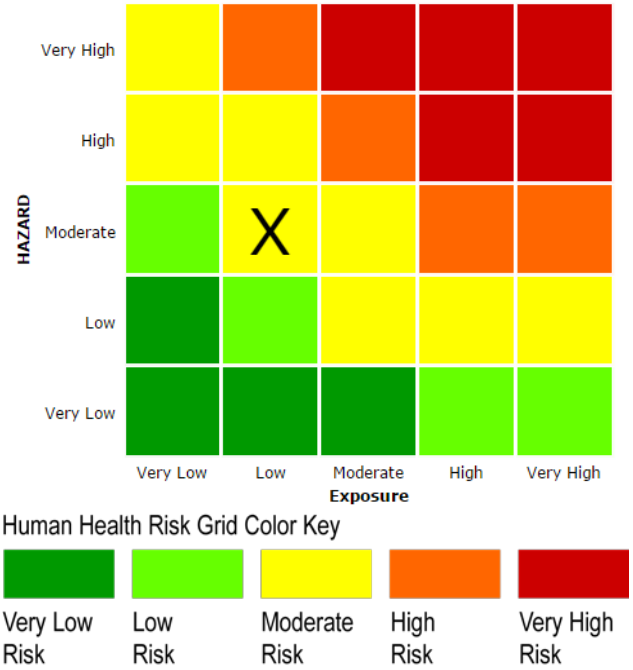
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



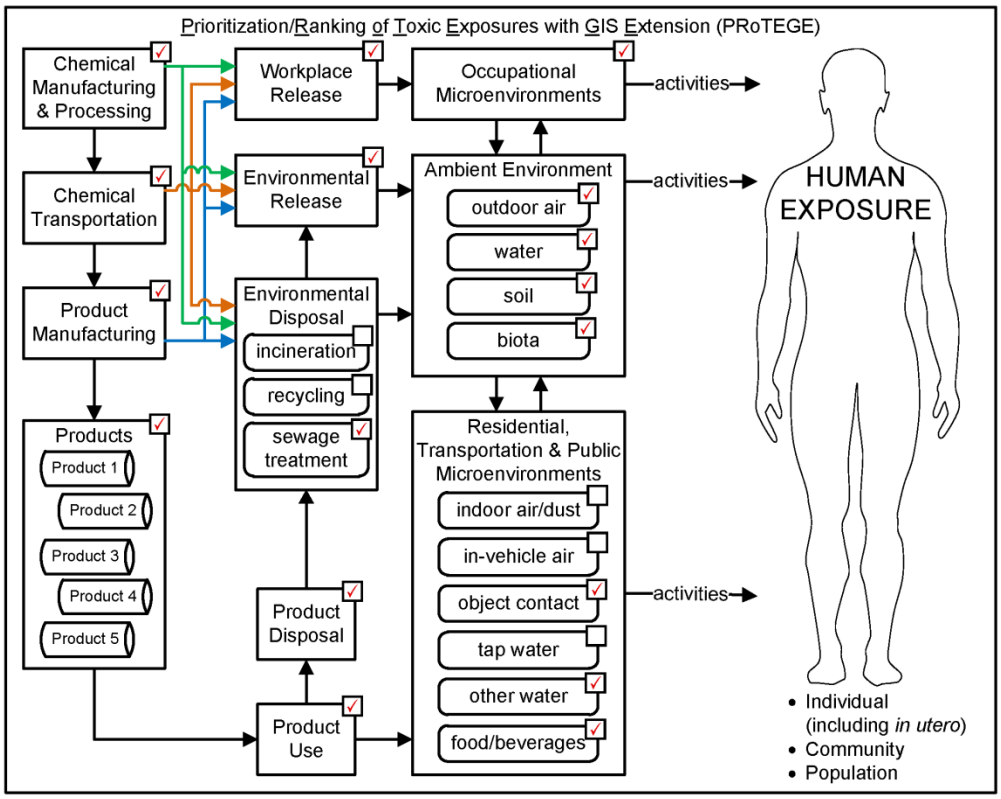
(a) Human Hazard
Estimated ranking of human hazard risk from 2,4,5-Trichlorophenoxyacetic acid, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of 2,4,5-Trichlorophenoxyacetic acid (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from 2,4,5-Trichlorophenoxyacetic acid, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

PRoTEGE Results for 2,4-D



Summary Physico-Chemical Information	
Name	2,4-D
Other Names	Dichlorophenoxyacetic acid 2,4-Dichlorophenoxyacetic acid
Chemical Formula	$Cl_2C_6H_3OCH_2COOH$
Chemical Class	Herb
Identifier	CAS: 94-75-7
Chemical Forms	
Physical Properties	
Molecular weight: 221.0 Boiling point: Decomposes Melting point: 130°C Solubility: 0.05% Vapor pressure(160°C): 0.4 mmHg Vapor pressure(20°C): 8.25 ×10^{-8} mmHg Specific gravity: 1.57	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD (mg/kg/day): 0.01 (IRIS); IDLH: 100 mg/m³ (NIOSH)
Toxicological Effects: weakness, stupor, hyporeflexia and muscle twitch; convulsions; dermatitis
Exposure Limits: NIOSH REL: TWA 10 mg/m³; OSHA PEL: TWA 10 mg/m³
Chemical Use: Herbicide; used for broadleaf weed control in agricultural and nonagricultural settings; registered for use in both terrestrial and aquatic environments.
Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact (NIOSH)
Target Organs: Skin, central nervous system, liver, kidneys

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	1.2595E-07	8.16733E-05	0.0418	Data Source: Outdoor air – (5th, 50th, 95th %iles) - NATA 2002 county level average, 1192 out of 2173 county has annual data <LOD; Ground water(min, mean, max) – HSDB, 5 of 465 >LOD; Food – (5th, 50th, 95th %iles) – TDS ('91 – '02); Surface water – (min, mean, max) - HSDB, 100 of 327 >LOD; Tap water – [23] 99% of measurements <RL; Biota - HSDB	Air	1894.24 (NEI 2005) 1.00 (TRI 2008)	16.74% (NEI 2005) 0.47% (TRI 2008)
Ground water (µg/L)	0.01	4.0	24				
Food (ppb)	1	3	8		Surface Water	0.03 (TRI 2008)	0.12% (TRI 2008)
Indoor Air (ng/m³)	NA				Ground Water	0.20 (TRI 2008)	0.03% (TRI 2008)
Surface water (µg/L)	0.01	0.33-0.36	10-15		Soil	22.77 (TRI 2008)	0.06% (TRI 2008)
Tap water (µg/L)	<RL	<RL	<RL				
Soil (µg/kg)	<LOD		38				
Dust	NA				Chemical Production and Use		
Surfaces	NA				Production	50 to < 100 million lbs/yr	Data Source: IUR
Biota(ppm)	0.001	0.013	0.22				
Human Biomarkers				Data Source: Urine - HSDB			
Urine (ppb)	<LOD		9				
Blood	NA						
Other	NA						

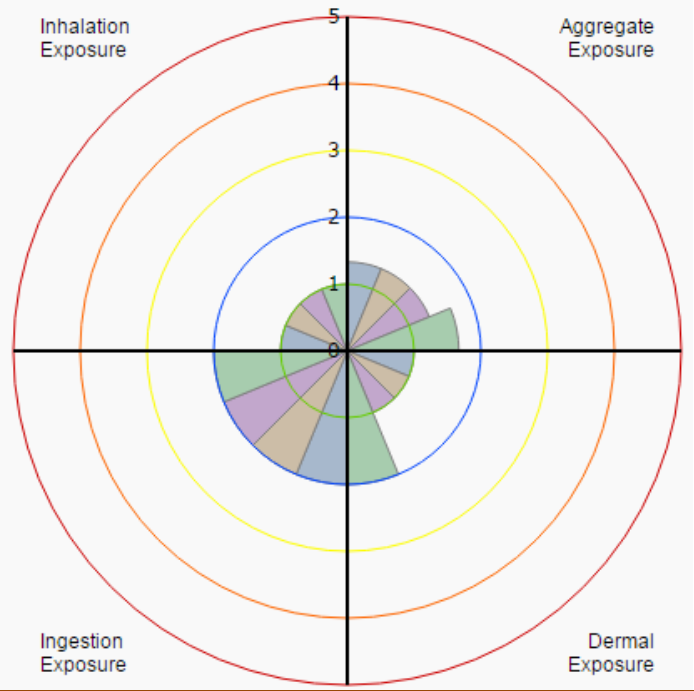
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		
Pro[illegible]tion and Use	SIDS		
	EHPV		○
	HPD		●
	IUR		●
	ECD		○
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	N[illegible]A		
	NAWQA		●
	AQS		○
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and [illegible]cologica	[illegible]DS		●
	SDWIS		●
	NHANES	03-04	u
		05-06	(u)
		07-08	(u)
		09-10	(u)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PKm (R/r) [24]
	BME		● [25]
	ERDEM		

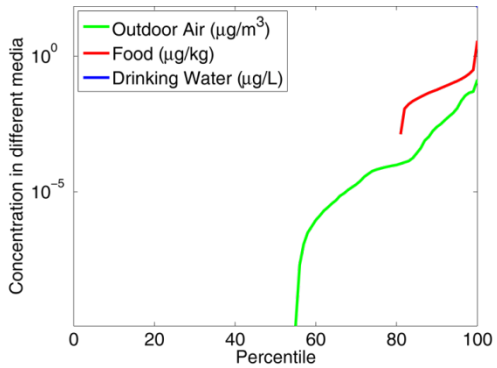
"Tier 1" Exposure Ranking for 2,4-D

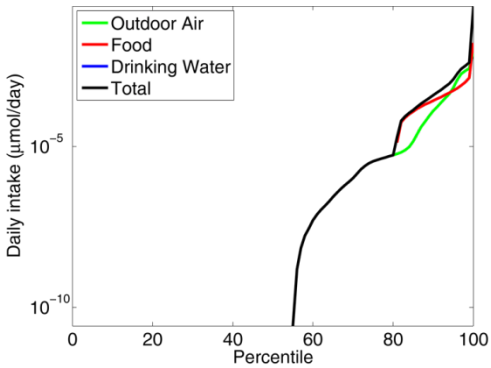
Semi-Quantitative Exposure Ranking	Pervasivenes	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for 2,4-D





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0	0	NA	0
90 % tile	0.000122	0.00028	NA	0.000437
% over 0.1 μmol/day	0	0	NA	0
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

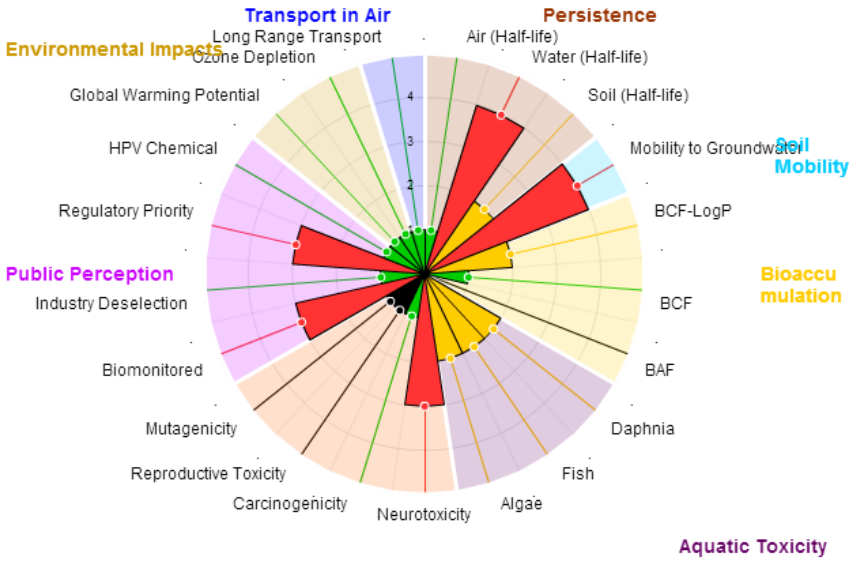
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for 2,4-D

		CAS # 94-75-7
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 1.614 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 0% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 0%, Max. BOD = 0%).
	Soil (Half-life)	Moderate persistence in Soil (Estimated Half-life = 75 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 1.468
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=2.81
	BCF	Low bioconcentration potential based on Estimated LogBCF = 0.5
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 478.931 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R52/53 (Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 428.226 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R52/53 (Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R52/53 (Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	CLASS A4 - Not Classifiable as a Human Carcinogen [ACGIH]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	0 out of 6 lists
	Regulatory Priority	2 out of 10 lists (JDES_LST; JMON3)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Tansport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 144.936 km - A_TRNSPRT)



SHR

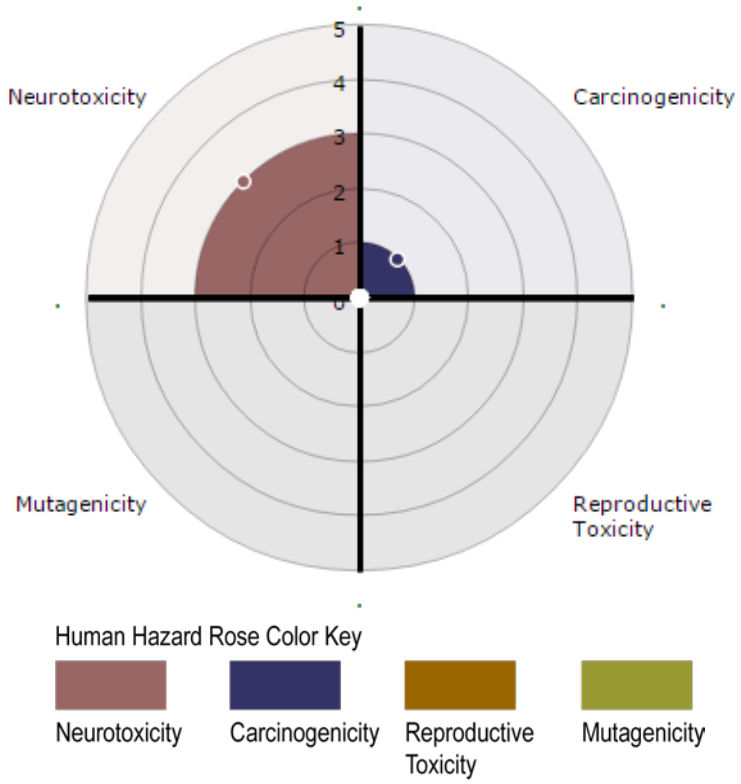
Key

- Potential for High level of concern (**3-4**)
- Potential for Moderate level of concern (**2**)
- Potential for Low level of concern (**1**)

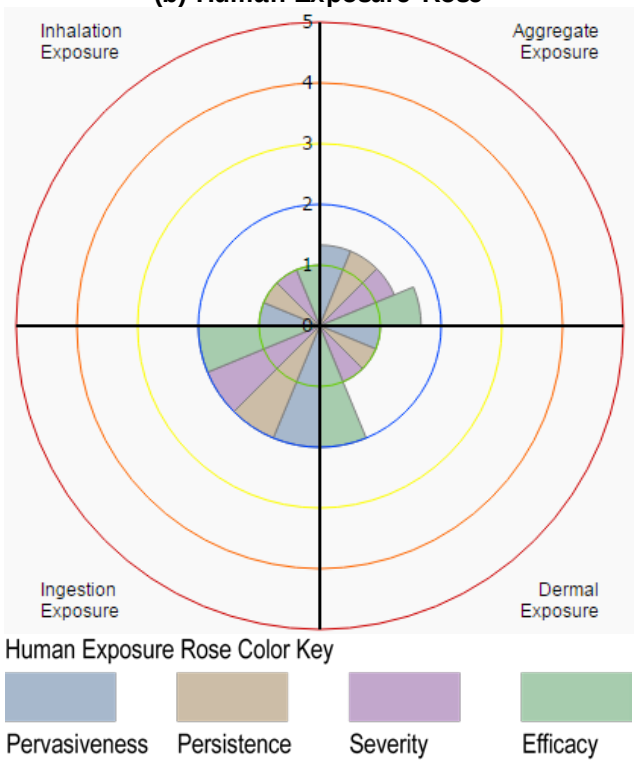
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for 2,4-D

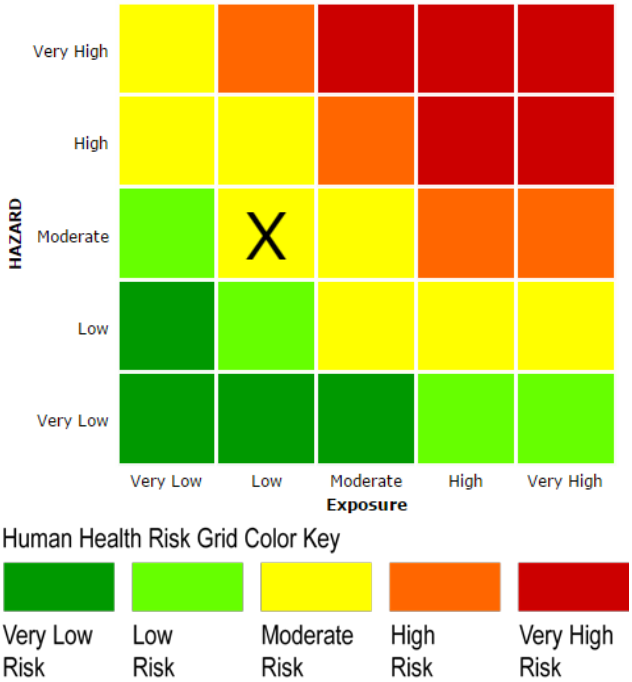
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



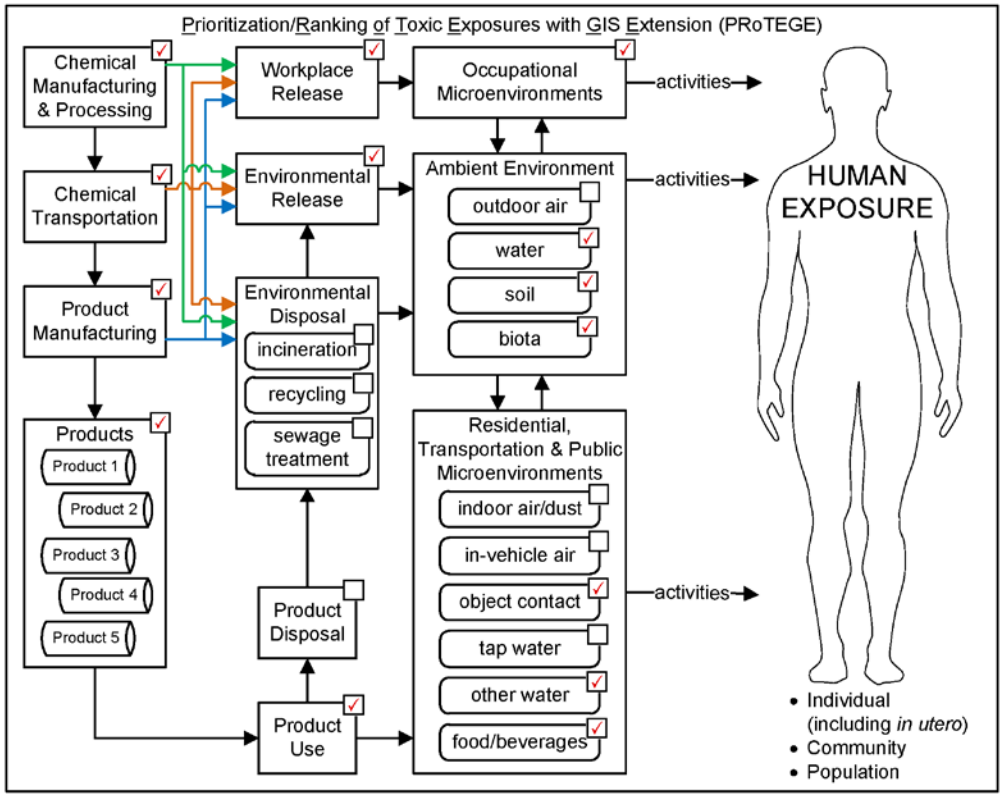
(a) Human Hazard
Estimated ranking of human hazard risk from 2,4-D, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of 2,4-D (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from 2,4-D, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Aldicarb



Summary Physico-Chemical Information	
Name	Aldicarb
Other Names	
Chemical Formula	$C_7H_{14}N_2O_2S$
Chemical Class	CarP
Identifier	CAS: 116-06-3
Chemical Forms	Crystals from isopropyl ether
Physical Properties	
Molecular weight: 190.27 Melting point: 99-100°C Solubility (25 °C): in water 0.6% Vapor pressure(20 °C): 9.75×10^{-5} mm Hg Specific gravity (25 °C / 20 °C): 1.1950	
Additional Notes	
Decomposes above 100°C	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.001 mg/kg/day (IRIS); Lowest Observed Effect Level (LOEL) for subclinical blood cholinesterase depression 0.025 mg/kg (HSDB)
Toxicological Effects: cholinergic symptoms, diarrhea, CNS depression and conduction abnormalities
Exposure Limits:
Chemical Use: Insecticide, acaricide, nematocide
Exposure Routes: ingestion of contaminated food, inhalation and skin contact
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	NA			Data Source: Ground water – HSDB, 0.04% of 2,306 groundwater samples (1992-1996) > LOD, max conc of 0.01 µg/L, high conc from aldicarb applied to farmland; Food – aldicarb was not measured in the TDS ('91 – '03); Surface water – HSDB, 14/92 > LOD; Tap water - NCOD, 24 detected out of 30,564 analyses*; Soil – HSDB, farmland; Biota - HSDB	Air	0.0575 (TRI 2008)	0.06% (TRI 2008)
Ground water (µg/L)	<LOD	<0.01	515				
Food (ppm)	<LOD				Surface Water		
Indoor Air (ng/m³)	NA				Ground Water		
Surface water (ppb)	1		4		Soil	0.0015 (TRI 2008)	0.03% (TRI 2008)
Tap water (µg/L)	<LOD						
Soil (ppm)	0.0048-0.0052	2	1330		Chemical Production and Use		
Dust (µg/cm²)	NA				Production		
Surfaces (µg/cm²)	NA						
Biota (ppm)	0.03-0.05	1.40	8.89				
Human Biomarkers							
Urine	NA						
Blood	NA						
Other	NA						

*Metabolites aldicarb sulfone and aldicarb sulfonide were detected in NCOD (detects/total; min; mean; max): aldicarb sulfone (34/30,498; 0.10; 0.408; 1.14); aldicarb sulfoxide (35/30,467; 0.40; 3.592; 8.80)

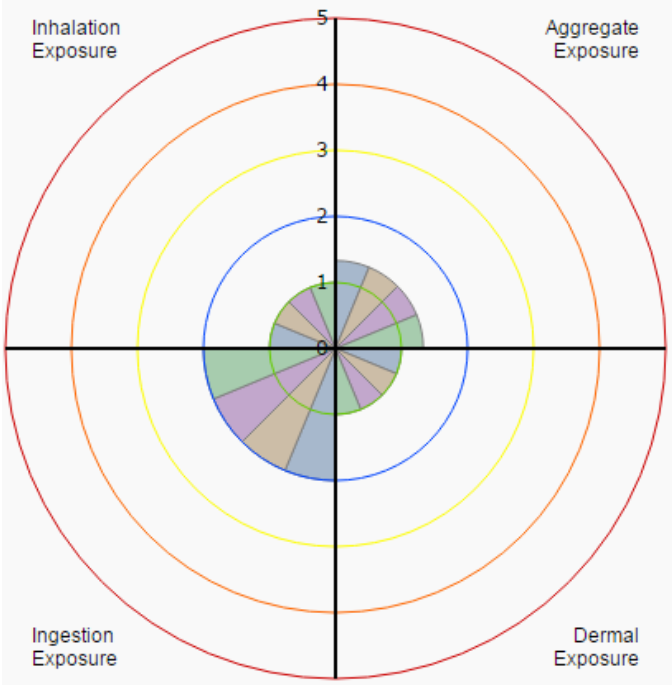
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		
	ICSC		●
	Tox Profs		
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		
	IARC		
	PSAP		
	NTP		●
	REACH		
	PFD		●
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		
	IUR		
	ECD		
	SRD		
Releases	TRI		●
	NEI		
Environmental Quality	NGA		
	NAWQA		●
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		○
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [26]
	BME		
	ERDEM		

"Tier 1" Exposure Ranking for Aldicarb

Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	1
Aggregate	1.33	1.33	1.33	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Aldicarb

insufficient data for analysis

insufficient data for analysis

	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0	0	NA	0
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

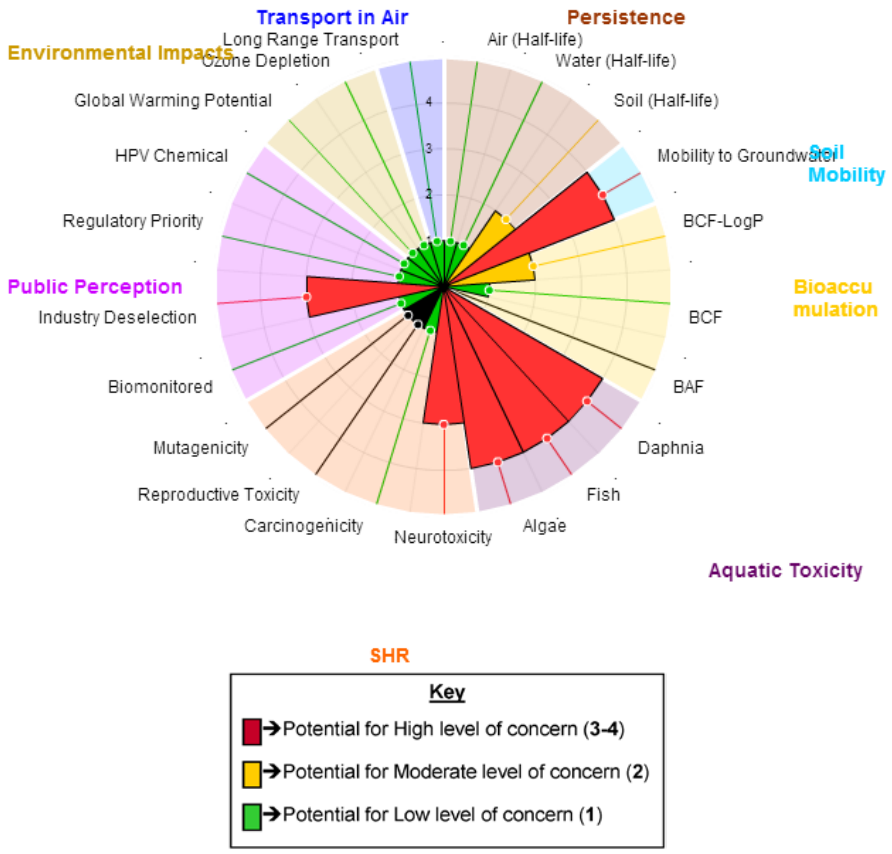
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Aldicarb

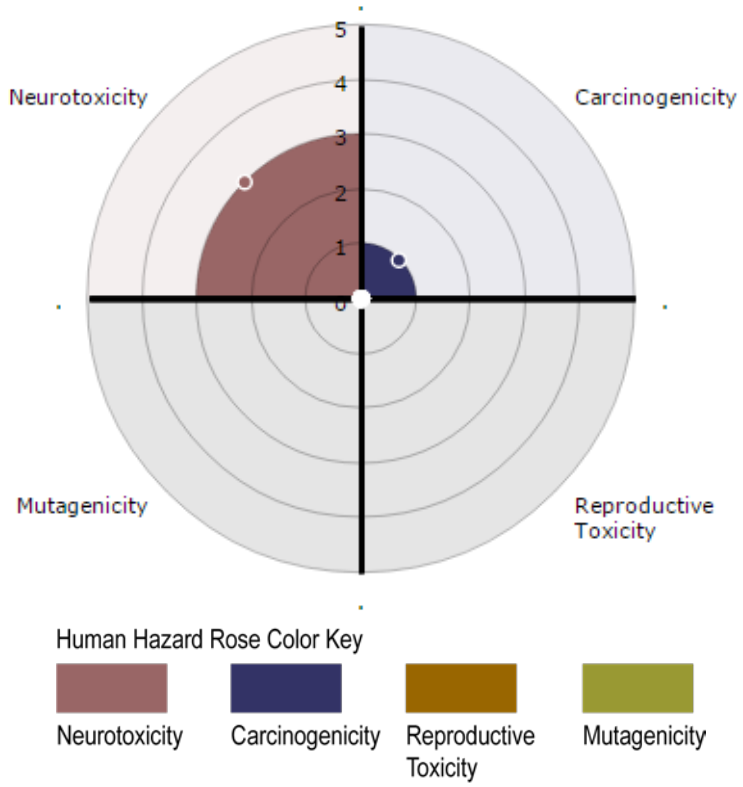
		CAS # 116-06-3
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 1.162 days)
	Water (Half-life)	Low persistence in Water (Estimated Half-life = 37.5 days)
	Soil (Half-life)	Moderate persistence in Soil (Estimated Half-life = 75 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 1.512
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=1.13
	BCF	Low bioconcentration potential based on Estimated LogBCF = 0.17
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 577.766 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 563.575 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	Not classifiable [IARC_OE]; D (Not classifiable as to human carcinogenicity) [1986 Guidelines] [IRIS]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (RC_PIC)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 8.30014 km - A_TRNSPRT)



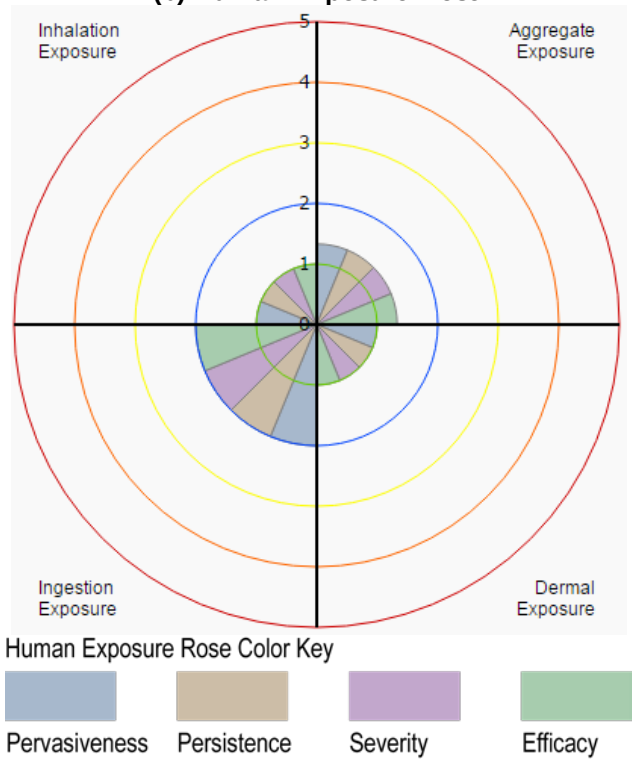
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Aldicarb

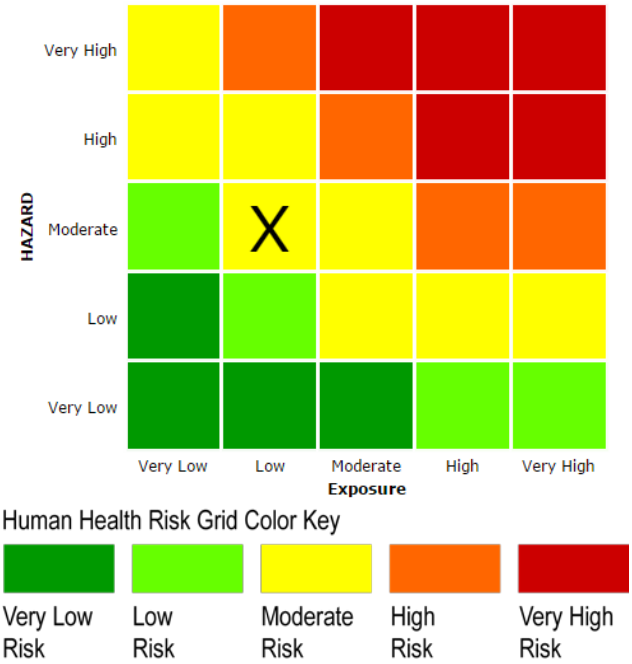
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



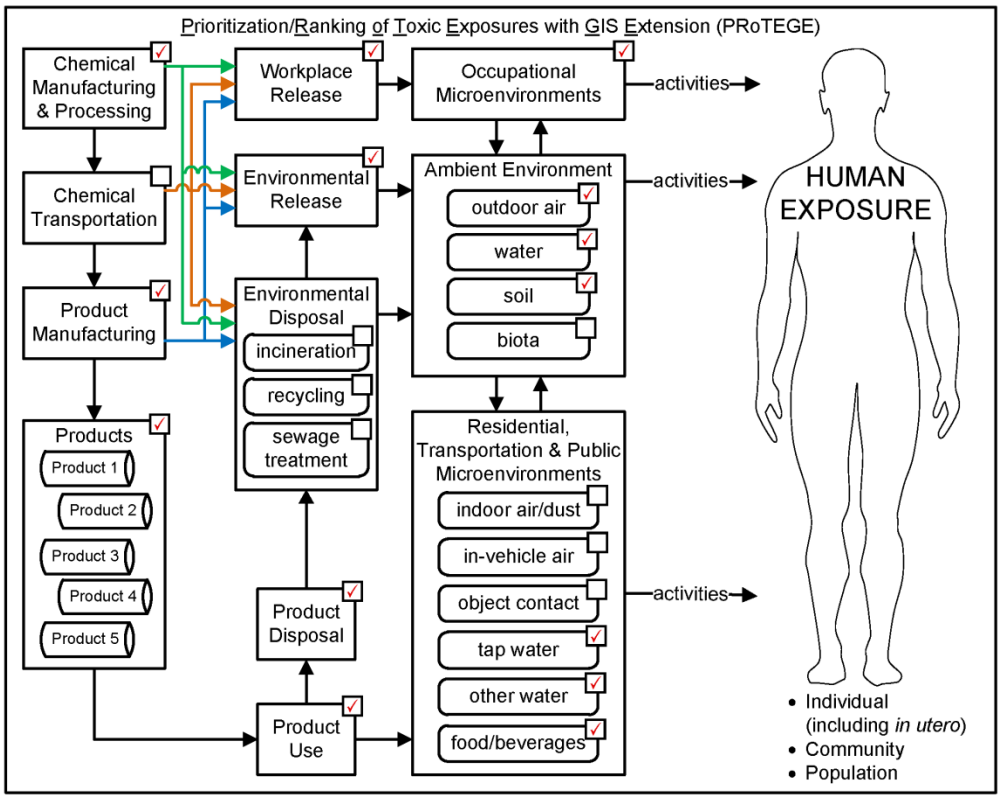
(a) Human Hazard
Estimated ranking of human hazard risk from Aldicarb, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Aldicarb (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Aldicarb, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Aroclor_1254



Summary Physico-Chemical Information	
Name	Aroclor_1254
Other Names	Chlorodiphenyl;PCB; Polychlorinated biphenyl
Chemical Formula	$C_6H_3Cl_2C_6H_2Cl_3$
Chemical Class	PCBs
Identifier	CAS: 11097-69-1
Chemical Forms	Mixture of many PCBs
Physical Properties	
Molecular weight: 326 Solubility: Insoluble Vapor pressure: 0.00006 mmHg Specific gravity (25°C): 1.38	
Additional Notes	
Nonflammable Liquid, but exposure in a fire results in the formation of a black soot containing PCBs, polychlorinated dibenzofurans, and chlorinated dibenzo-p-dioxins.	

Exposure and Toxicity Information
Toxicity Limits: RfD: 2E-5 mg/kg-day (monkey), RfD: 0.00002 mg/kg (IRIS), MRL: 0.03 mg/kg/day (Int); 0.02 mg/kg/day (Chr) (ATSDR)
Toxicological Effects: irritation eyes, chloracne; liver damage; reproductive effects; potential occupational carcinogen;
Exposure Limits: NIOSH REL: Ca TWA 0.001 mg/m³; OSHA PEL: TWA 0.5 mg/m³
Chemical Use: rubber plasticizers
Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs: Skin, eyes, liver, reproductive system (Cancer Site: [in animals: tumors of the pituitary gland & liver, leukemia])

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ng/m³)	0.45	1.5	9.3	Data Sources: Outdoor air – HSDB [27]; Ground water – HSDB (NJ, 1981, 30/1040 >LOD); Food – [28]; Surface water – HSDB, 9% of 1186 observation stations >LOD based on STORET; Tap water – [23]; Soil – HSDB; Biota - HSDB	Air		
Ground water (ppb)	<LOD		0.4				
Food (ng/kg)	<LOD	0.200	0.955		Surface Water		
Indoor Air (ng/m³)	NA				Ground Water		
Surface water (ppb)		0.3	127		Soil		
Tap water (µg/L)	< LOD	< LOD	0.214 (99% tile)				
Soil (µg/kg)	77-93	215-482	574-880		Chemical Production and Use		
Dust	NA				Production	Not been commercially produced in USA since 1977	HSDB
Surfaces (µg/cm²)	NA						
Biota (ppm)	< 0.1	0.74	2.6				
Human Biomarkers							
Urine							
Blood							
Other							

Environmental concentrations of Arcolor_1254 were assumed to be the total of all measured PCBs.

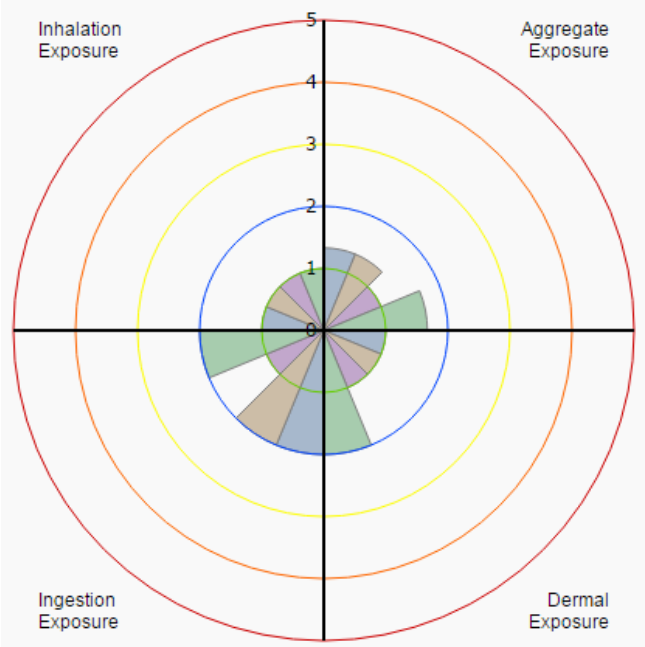
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		●
	ICSC		●
	Tox Profs		○
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		●
Production and Use	SIDS		
	EHPV		
	HPD		
	IUR		
	ECD		
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		●
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		□
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (R) [29]
	BME		
	ERDEM		

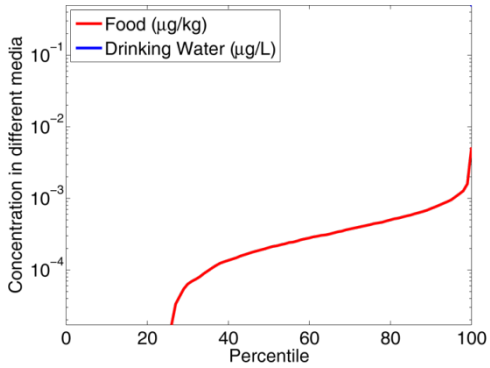
"Tier 1" Exposure Ranking for Aroclor_1254

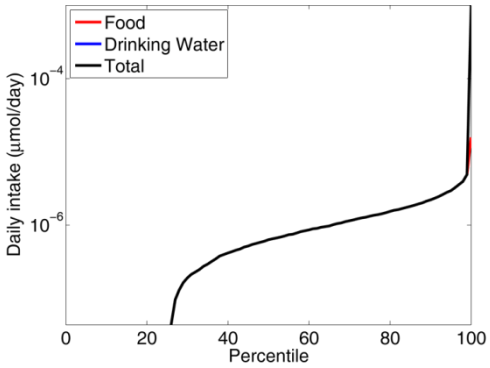
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	1	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Aroclor_1254





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	6.33E-07	NA	6.33E-07
90 % tile	0	2.24E-06	NA	2.28E-06
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

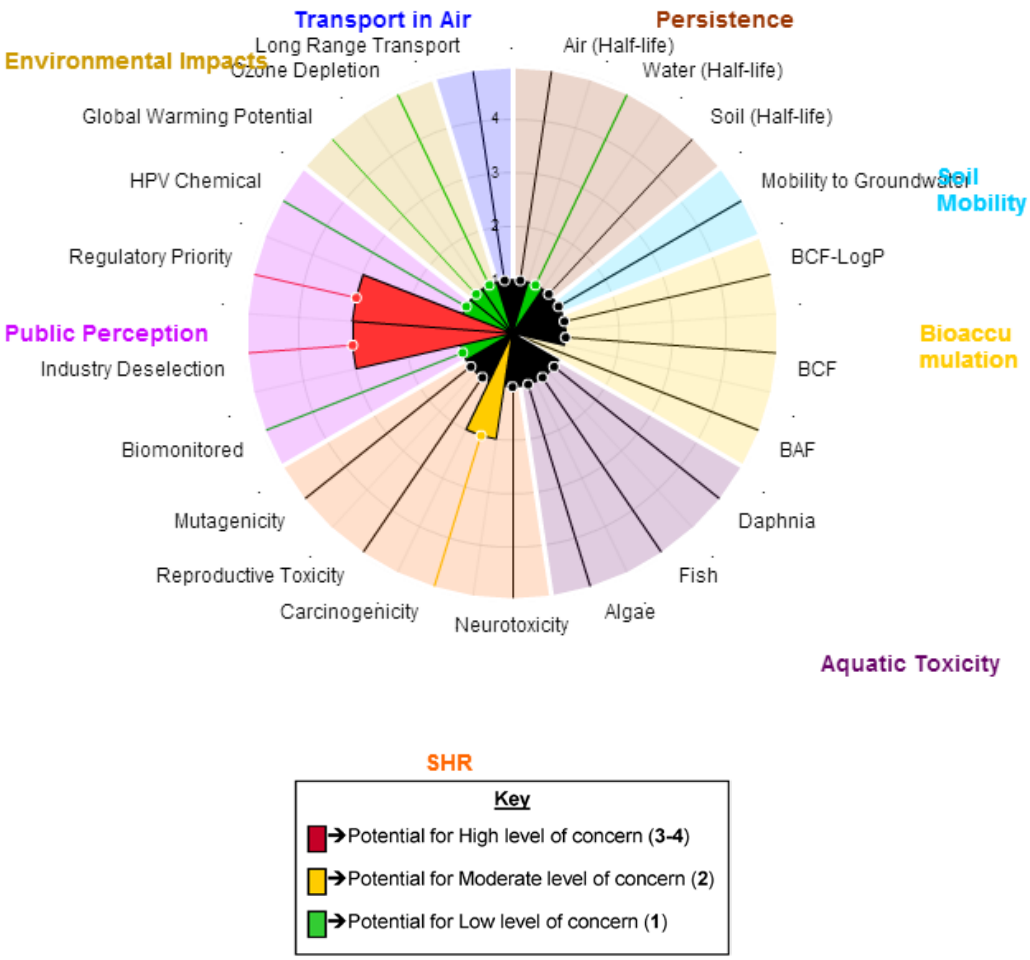
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Aroclor_1254

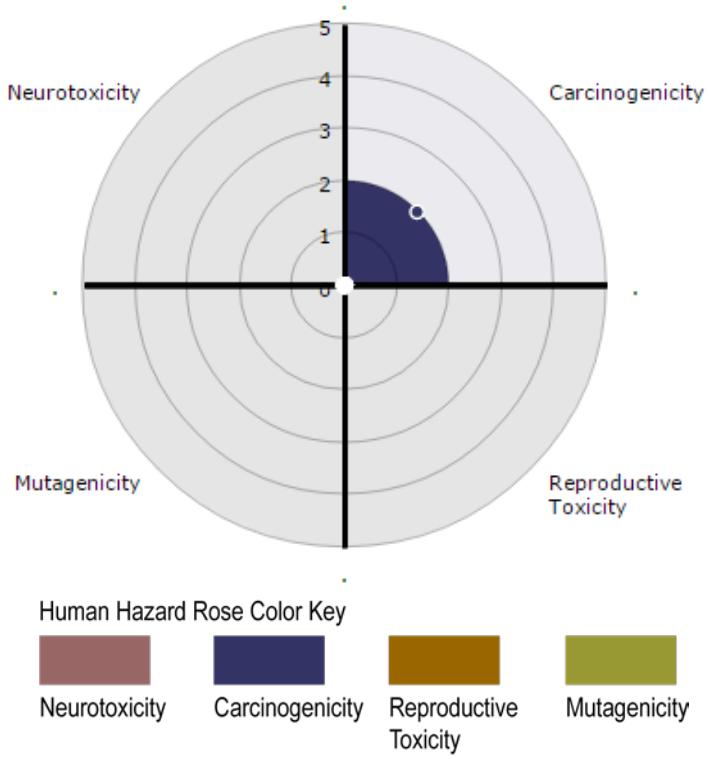
		CAS # 11097-69-1
Persistence	Air (Half-life)	Persistence in Air has not been calculated for this compound
	Water (Half-life)	Persistence in Water has not been calculated for this compound.
	Soil (Half-life)	Persistence in Soil has not been calculated for this compound.
Soil Mobility	Mobility to Groundwater	Soil mobility has not been calculated for this compound
Bioaccumulation	BCF-LogP	BCF value based on LogP has not been calculated for this compound
	BCF	BCF value has not been calculated for this compound
	BAF	
Aquatic Toxicity	Daphnia	No toxicity estimate.
	Fish	No toxicity estimate.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	
	Carcinogenicity	CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (GADSL)
	Regulatory Priority	1 out of 10 lists (JCL1_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Long Range Transport in Air has not been calculated for this compound



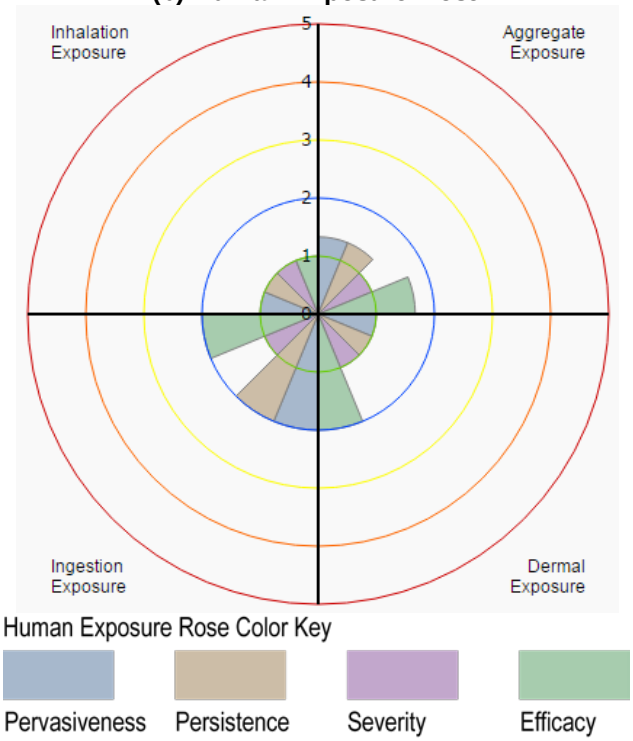
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Aroclor_1254

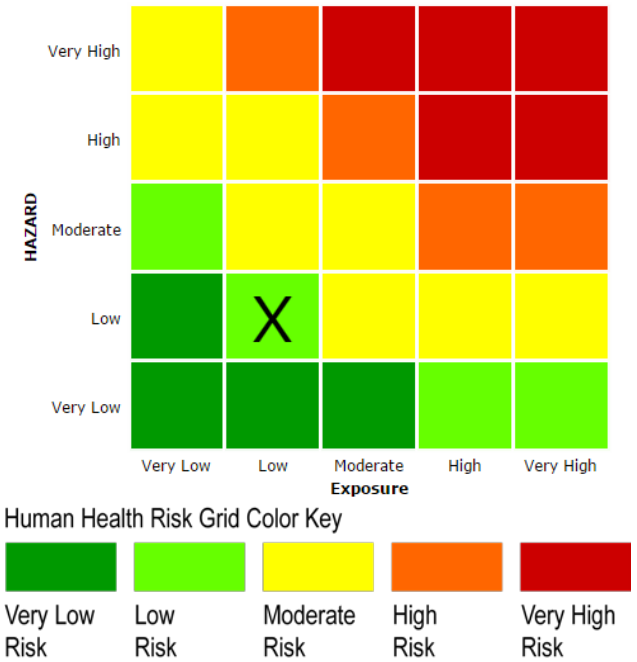
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



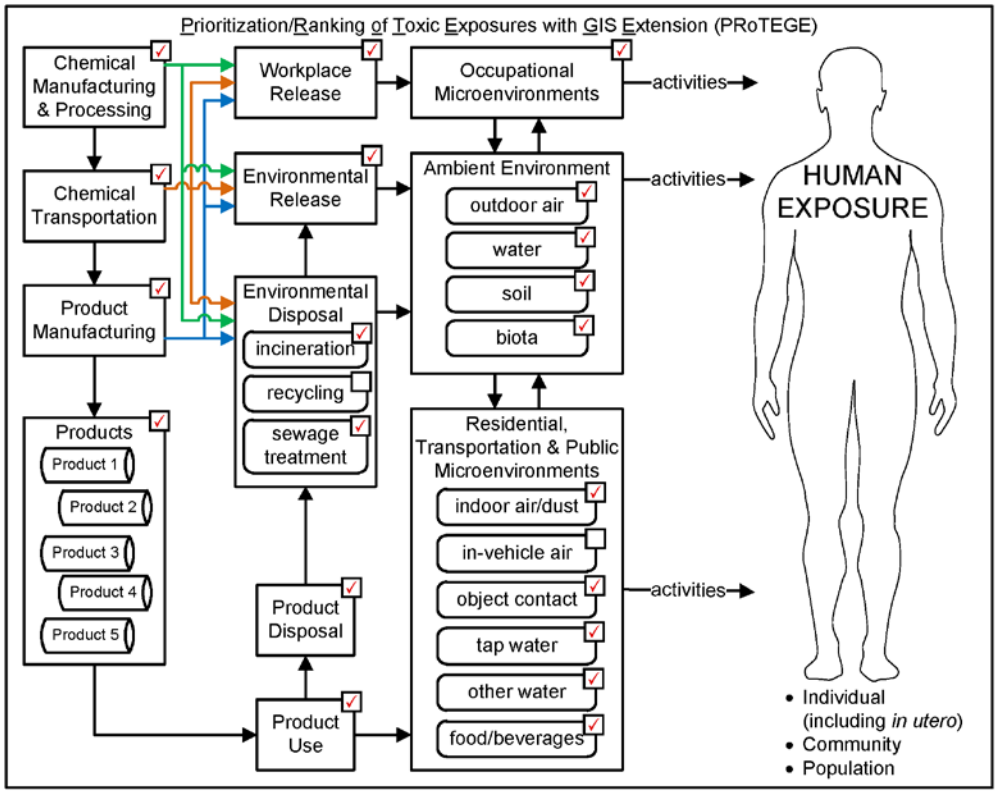
(a) Human Hazard
Estimated ranking of human hazard risk from Aroclor_1254, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Aroclor_1254 (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Aroclor_1254, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Arsenic (and As compounds)



Summary Physico-Chemical Information	
Name	Arsenic
Other Names	
Chemical Formula	As
Chemical Class	Mtd/MU
Identifier	CAS: 7440-38-2; RTECS: CG0525000; UN: 1558; EC No: 033-001-00-X
Chemical Forms	Many compounds including arsenate salts (Ca, Cu, Na, Pb), arsenic sulfides, arsenic trioxide, arsenide alloys (Al, Cd, Ga, In), arsenic minerals (Fe, Ni, Co), gaseous arsine and organic forms (arsenobetaine and methylated arsenic)
Physical Properties	
Molecular weight: 74.9 Solubility in water: high solubility as arsenate Vapor pressure: negligible at 20°C Density: 5.727 g/cm^3 Sublimation point: 615 °C	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD 3 x 10^{-4} mg/kg-day (IRIS); Fatal human dose 70-180 mg As^{III}/70kg human
Toxicological Effects: Carcinogenic Classification – A human carcinogen (IRIS, ATSDR, IARC)
Exposure Limits: TLV: 0.01 mg/m^3 as TWA; NIOSH REL: CaC 0.002 mg/m^3 [15-minute]; OSHA PEL: [1910.1018]
Chemical Use: used in metallurgy, automotive and semiconductor industries; wood preservative, herbicide, pesticide
Exposure Routes: inhalation, skin absorption, skin and/or eye contact, ingestion
Target Organs: liver, kidney, lung, skin and bladder

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m^3)	7.76e-04	0.0011	0.005	Data sources: Outdoor air (5th, 50th, and 95th %iles) - '08 annual means @ AQS monitors; corresponding 2002 NATA county-level annual averages - 1.30e-4, 3.54e-4 and 4.22e-4. Food (5th, 50th, and 95th %iles) - TDS '94-'02. Indoor Air – 88% > LOD, Dust - 1-4 month accumulation and Surfaces (5th, 50th, and 95th %iles) [30]. Tap Water (5th, 50th, and 95th %iles) - NRDC '00. Surface water & soil (5th, 50th, and 95th %iles) - STORET.	Air	240.21 (NEI 2005) 0.4821 (TRI 2008)	99.4% 0.90%
Ground water							
Food (µg/g)	0.01	0.025	0.8796		Surface Water	1.19 (TRI 2008)	0.43%
Indoor Air (ng/m^3)	0.16	0.51	1.61		Ground Water	30.87 (TRI 2008)	0.06%
Surface water (µg/L)	0.351	2.2	5		Soil	1181.08 (TRI 2008)	0.47%
Tap water (µg/L)	0.80	2.9	9.5				
Soil (ppm)	1.33	5.72	8.40		Chemical Production and Use		
Dust (µg/cm^2)	1.8	7.48	30.5		Production	500,000 to < 1,000,000 lbs/yr	Data Source: IUR 2006
Surfaces (µg/cm^2)	0.44	5.77	75.9				
Biota							
Human Biomarkers				Data sources: Biomarkers- (5th, 50th, and 95th %iles) - NHANES 07-08 and 99.6% > LOD.			
Urine (µg/L)	1.6775	7.78	15.51				
Blood							
Other							

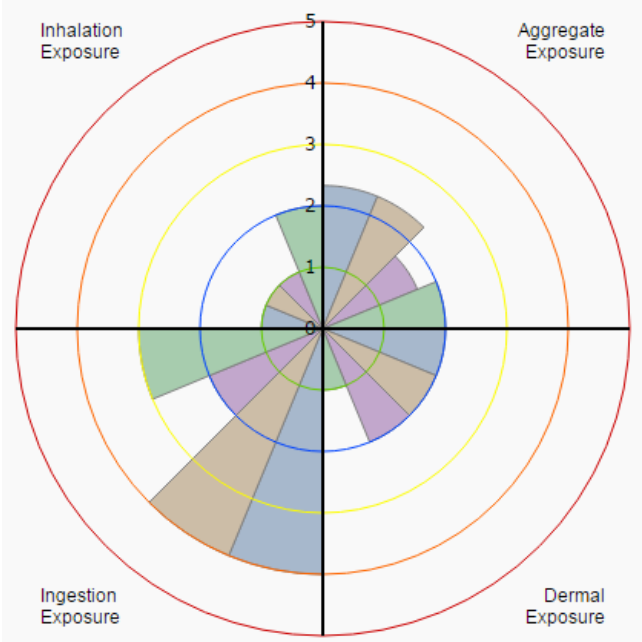
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		●
	IARC		●
	PSAP		●
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		●
	ECD		○
	SRD		
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		●
	NAWQA		●
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		●
	NHANES	03-04	
		05-06	
		07-08	u
		09-10	(u)
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [31]
	BME		● [32]
	ERDEM		

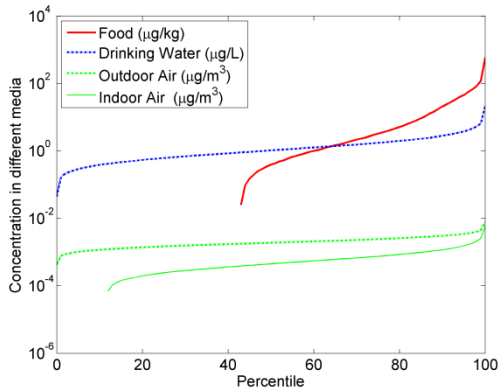
"Tier 1" Exposure Ranking for Arsenic (and As compounds)

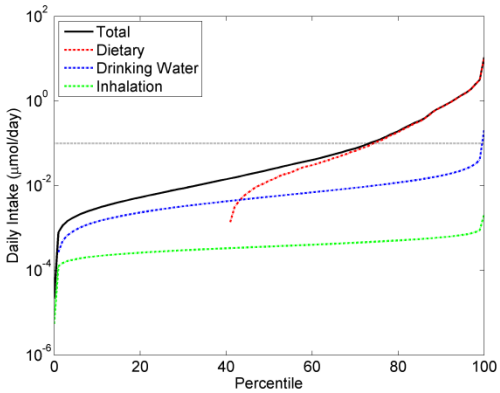
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	2
Ingestion	4	4	2	3
Dermal	2	2	2	1
Aggregate	2.33	2.33	1.66	2

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Arsenic (and As compounds)





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.000426	0.0174	NA	0.0178
90 % tile	0.00157	0.36	NA	0.384
% over 0.1 μmol/day	0	20	NA	20.4
% over 1 μmol/day	0	2.79	NA	3.32

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

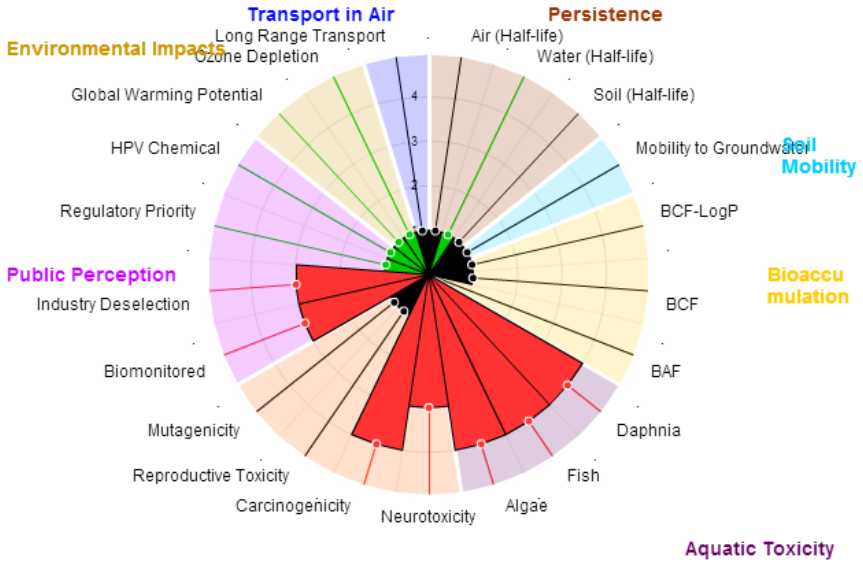
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Arsenic (and As compounds)

		CAS # 7440-38-2
Persistence	Air (Half-life)	Persistence in Air has not been calculated for this compound
	Water (Half-life)	Persistence in Water has not been calculated for this compound.
	Soil (Half-life)	Persistence in Soil has not been calculated for this compound.
Soil Mobility	Mobility to Groundwater	Soil mobility has not been calculated for this compound
Bioaccumulation	BCF-LogP	BCF value based on LogP has not been calculated for this compound
	BCF	BCF value has not been calculated for this compound
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 983.992 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 1005.985 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	CLASS A1 - Confirmed Human Carcinogen [ACGIH]; Known Carcinogen - human studies indicate a causal relationship between exposure and human cancer [NTPLIST]; Carcinogenic to humans [IARC_OE]; A (Human carcinogen) [1986 Guidelines] [IRIS]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	2 out of 6 lists (GADSL; EUC2)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Long Range Transport in Air has not been calculated for this compound



SHR

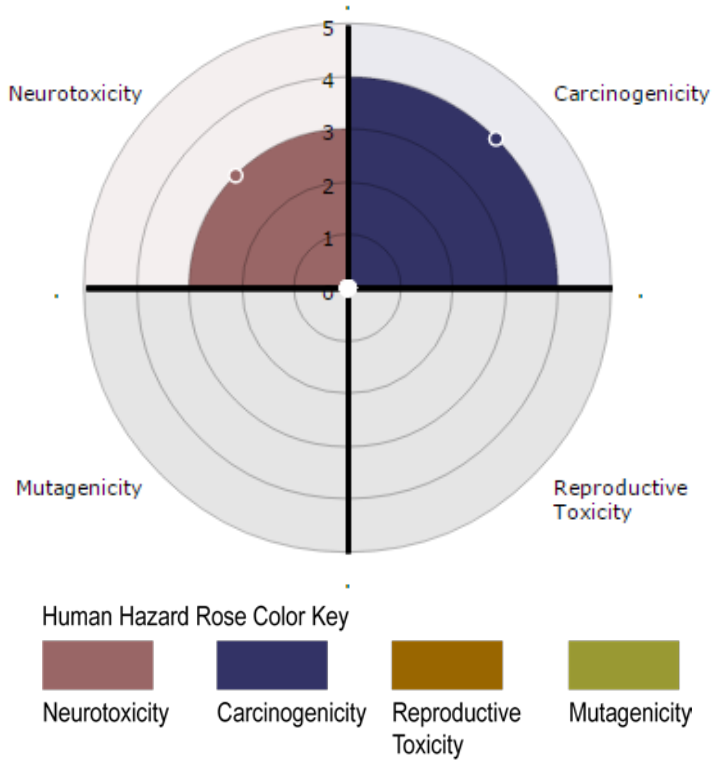
Key

- Potential for High level of concern (**3-4**)
- Potential for Moderate level of concern (**2**)
- Potential for Low level of concern (**1**)

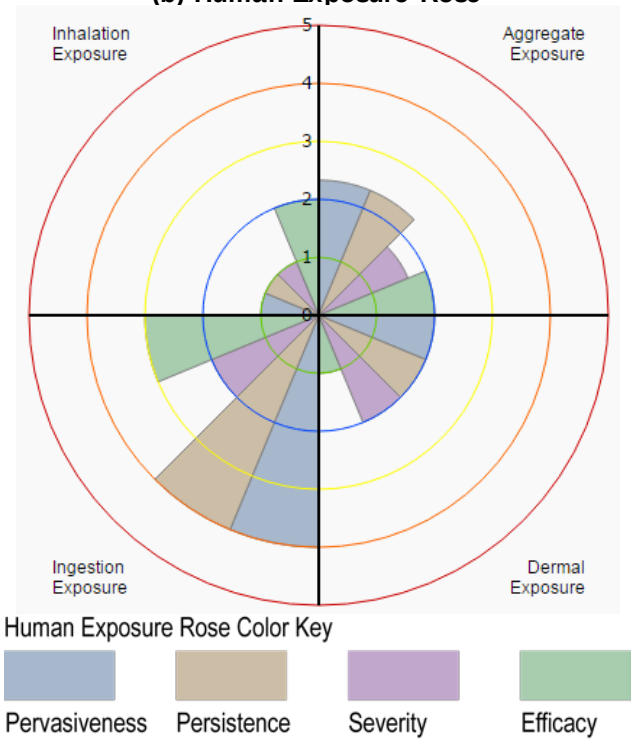
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Arsenic (and As compounds)

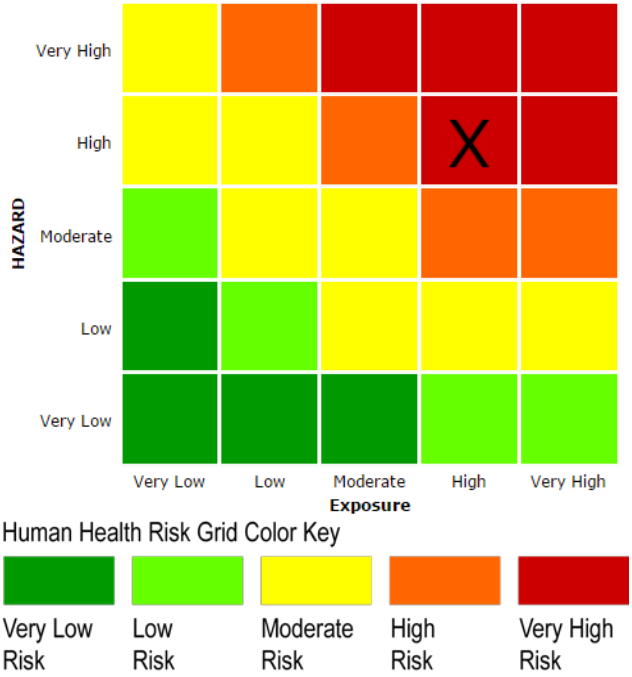
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



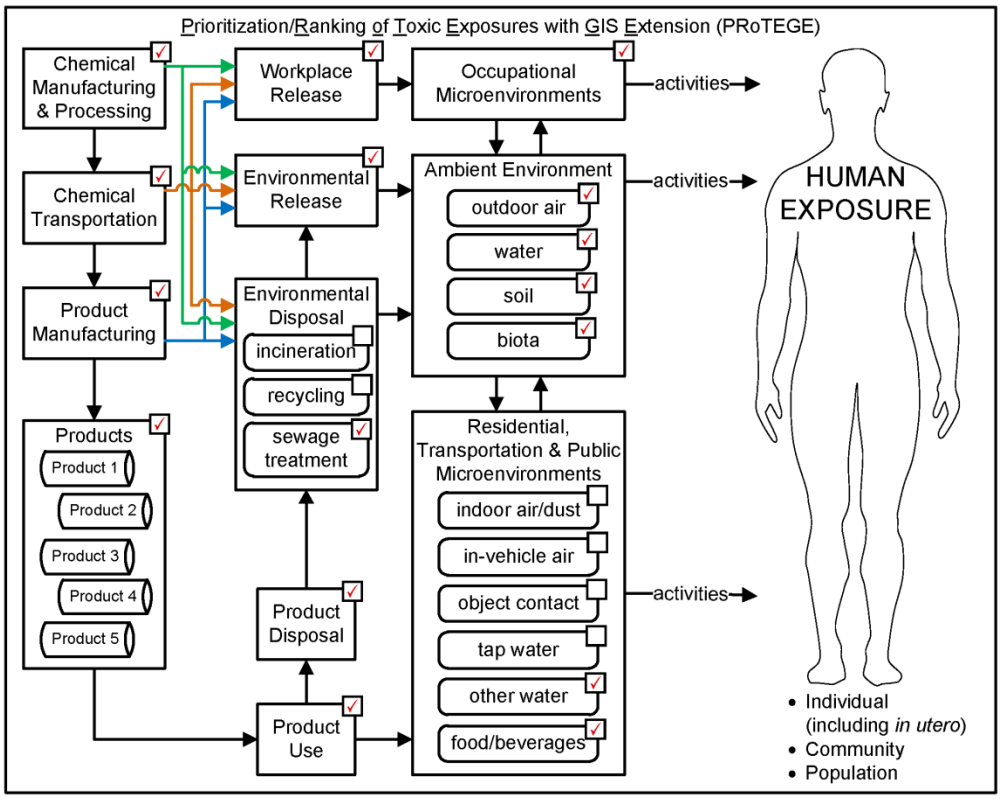
(a) Human Hazard
Estimated ranking of human hazard risk from Arsenic, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Arsenic (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Arsenic, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Atrazine



Summary Physico-Chemical Information	
Name	Atrazine
Other Names	2-Chloro-4-ethylamino-6-isopropylamino-s-triazine; 6-Chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine
Chemical Formula	$C_8H_{14}ClN_5$
Chemical Class	Herb
Identifier	CAS: 1912-24-9
Chemical Forms	
Physical Properties	
Molecular weight: 215.7 Boiling point: Decomposes Melting point: 171°C Solubility: 0.003% Vapor pressure: 0.0000003 mmHg Specific gravity: 1.19	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD (mg/kg/day): 0.035 (IRIS), MRL: 0.01 mg/kg/day (Ac); 0.003 mg/kg/day (Int) (ATSDR)
Toxicological Effects: Carcinogenic classification: 3 (O), 3 (I) (IARC); irritation eyes, skin; dermatitis, sensitization skin; dyspnea (breathing difficulty), lassitude (weakness, exhaustion), incoordination, salivation; hypothermia; liver injury (NIOSH)
Exposure Limits: NIOSH REL: TWA 5 mg/m^3
Chemical Use: Restricted US herbicide
Exposure Routes: inhalation, ingestion, skin and/or eye contact (NIOSH)
Target Organs: Eyes, skin, respiratory system, central nervous system, liver

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ng/m^3)	0.019	0.42	2.6	Data Source: Outdoor air – HSDB; Ground water – HSDB; Food – TDS 1991-3 to 2003-4, 2 out of 88 samples >LOD; Surface water – HSDB; Tap water – [23,33] (5, 50, and 95%tiles); Soil – HSDB	Air	231.03 (NEI 2005) 20.65 (TRI 2008)	2.20% (NEI 2005) 0.47% (TRI 2008)
Ground water (µg/L)	0.1	0.4	4.2				
Food (ppb)	0.905	0.95	0.995		Surface Water	0.05 (TRI 2008)	0.06% (TRI 2008)
Indoor Air (ng/m^3)	NA				Ground Water		
Surface water (µg/L)	0.0074-0.016	0.2-2.74	18		Soil	172.14 (TRI 2008)	0.09% (TRI 2008)
Tap water (µg/L)	0.0064	0.050	0.39				
Soil (µg/kg)	<0.1		82		Chemical Production and Use		
Dust	NA				Production		
Surfaces	NA						
Biota	NA						
Human Biomarkers							
Urine							
Blood							
Other							

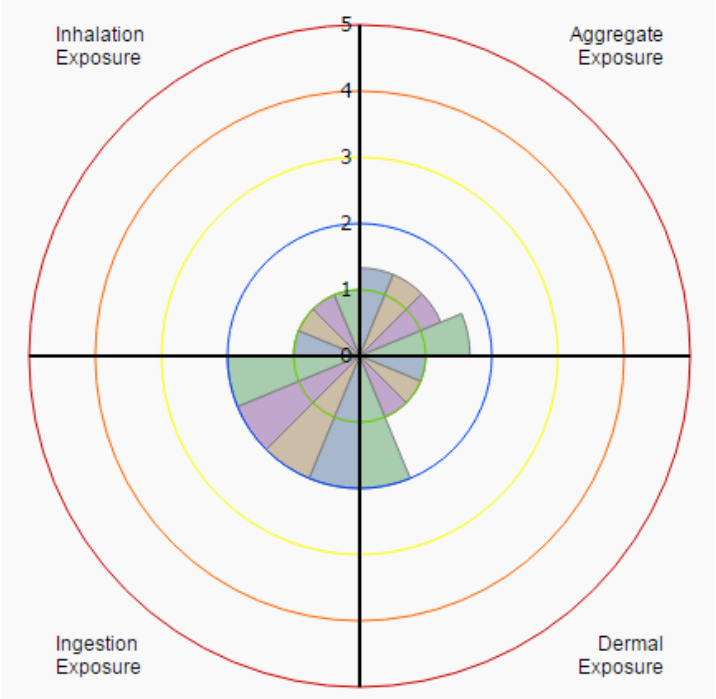
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		●
	PSAP		
	NTP		
	REACH		
	PFD		●
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		○
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		
	CEBS		●
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		○
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		●
	NHANES	03-04	(s),u
		05-06	(s,u)
		07-08	(s,u)
		09-10	(,u)
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PBPKm (R) [34]
	BME		
	ERDEM		

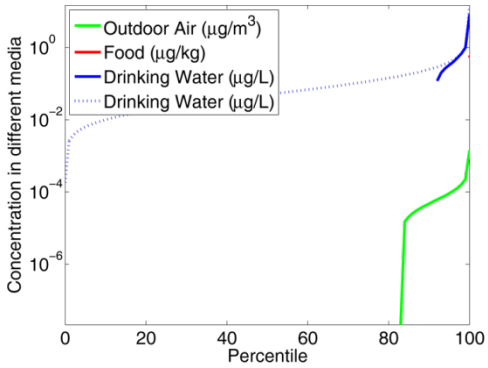
"Tier 1" Exposure Ranking for Atrazine

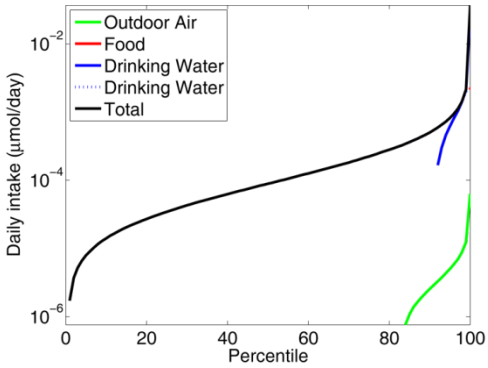
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Atrazine





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0.000105	NA	0.000105
90 % tile	2.57E-06	0.000761	NA	0.000792
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

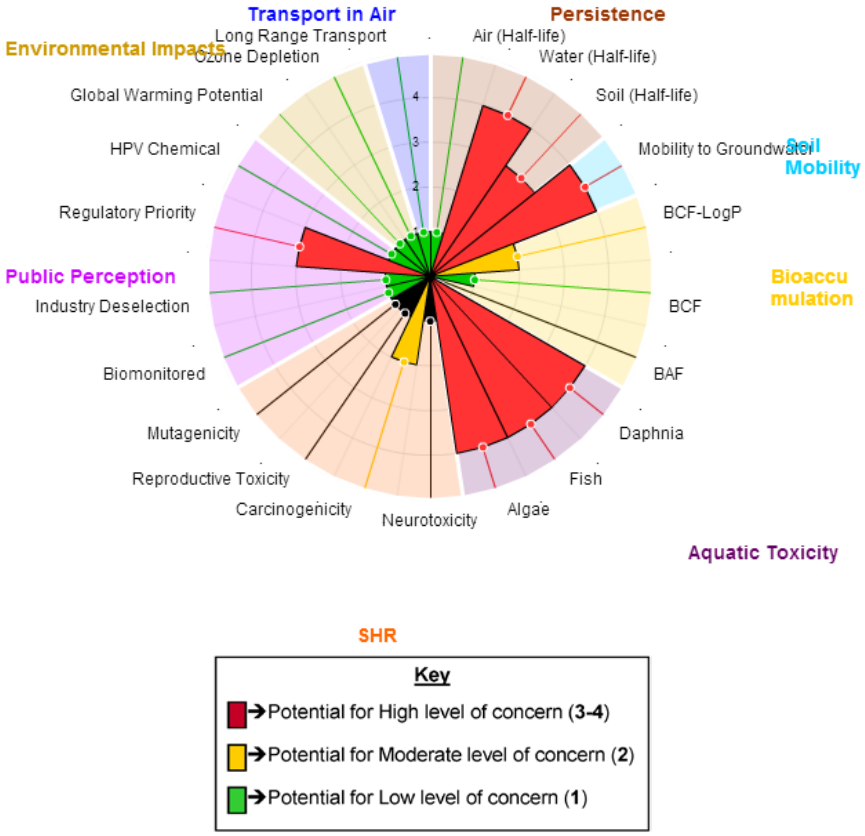
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Atrazine

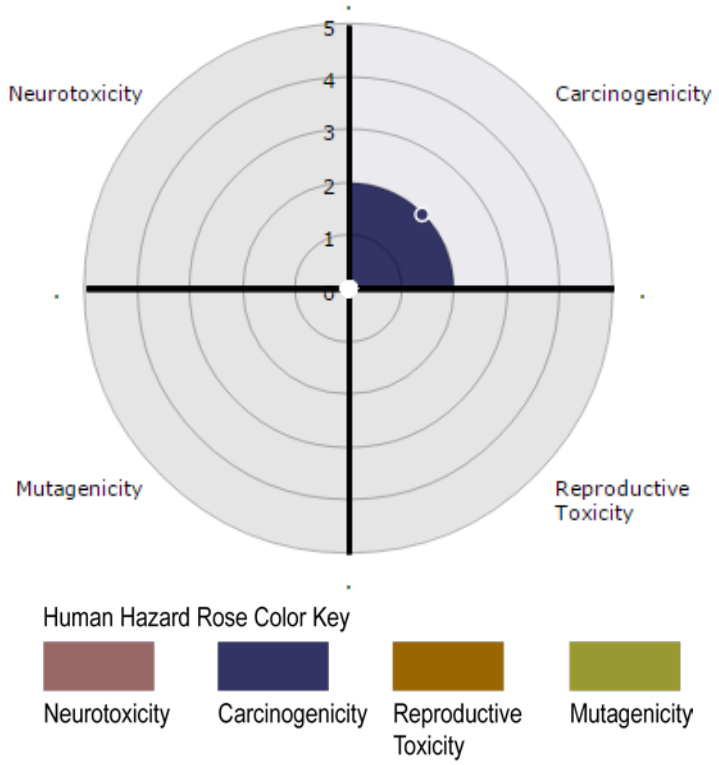
		CAS # 1912-24-9
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.3911 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 1% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 0%, Max. BOD = 3%).
	Soil (Half-life)	High persistence in Soil (Estimated Half-life = 120 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 2.362
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=2.61
	BCF	Low bioconcentration potential based on Experimental LogBCF = 0.9
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 30.734 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 27.103 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]; Not classifiable [IARC_OE]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	0 out of 6 lists
	Regulatory Priority	2 out of 10 lists (JDES_LST; JMON3)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 12.869 km - A_TRNSPRT)



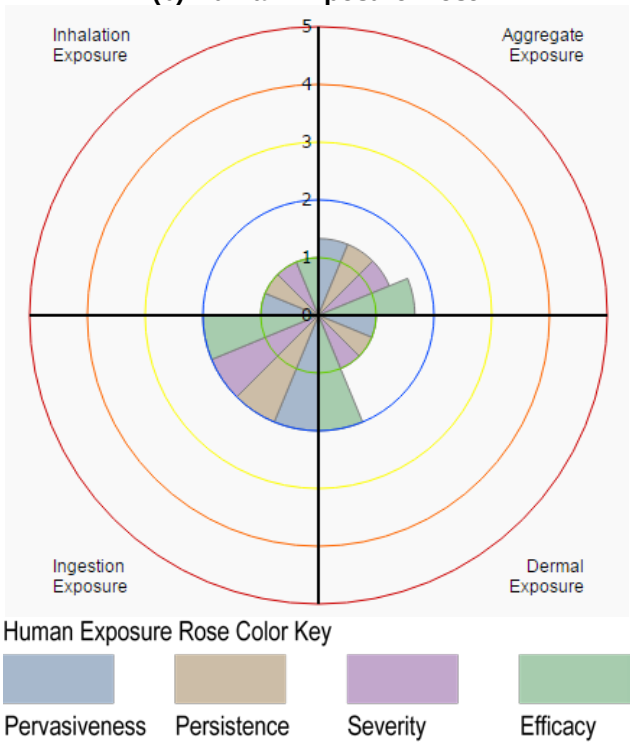
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Atrazine

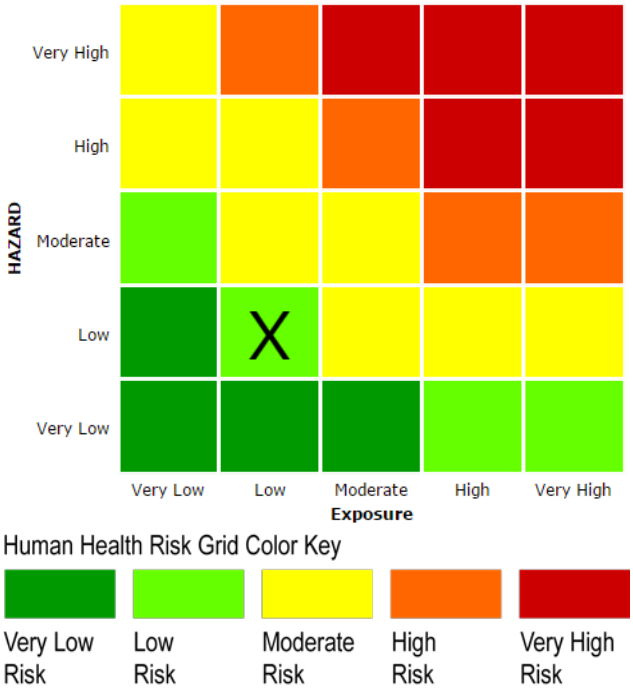
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



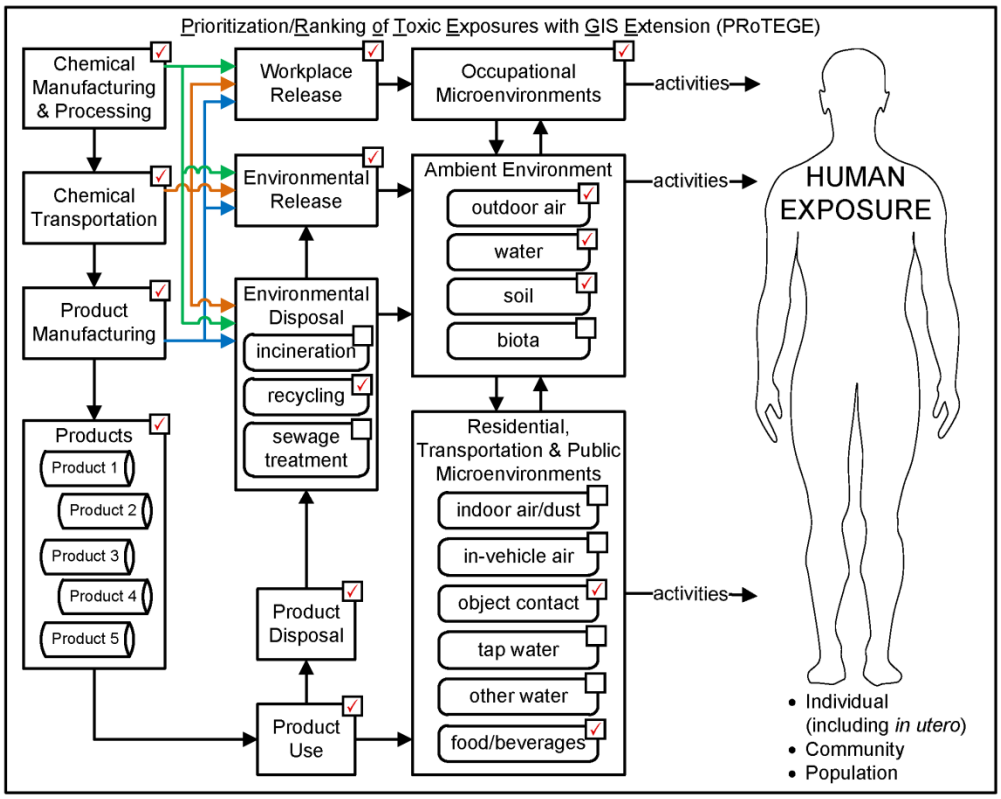
(a) Human Hazard
Estimated ranking of human hazard risk from Atrazine, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Atrazine (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Atrazine, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Ranking for Bisphenol-A



Summary Physico-Chemical Information	
Name	Bisphenol-A
Other Names	4,4'-dihydroxy-2,2-diphenylpropane
Chemical Formula	$C_{15}H_{16}O_2$
Chemical Class	Plzr
Identifier	CAS:80-05-7
Chemical Forms	
Physical Properties	
Molecular weight: 228.29 Melting point: 150-155 deg C (solidification range) (HSDB)	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD (mg/kg/day): 0.05 (IRIS), NOAEL: 10 mg/m3 (repeated I); 50 mg/kg (repeated O) (REACH)
Toxicological Effects:
Exposure Limits:
Chemical Use: plasticizer, fungicide, flame retardant, rubber chemicals
Exposure Routes: inhalation, ingestion, dermal contact
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ng/m³)	0.02	0.51	1.92	Data Source: Outdoor air – [74]; Ground water – HSDB, landfill or waste water treatment plant data; Food – [75] (5, 50, 95%tile), canned food; Surface water – HSDB, USGS 1999-2000, 41.2% of 139 streams >LOD; Tap water - [76]; Indoor Air - [77]; Surface water - [76]; Dust - [76]	Air	53.05 (TRI 2008)	1.98% (TRI 2008)
Ground water (µg/L)	0.003		1.41				
Food (mg/kg)	<LOD	<LOD	1.5		Surface Water	2.87 (TRI 2008)	0.28% (TRI 2008)
Indoor Air (ng/L)	<LOD		<LOD		Ground Water		
Surface water (µg/L)		0.14	12		Soil	95.74 (TRI 2008)	0.12% (TRI 2008)
Tap water (ng/L)	0.5	1.1	2				
Soil (ppm)	ND				Chemical Production and Use		
Dust (µg/g)	0.2	0.821	17.6		Production	1 billion lbs and greater	IUR
Surfaces (µg/cm²)	NA						
Biota	NA						
Human Biomarkers							
Urine							
Blood							
Other							

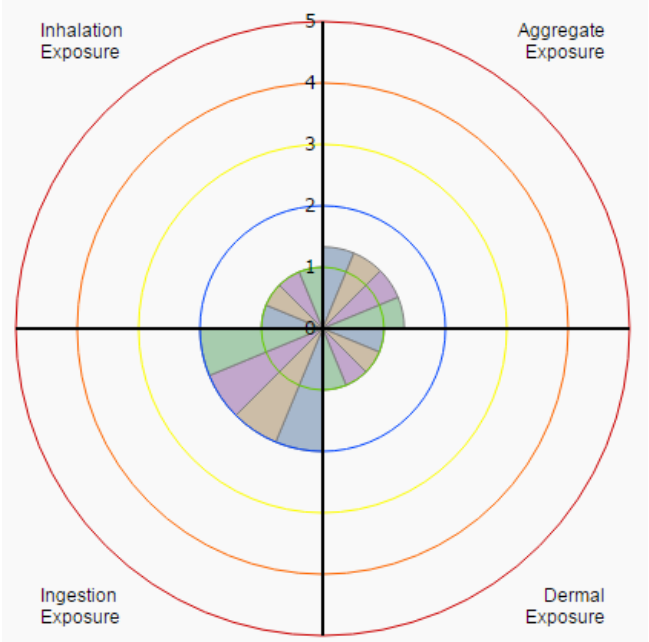
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		
	ICSC		●
	Tox Profs		□
	IRIS		●
	HSDB		●
	ITER		●
	McKay		
	Howard		●
	RIVM rprts		
	IARC		
	PSAP		
	NTP		●
	REACH		●
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	●
	Tox RefDB		●
	CEBS		●
Production and Use	SIDS		●
	EHPV		
	HPD		●
	IUR		●
	ECD		●
	SRD		
Releases	TRI		●
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	u
		05-06	u
		07-08	u
		09-10	(u)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (R, H) [26]
	BME		● [32]
	ERDEM		

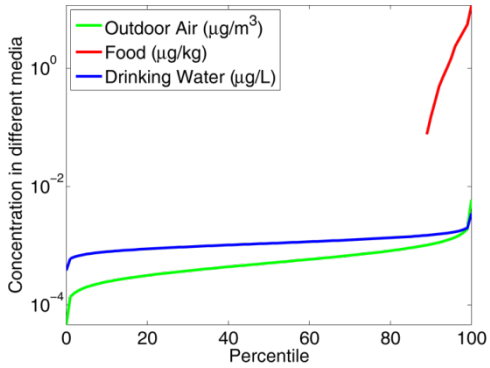
"Tier 1" Exposure Ranking for Bisphenol-A

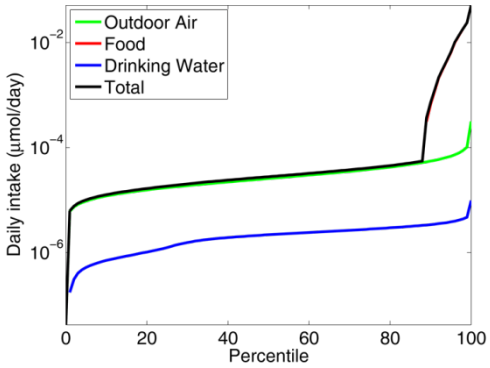
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	1
Aggregate	1.33	1.33	1.33	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Bisphenol-A





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	2.59E-05	2.35E-06	NA	2.82E-05
90 % tile	5.52E-05	0.000789	NA	0.00107
% over 0.1 μmol/day	0	0	NA	0
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

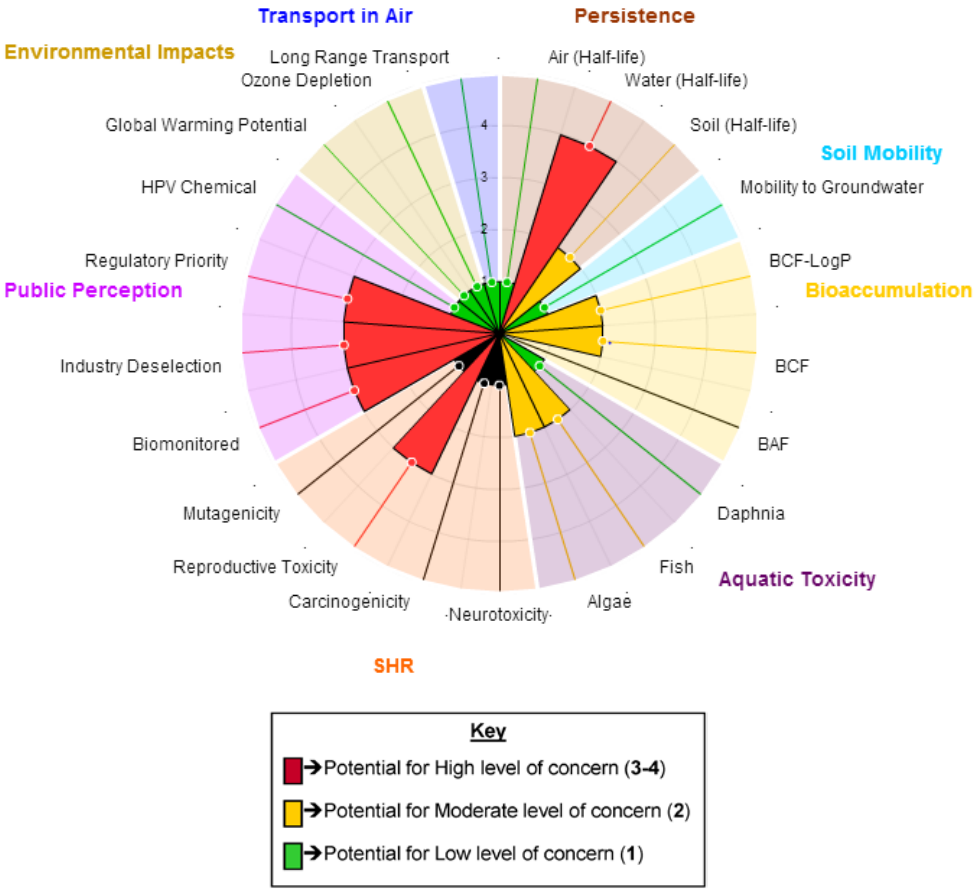
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Bisphenol-A

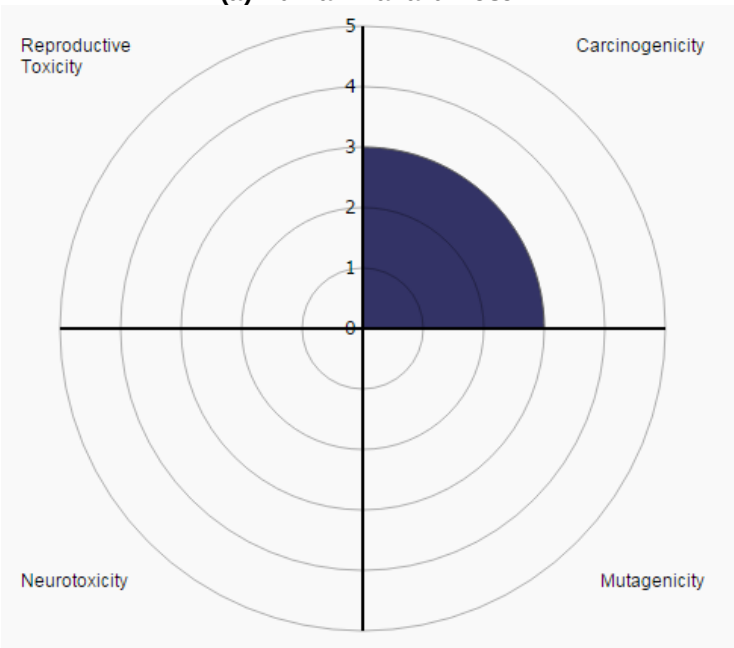
		CAS # 80-05-7
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.1327 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 0% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 0%, Max. BOD = 0%).
	Soil (Half-life)	Moderate persistence in Soil (Estimated Half-life = 75 days)
Soil Mobility	Mobility to Groundwater	Low mobility to groundwater based on LogKoc = 4.876
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=3.32
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 1.57
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) = 13 mg/L indicates a Low toxicity to Daphnia.
	Fish	A measured LC50 (96-hr) = 8 mg/L indicates a Moderate toxicity to Fish.
	Algae	A measured EC50 (72-hr) = 4.8 mg/L indicates a Moderate toxicity to Algae.
SHR	Neurotoxicity	
	Carcinogenicity	[EU_GHS]
	Reproductive Toxicity	TOXIC TO REPRODUCTION - Hazard category 2 [EU_GHS]
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	2 out of 6 lists (EUC2; SINLIST)
	Regulatory Priority	3 out of 10 lists (EU_RRAP; JDES_LST; JMON3)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 0.0727834 km - A_TRNSPRT)



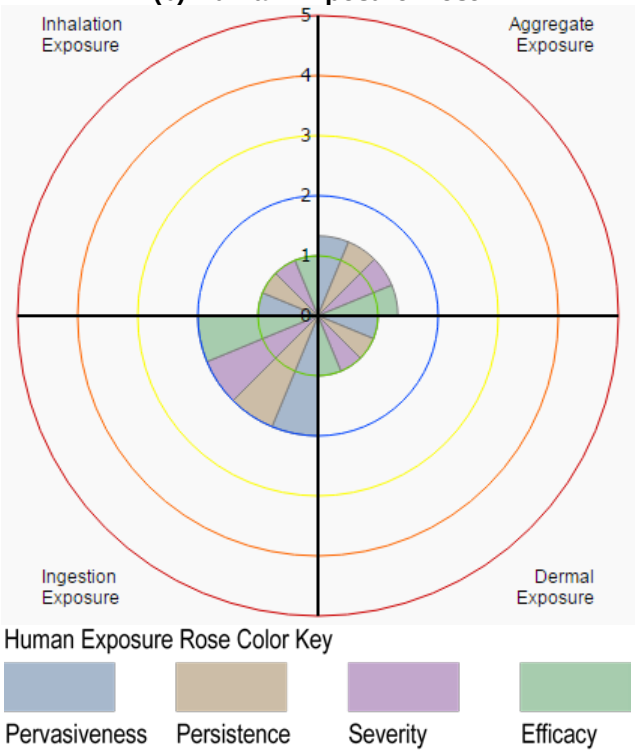
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Bisphenol-A

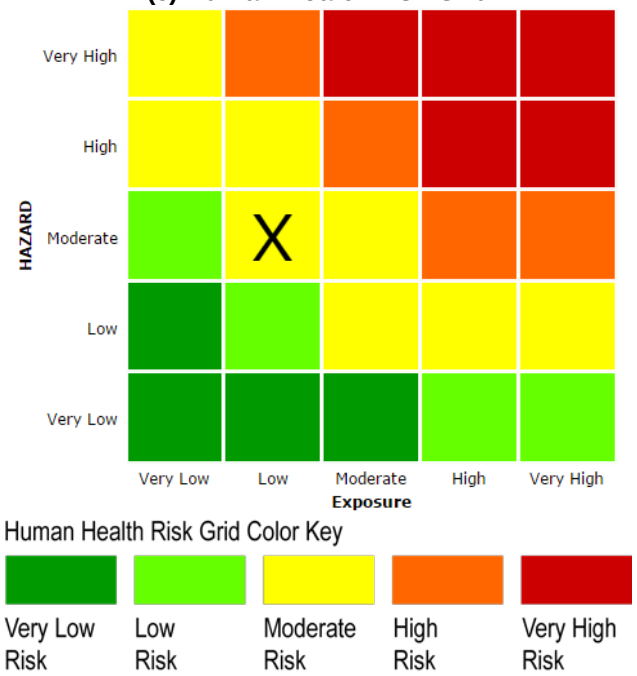
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



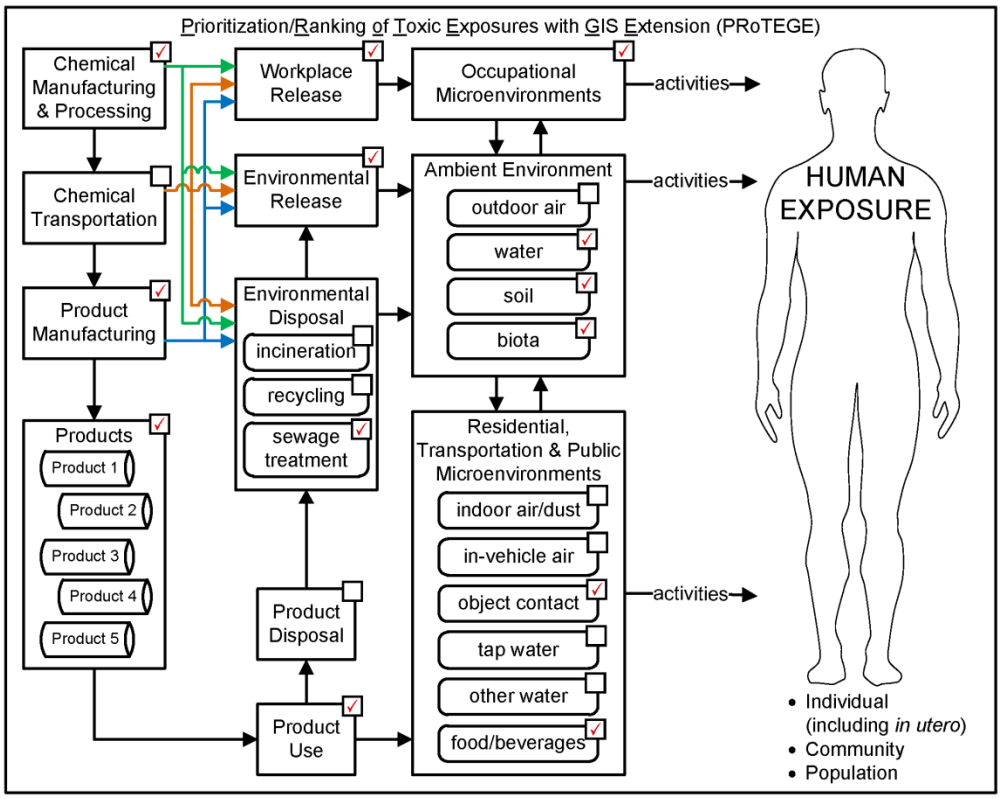
(a) Human Hazard
Estimated ranking of human hazard risk from Bisphenol-A, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Bisphenol-A (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Bisphenol-A, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

PRoTEGE Ranking for C10-13 Chloroalkanes



Summary Physico-Chemical Information	
Name	C10-13 Chloroalkanes
Other Names	Chlorinated paraffin (C10-13); Short-chained chlorinated parraffins
Chemical Formula	$C_xH_{(2x-y+2)}Cl_y$, where x = 10-13 and y = 1 to x
Chemical Class	SCCP
Identifier	CAS: 85535-84-8
Chemical Forms	Mixtures
Physical Properties	
Molecular weight: ~ 320-500 Boiling point: > 200 °C at 1013 hPa Melting point: -30 ~ 20 °C Solubility: 0.15~0.47 mg/L at 20°C Vapor pressure: 0.000213 mmHg at 40 °C	
Additional Notes	
Non-flammable viscous liquid	

Exposure and Toxicity Information
Toxicity Limits: 100 mg/kg/day - repeated doses and carcinogenicity (REACH-NOAEL)
Toxicological Effects: Very toxic to aquatic organisms; may cause long-term adverse effects in the aquatic environment. Liver - changes in liver weight. Biochemical - Enzyme inhibition, induction, or change in blood or tissue levels - hepatic microsomal mixed oxidase (dealkylation, hydroxylation, etc.)
Exposure Limits:
Chemical Use: Lubricant in metal work, rubber, leather, glue
Exposure Routes: Skin absorption, ingestion, skin and/or eye contact. Intraperitoneal. Repeated exposure may cause skin dryness or cracking
Target Organs: liver

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air					Air		
Ground water							
Food					Surface Water		
Indoor Air					Ground Water		
Surface water					Soil		
Tap water							
Soil					Chemical Production and Use		
Dust					Production	Aggregated production volume 15,000 tons	EU (1995)
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

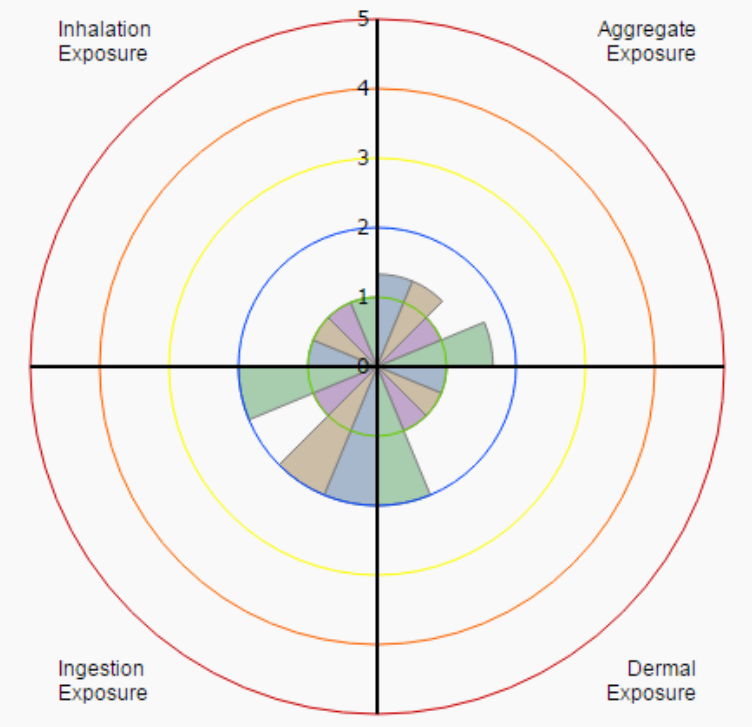
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		
	Tox Profs		
	IRIS		
	HSDB		
	ITER		
	McKay		
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		●
	PFD		
	MSDS		●
	DSSTox		
	TMI		
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		
	ECD		●
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		
	BME		
	ERDEM		

"Tier 1" Exposure Ranking for C10-13 Chloroalkanes

Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	1	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for C10-13 Chloroalkanes

insufficient data for analysis

insufficient data for analysis

	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0	0	NA	0
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

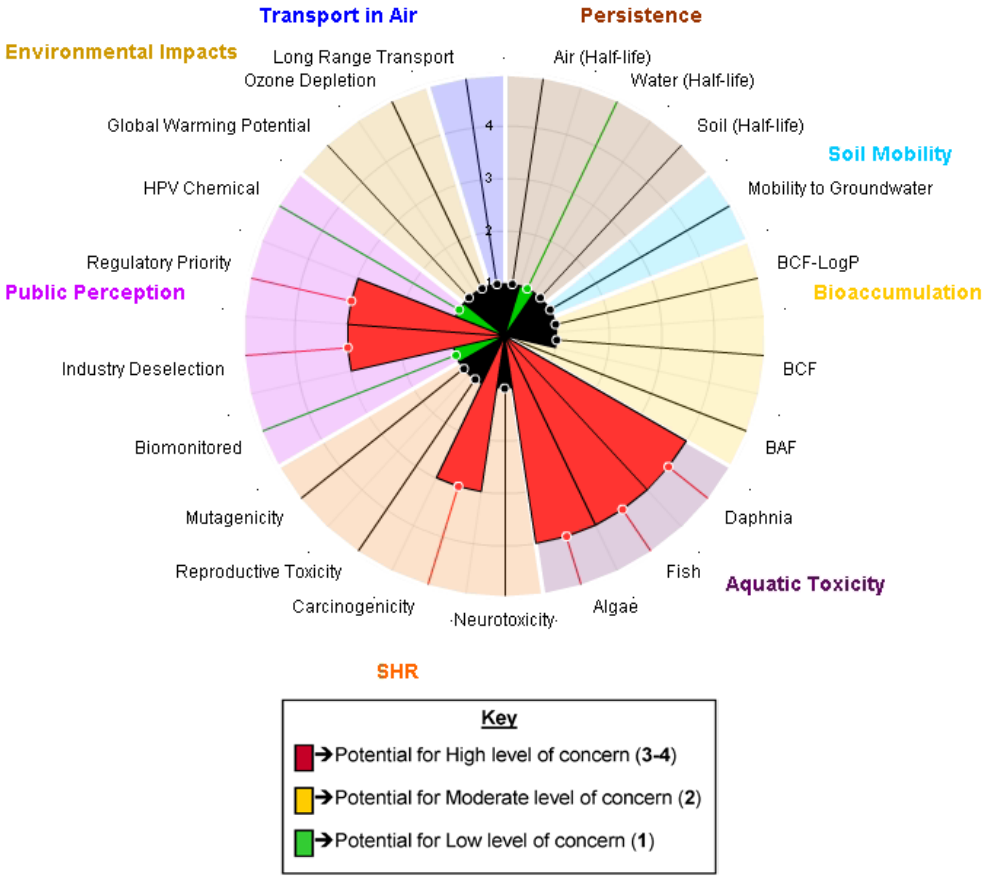
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for C10-13 Chloroalkanes

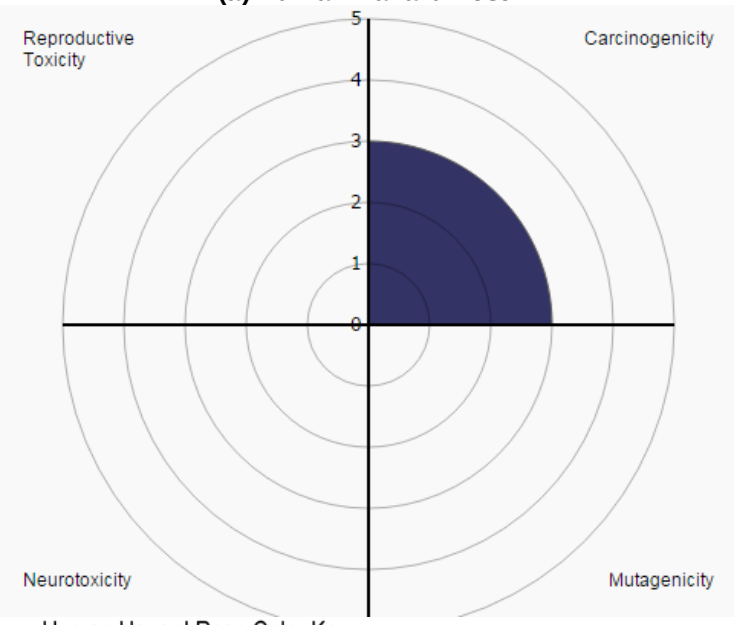
		CAS # 85535-84-8
Persistence	Air (Half-life)	Persistence in Air has not been calculated for this compound
	Water (Half-life)	Persistence in Water has not been calculated for this compound.
	Soil (Half-life)	Persistence in Soil has not been calculated for this compound.
Soil Mobility	Mobility to Groundwater	Soil mobility has not been calculated for this compound
Bioaccumulation	BCF-LogP	BCF value based on LogP has not been calculated for this compound
	BCF	BCF value has not been calculated for this compound
	BAF	
Aquatic Toxicity	Daphnia	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	[EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	3 out of 6 lists (GADSL; EUC2; SINLIST)
	Regulatory Priority	1 out of 10 lists (EU_CAND)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	Long Range Transport in Air has not been calculated for this compound



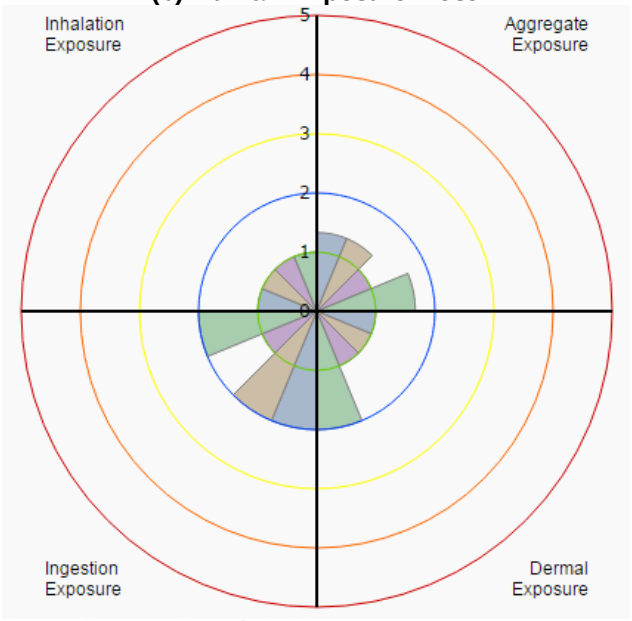
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for C10-13 Chloroalkanes

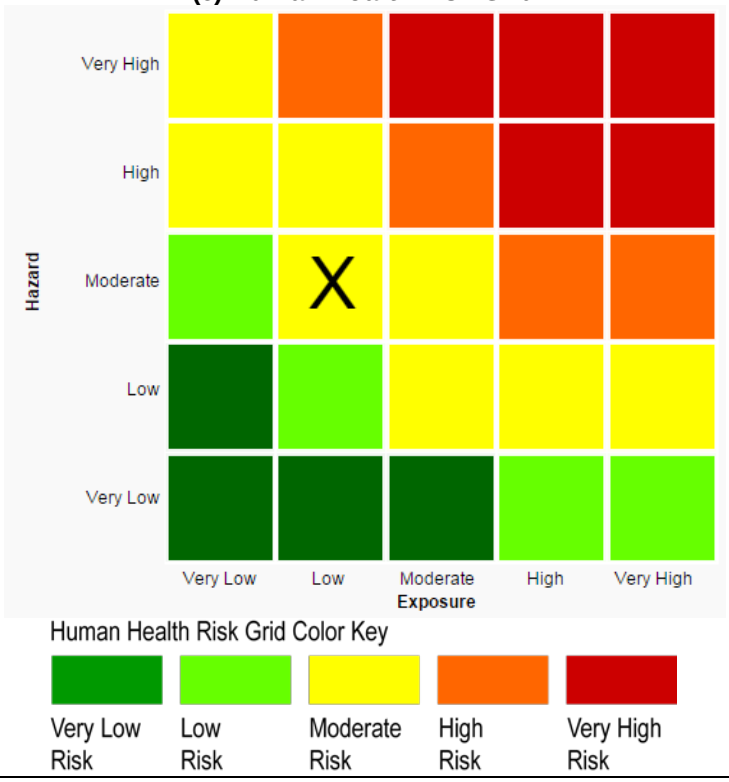
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



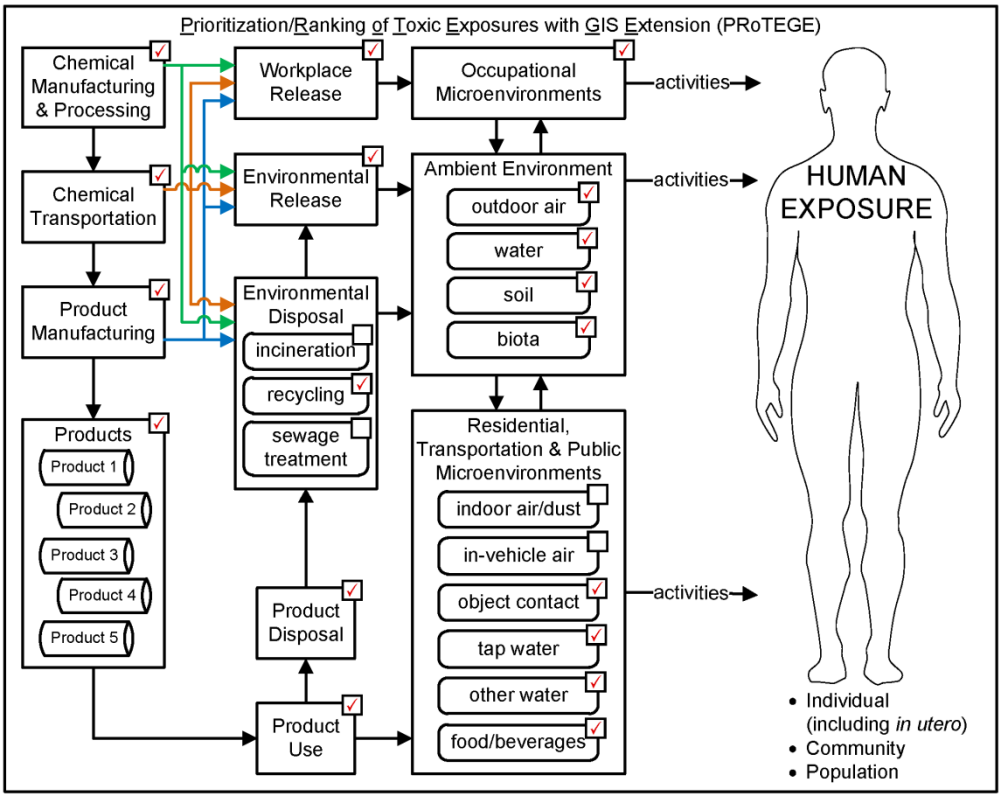
(a) Human Hazard
Estimated ranking of human hazard risk from C10-13 Chloroalkanes, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of C10-13 Chloroalkanes (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from C10-13 Chloroalkanes, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Cadmium



Summary Physico-Chemical Information	
Name	Cadmium
Other Names	
Chemical Formula	Cd
Chemical Class	Mt/MU
Identifier	CAS:7440-43-9
Chemical Forms	
Physical Properties	
Molecular weight: 112.41 Boiling point: 765°C Melting point: 321°C Solubility: 0.05% Specific gravity: 8.65	
Additional Notes	
Recycling cadmium batteries is most prominent. Average Daily Intake: 50 µg (HSDB)	

Exposure and Toxicity Information
Toxicity Limits: RfD (mg/kg/day): 0.0005(water),0.001(food) (IRIS). Average concentrations responsible for fatal cases have been estimated at 50 mg/m³ and 40 mg/m³, both for exposures of 1 hr; and 9 mg/m³ for 5 hr. (HSDB)
Toxicological Effects: Potential symptoms of acute poisoning from the inhalation of cadmium dusts or fumes include headache, chest pains, cough, metal fume fever, weakness. Potential symptoms of acute poisoning from ingestion of cadmium salts are GI disturbances, headache, muscular cramps, vertigo, and convulsions. Chronic inhalation may cause pulmonary emphysema and chronic bronchitis.
Exposure Limits: OSHA PEL*: [1910.1027] TWA 0.005 mg/m³ (NIOSH)
Chemical Use: Batteries, fungicide, colorant
Exposure Routes: inhalation, ingestion
Target Organs: Respiratory system, kidneys, prostate, blood; cancer site: prostate and lung cancer

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	0.0001	0.000715	0.002302	Data Sources: Outdoor air (5th, 50th, 95th, %iles)- '08 annual means @ AQS monitor); Ground water – HSDB; Food –(5th, 50th, 95th %iles)- TDS ('94 – '02), 3884 out of 10373 samples <LOD; Surface water - STORET, 1256 detects, 15127 non-detects; Tap water – [23]; Soil – HSDB, min, geometric mean, max; Biota – HSDB	Air	54.14 (NEI 2005) 0.50 (TRI 2008)	99.94% (NEI 2005) 0.56% (TRI 2008)
Ground water (µg/L)	<0.01	0.05	1.0				
Food (mg/kg)	0.002	0.01	0.046		Surface Water	0.05 (TRI 2008)	0.16% (TRI 2008)
Indoor Air					Ground Water	68.20 (TRI 2008)	0.09% (TRI 2008)
Surface water (µg/L)	0.004	0.51	170		Soil	156.58 (TRI 2008)	0.31% (TRI 2008)
Tap water (ng/L)	<RL	<RL	0.2				
Soil (µg/g)	<0.2	0.53	5.9		Chemical Production and Use		
Dust (µg/cm²)	NA				Production	1 to < 10 million	EU (1996), 5808 44% of them converted into CdO
Surfaces (µg/cm²)	NA						
Biota (µg/g)	0.05	0.20	1.62				
Human Biomarkers				Urine 89.9% of total that are above LOD (NHANES 07-08) Blood 67.1% of total that are above LOD (NHANES 03-04)			
Urine							
Blood							
Other							

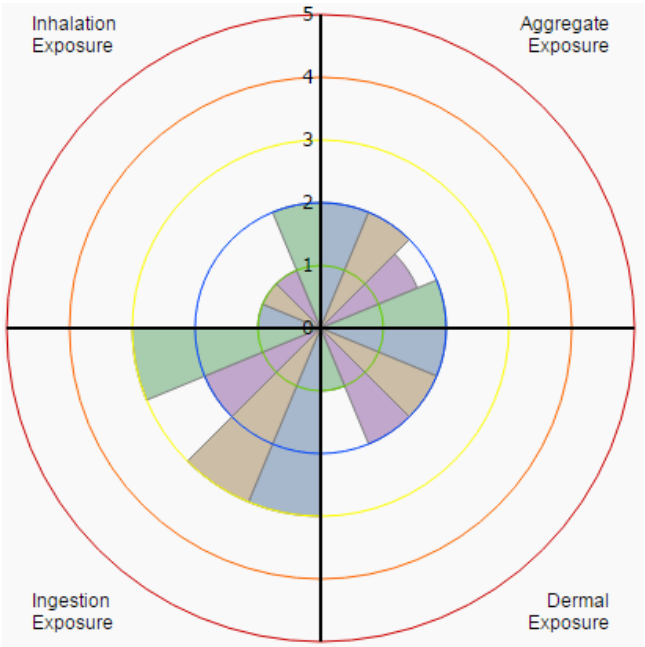
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		●
	IARC		●
	PSAP		●
	NTP		
	REACH		●
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		●
	IUR		●
	ECD		●
	SRD		
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		●
	NHANES	03-04	b,u
		05-06	(b),u
		07-08	(b),u
		09-10	(b,u)
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PKm (H) [7]
	BME		● [35]
	ERDEM		

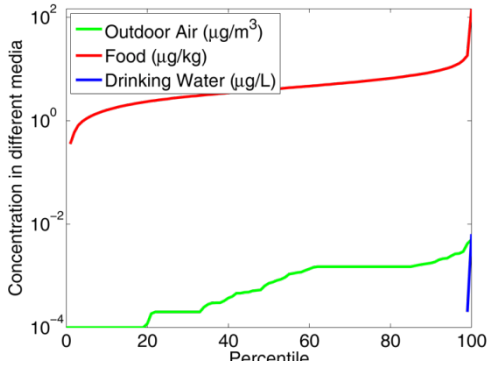
"Tier 1" Exposure Ranking for Cadmium

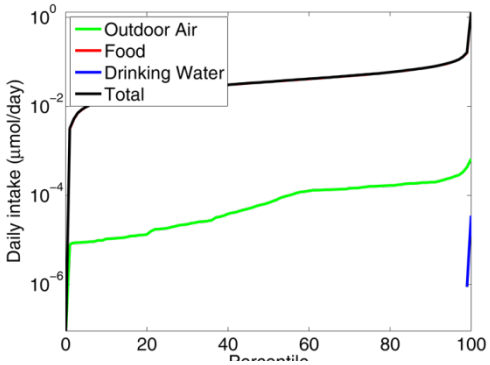
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	2
Ingestion	3	3	2	3
Dermal	2	2	2	1
Aggregate	2	2	1.66	2

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Cadmium





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	6.77E-05	0.0359	NA	0.036
90 % tile	0.000198	0.0767	NA	0.0781
% over 0.1 μmol/day	0	4.69	NA	5.2
% over 1 μmol/day	0	0.271	NA	0.532

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

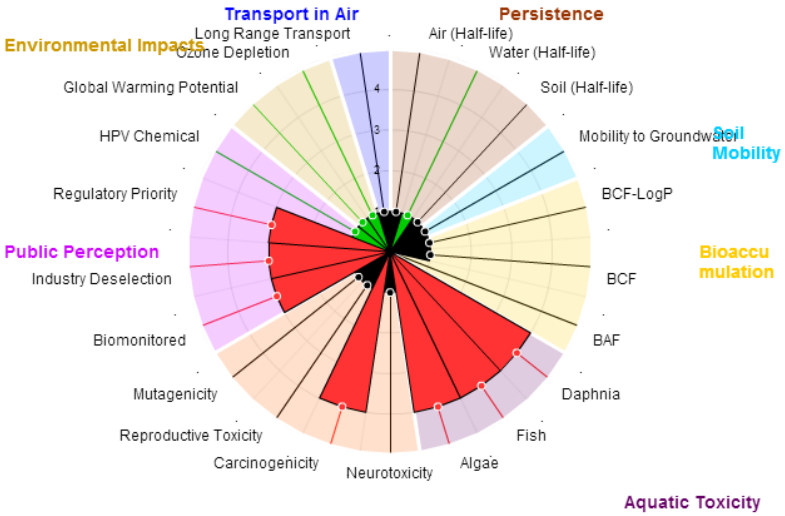
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Cadmium

		CAS # 7440-43-9
Persistence	Air (Half-life)	Persistence in Air has not been calculated for this compound
	Water (Half-life)	Persistence in Water has not been calculated for this compound.
	Soil (Half-life)	Persistence in Soil has not been calculated for this compound.
Soil Mobility	Mobility to Groundwater	Soil mobility has not been calculated for this compound
Bioaccumulation	BCF-LogP	BCF value based on LogP has not been calculated for this compound
	BCF	BCF value has not been calculated for this compound
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 6831.386 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.). This compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 7355.443 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.). This compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.). This compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	Known Carcinogen - human studies indicate a causal relationship between exposure and human cancer [NTPLIST]; Carcinogenic to humans [IARC_OE]; CLASS A2 - Suspected Human Carcinogen [ACGIH]; B1 (Probable human carcinogen - based on limited evidence of carcinogenicity in humans and sufficient evidence of carcinogenicity in animals) [1986 Guidelines] [IRIS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	3 out of 6 lists (GADSL; EUC2; SINLIST)
	Regulatory Priority	1 out of 10 lists (EU_CAND)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Long Range Transport in Air has not been calculated for this compound



SHR

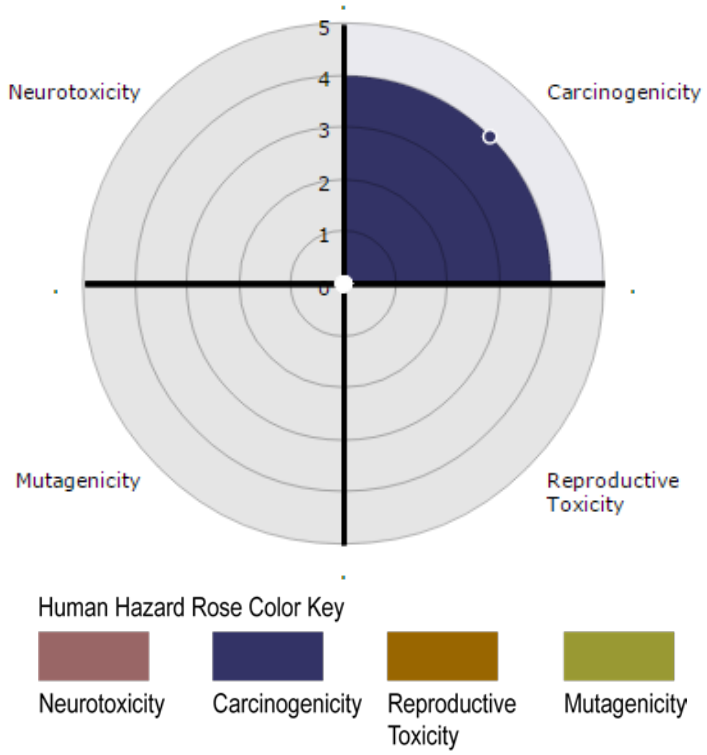
Key

- → Potential for High level of concern (**3-4**)
- → Potential for Moderate level of concern (**2**)
- → Potential for Low level of concern (**1**)

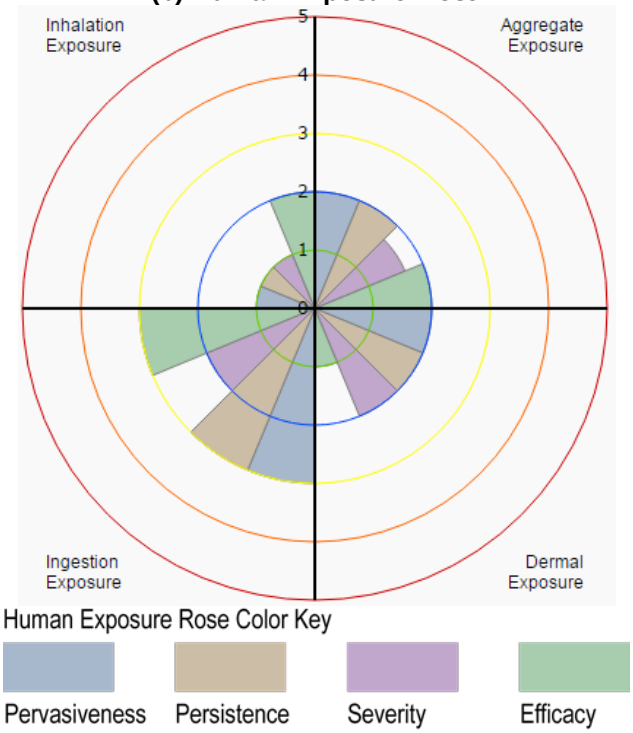
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Cadmium

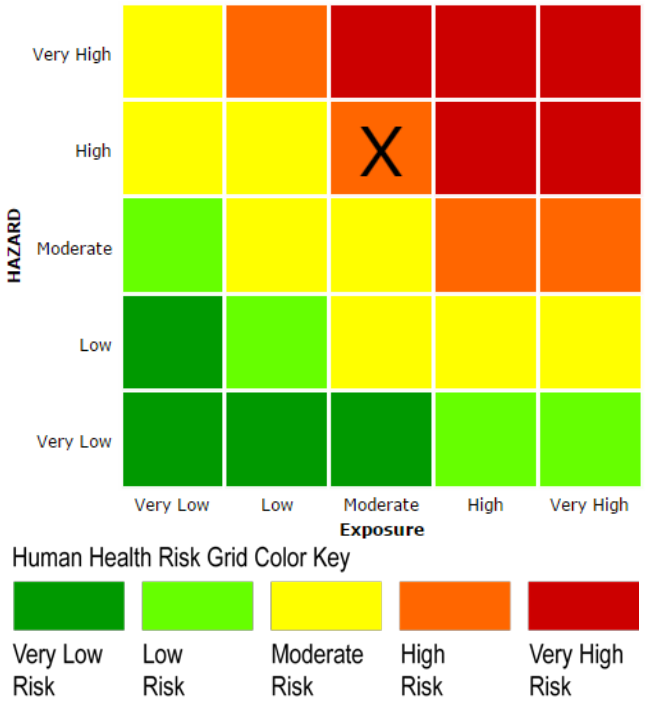
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



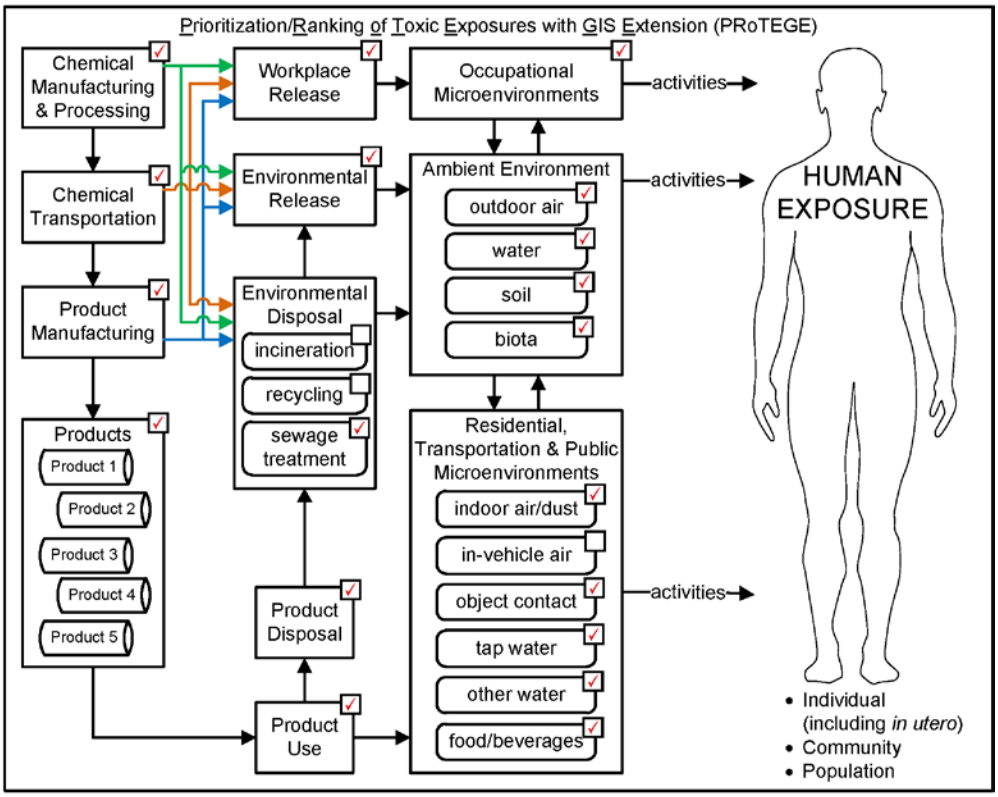
(a) Human Hazard
Estimated ranking of human hazard risk from Cadmium, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Cadmium (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Cadmium, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Ranking for Carbaryl



Summary Physico-Chemical Information	
Name	Carbaryl
Other Names	1-naphthyl methylcarbamate, Sevin
Chemical Formula	$CH_3NHCOOC_{10}H_7$
Chemical Class	CarP
Identifier	CAS: 63-25-2; RTECS: FC5950000; UN: 2757; EC: 006-011-00-7
Chemical Forms	
Physical Properties	
Molecular weight: 201.2 Melting point: 142°C Density: 1.2 g/cm³ Solubility in water: 0.04 - 0.12 g/L (at 30°C) Vapor pressure: negligible at 20°C Flash point: 193-202°C Octanol/water partition coefficient as log Pow: 1.59	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD 1 x10^{-1} mg/kg/day (IRIS); RfC: NA (IRIS); TDI 3 x10^{-3} mg/kg/day (RIVM)
Toxicological Effects: Carcinogenic classification – A4 (ACGIH 2004), Category (4); (DFG 2003)
Exposure Limits: NIOSH REL: TWA 5 mg/m³; OSHA PEL: TWA 5 mg/m³
Chemical Use: Pesticide
Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ppb)	3.04e-07	5.23e-06	1.26e-05	Data sources: Outdoor air (5th, 50th, and 95th %iles) - 2002 NATA county-level annual averages. Surface and biota - HSDB. Food (5th, 50th, and 95th %iles) - TDS '94-'02. Indoor Air (min, mean, and max) [77] 19% of samples were >LOD. Tap water - (min, mean, max) NCOD 0.09% of samples were >LOD.	Air	21.99 (NEI 2005) 0.27 (TRI 2008)	7.97% (NEI 2005) 0.28% (TRI 2008)
Ground water							
Food (µg/g)	0.002	0.007	0.14		Surface Water	0.01 (TRI 2008)	0.09%
Indoor Air (ng/m³)	0.89	1.5	22		Ground Water	21.99 (TRI 2008)	7.97%
Surfaces (µg/L)	<0.046-1.5		0.15-2.5		Soil		
Tap water (µg/L)	0.18	0.56	3.0				
Soil					Chemical Production and Use		
Dust					Production		
Biota (µg/cm²)	0.07		0.18				
Outdoor air (ppb)	3.04e-07	5.23e-06	1.26e-05				
Human Biomarkers							
Urine							
Blood							
Other							

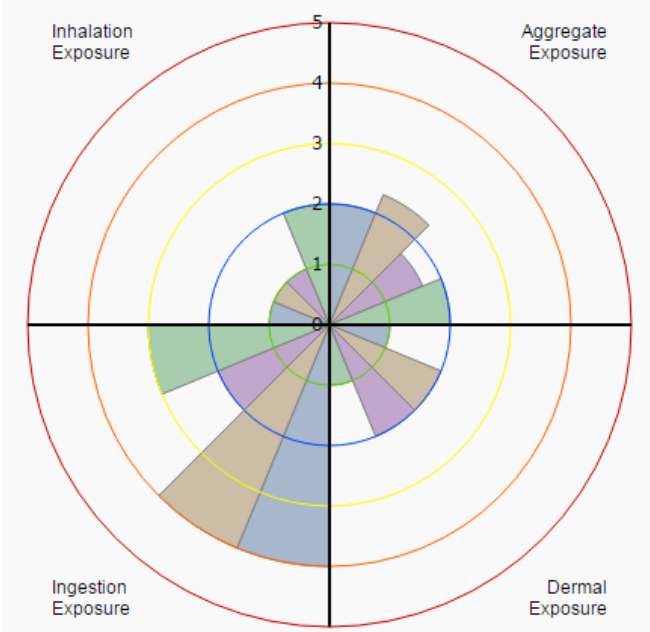
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		○
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PBPKm (R) [28]
	BME		
	ERDEM		● PKd

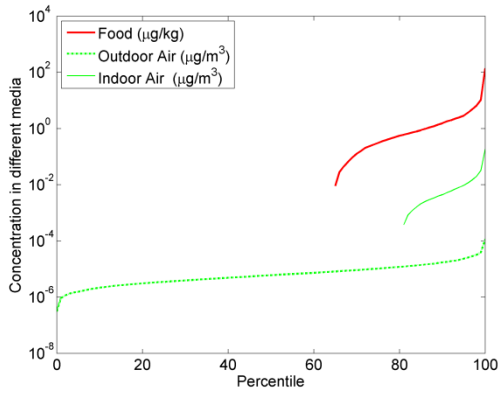
"Tier 1" Exposure Ranking for Carbaryl

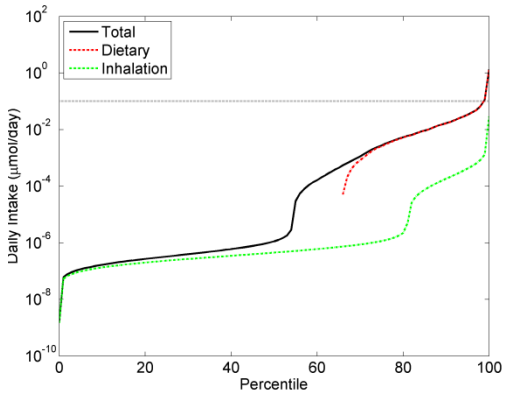
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	2
Ingestion	4	4	2	3
Dermal	1	2	2	1
Aggregate	2	2.33	1.66	2

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Carbaryl





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0	0	NA	0
90 % tile	0.000197	0.00742	NA	0.008
% over 0.1 μmol/day	0	0.947	NA	1.88
% over 1 μmol/day	0	0.0231	NA	0.0892

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

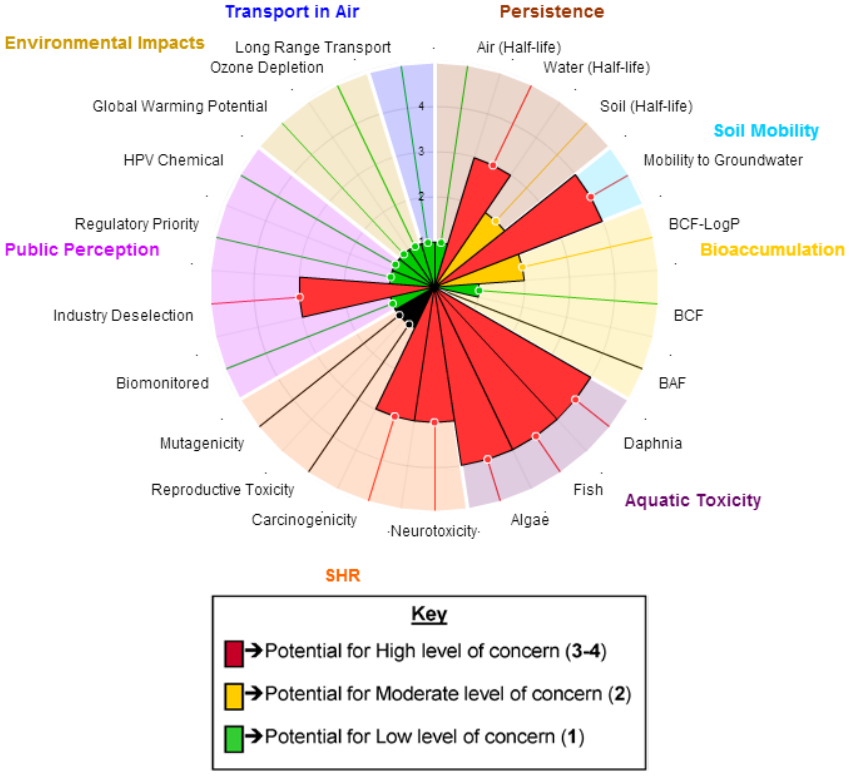
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Carbaryl

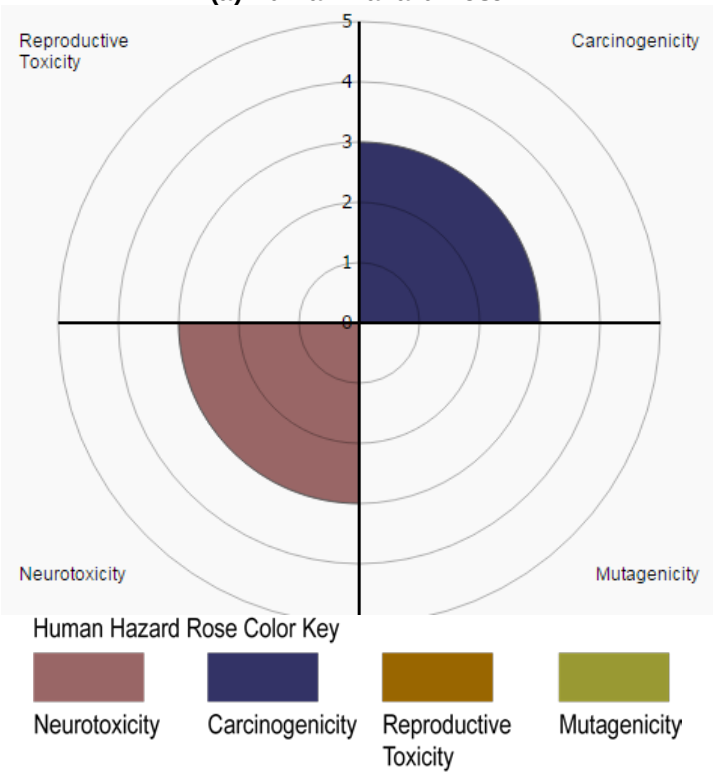
		CAS # 63-25-2
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.4114 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 27% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is persistent in water (Min. BOD = 8%, Max. BOD = 65%).
	Soil (Half-life)	Moderate persistence in Soil (Estimated Half-life = 75 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 2.383
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=2.36
	BCF	Low bioconcentration potential based on Experimental LogBCF = 0.95
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 76.769 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R50 (Very toxic to aquatic organisms.).
	Fish	An estimated LC50(96-hr) = 19.790 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R50 (Very toxic to aquatic organisms.).
	Algae	No toxicity estimate. However, this compound is classified as R50 (Very toxic to aquatic organisms.).
SHR	Neurotoxicity	Known Neurotoxin [Grandjean et al]
	Carcinogenicity	Carc. 2: [EU_GHS]; CLASS A4 - Not Classifiable as a Human Carcinogen [ACGIH]; Not classifiable [IARC_OE]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (EUC2)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 22.4446 km - A_TRNSPRT)



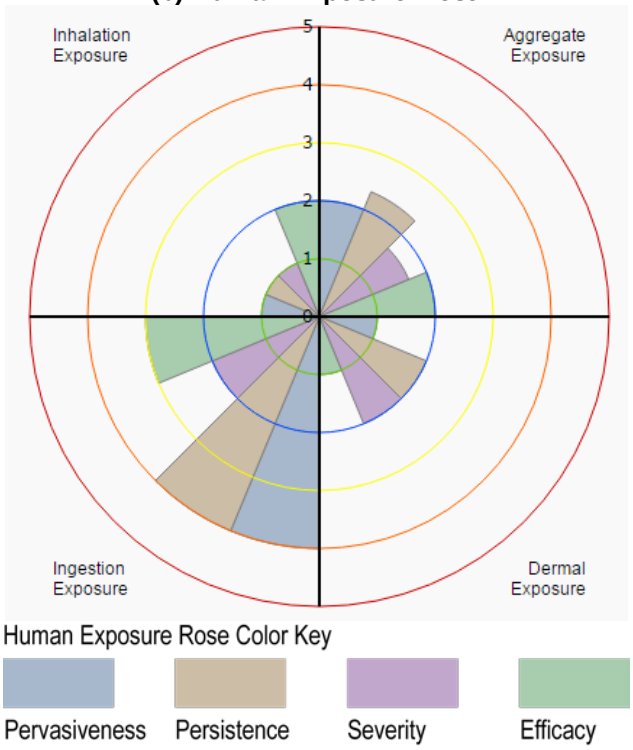
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Carbaryl

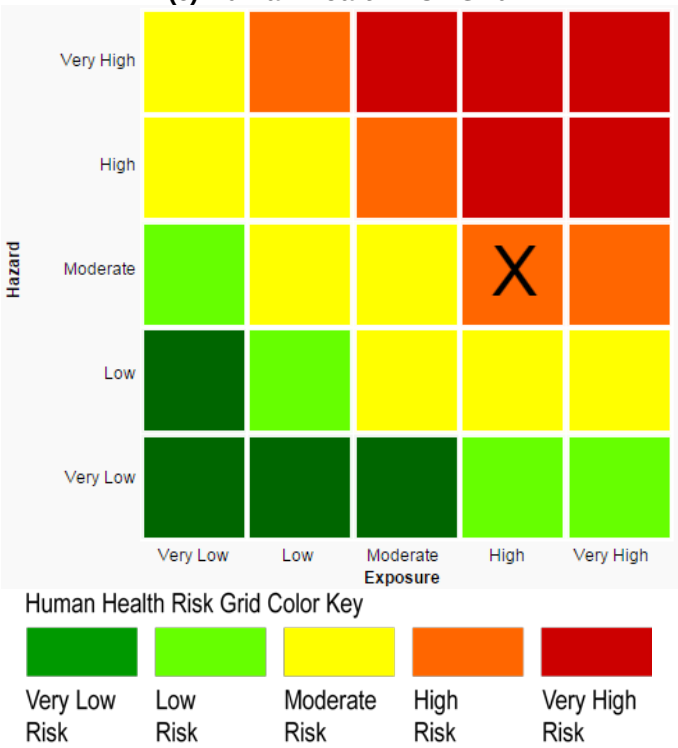
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



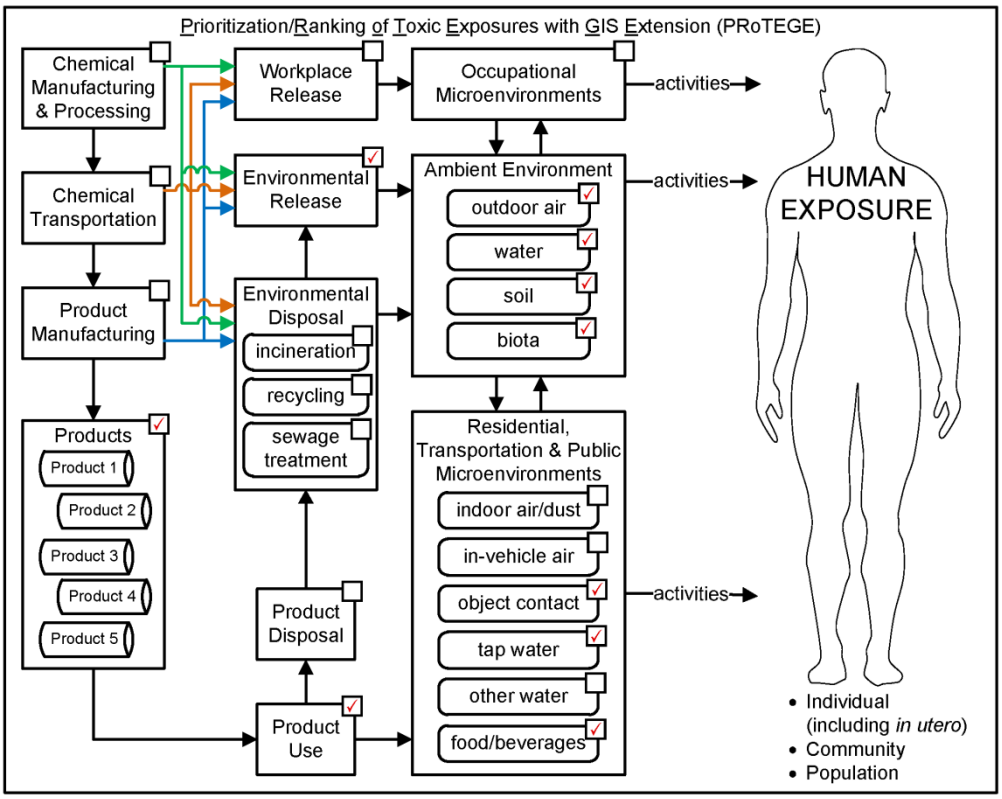
(a) Human Hazard
Estimated ranking of human hazard risk from Carbaryl, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Carbaryl (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Carbaryl, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for DDT



Summary Physico-Chemical Information	
Name	DDT
Other Names	p,p'-DDT; Dichlorodiphenyltrichloroethane; 1,1,1-Trichloro-2,2-bis(p-chlorophenyl)ethane
Chemical Formula	$(C_6H_4Cl)_2CHCCl_3$
Chemical Class	CAS: 50-29-3
Identifier	OCP
Chemical Forms	
Physical Properties	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.0005 mg/kg/day (IRIS); RfC: NA (IRIS)
Toxicological Effects: Carcinogenic classification: B2 (IRIS), numbness, paresthesias, malaise, headache, sore throat, fatigue, weakness, coarse tremors, convulsions and coma; death due to respiratory failure
Exposure Limits: NIOSH REL: Ca TWA 0.5 mg/m³ OSHA PEL: TWA 1 mg/m³ [skin]
Chemical Use: Contact insecticide
Exposure Routes: Inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, central nervous system, kidneys, liver, peripheral nervous system; Cancer site: [in animals: liver, lung and lymphatic tumors]

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (pg/m³)	7.7	36	169	Data Sources: Food –(5th, 50th, 95th %iles)-TDS('94 – '02), 10% samples > LOD based on TDS('91 – '03), DDE, DDT's natural degradation –(5th, 50th, 95th %iles)- is 0.2, 0.8, 9 (ppb) - TDS('94 – '02); Indoor air: [36] (5, 50, and 95%tiles); Outdoor air - [37] (5, 50, 95%tiles)	Air		
Ground water							
Food (µg/g)	0.1	0.7	5		Surface Water		
Indoor Air (ng/m³)	<LOD	<LOD	0.797		Ground Water		
Surface water					Soil		
Tap water							
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers				Data Source: Blood: 71.2% > LOD, serum (NHANES 03'-04')			
Urine							
Blood							
Other							

Data for DDT Metabolite DDE: Outdoor air - 2.08779E-09; 4.71729E-08; 1.00548E-06 µg /m³ (5th, 50th, 95th %iles)-NATA 2002 county level average, 265 out of 280 counties have annual data below LOD

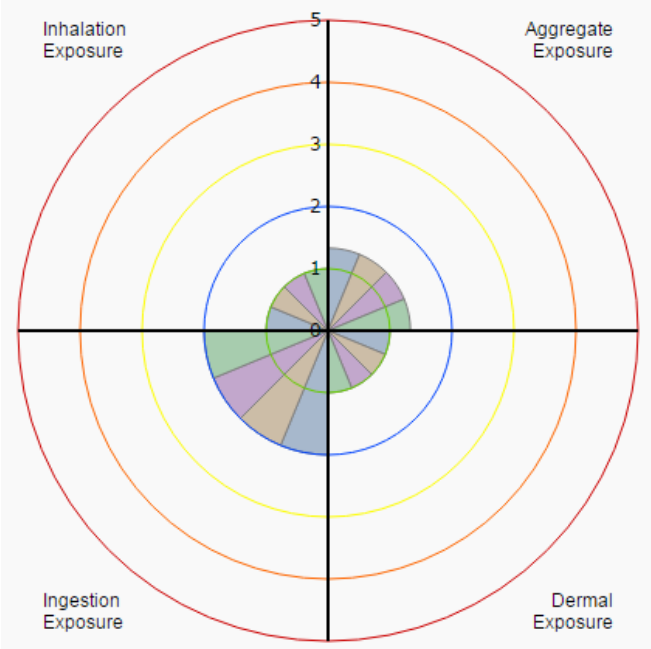
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		□
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		
	RIVM rprts		●
	IARC		
	PSAP		
	NTP		●
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	●
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		
	IUR		
	ECD		○
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		●
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		●1
	SDWIS		
	NHANES	03-04	s
		05-06	(s)
		07-08	(s)
		09-10	(s)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PKm (H) [38]
	BME		
	ERDEM		

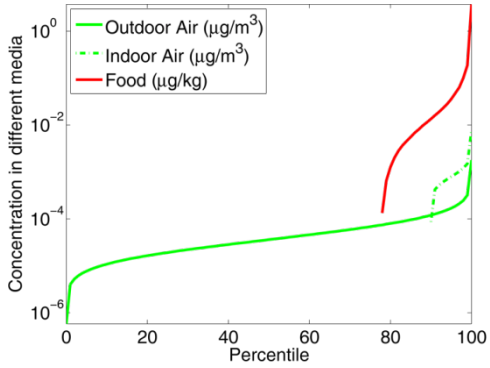
"Tier 1" Exposure Ranking for DDT

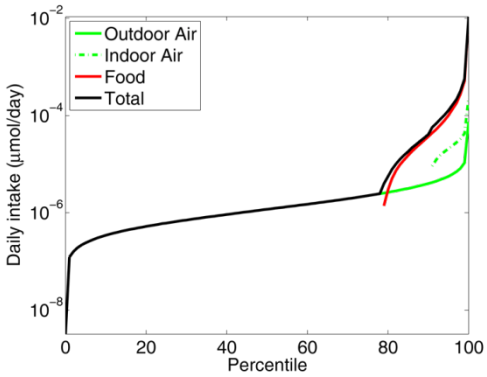
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	1
Aggregate	1.33	1.33	1.33	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for DDT





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	1.34E-06	0	NA	1.34E-06
90 % tile	1.04E-05	3.88E-05	NA	5.29E-05
% over 0.1 μmol/day	0	0	NA	0
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

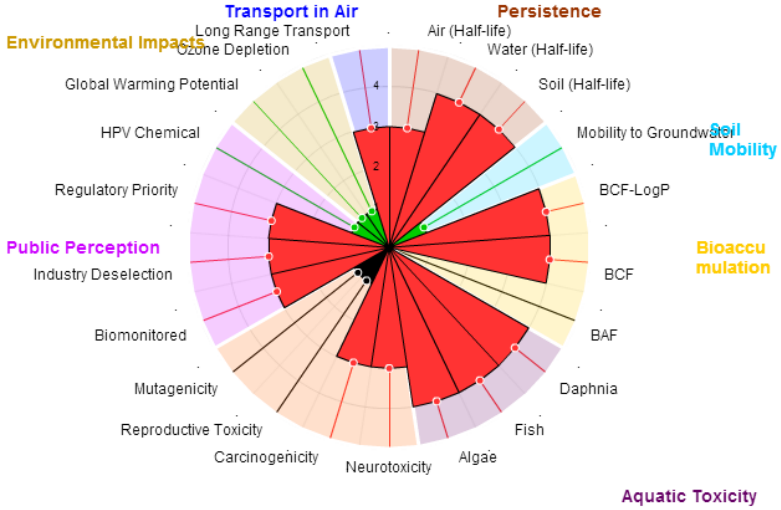
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for DDT

		CAS # 50-29-3
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 3.114 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 0% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 0%, Max. BOD = 0%).
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Low mobility to groundwater based on LogKoc = 5.343
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=6.91
	BCF	Very High bioconcentration potential based on Experimental LogBCF = 4.47
	BAF	
Aquatic Toxicity	Daphnia	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 0.103 mg/L indicates a Moderate toxicity to Fish [CLOGP]. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	Anticipated Carcinogen - there is limited evidence of carcinogenicity in humans or sufficient evidence of carcinogenicity in animals [NTP] [NTPLIST]; Possibly carcinogenic to humans [IARC_OE]; Carc. 2: [EU_GHS]; B2 (Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals) [1986 Guidelines] [IRIS]; CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	2 out of 6 lists (RC_PIC; EUC2)
	Regulatory Priority	2 out of 10 lists (EPA_PBT; JCL1_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 704.457 km - A_TRNSPRT)



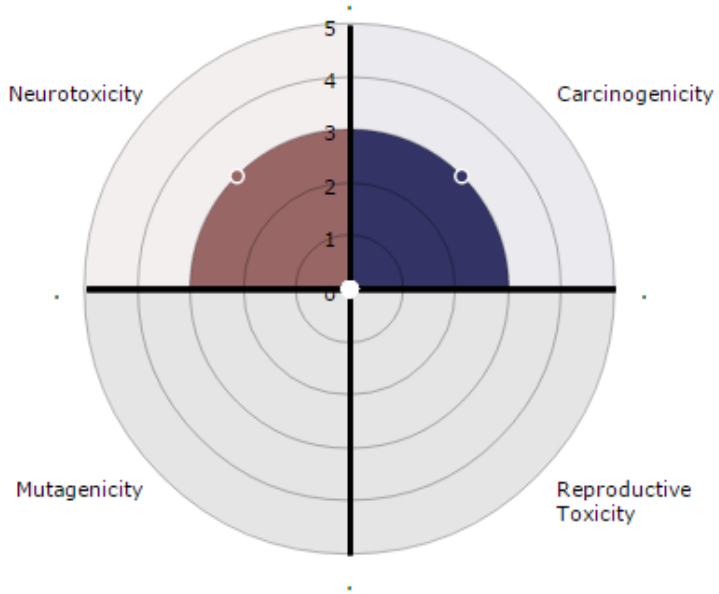
Key

- → Potential for High level of concern (**3-4**)
- → Potential for Moderate level of concern (**2**)
- → Potential for Low level of concern (**1**)

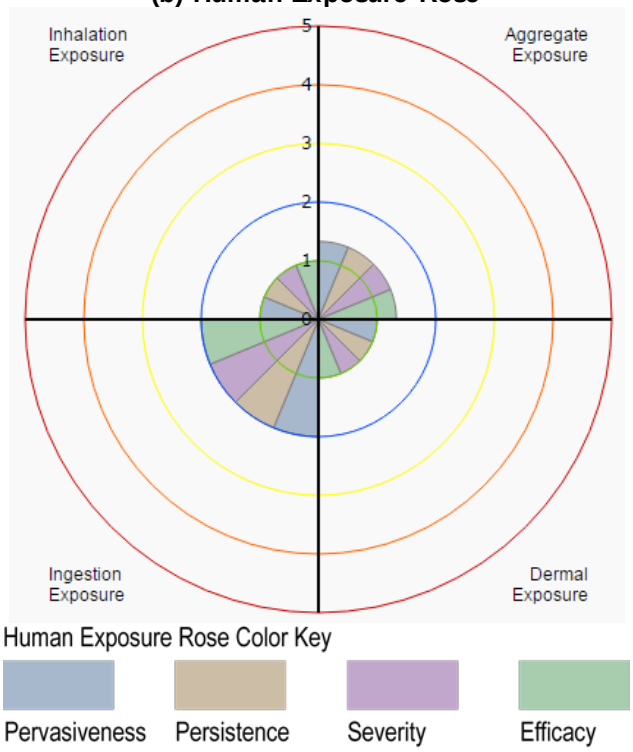
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for DDT

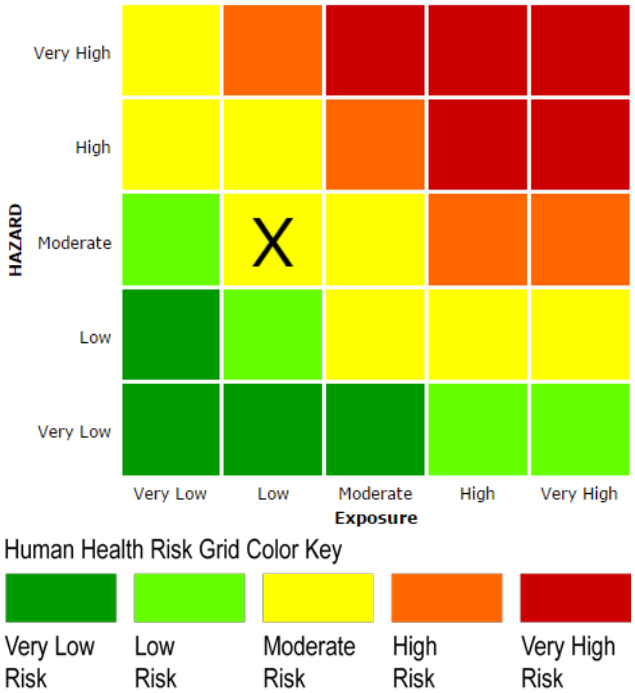
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



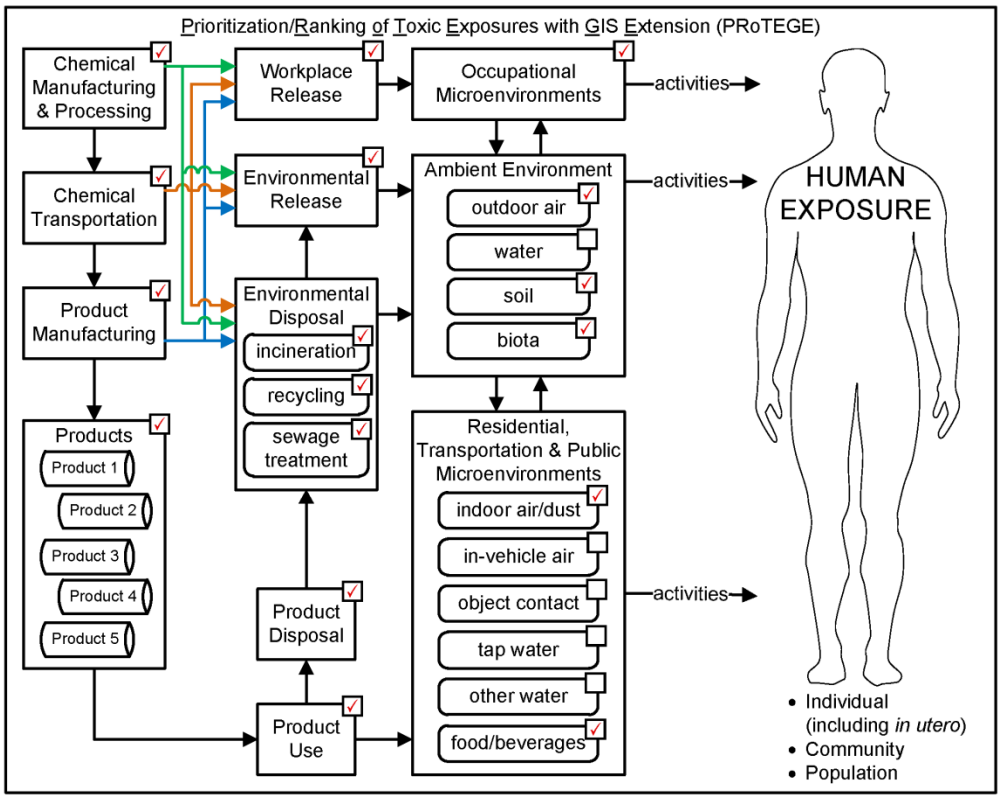
(a) Human Hazard
Estimated ranking of human hazard risk from DDT, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of DDT (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from DDT, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for decaBDE



Summary Physico-Chemical Information	
Name	decaBDE
Other Names	Decabromodiphenyl ether, 2,3,4,5,6-Pentabromo-1-(2,3,4,5,6-pentabromophenoxy)benzene; BDE 209
Chemical Formula	$C_{12}Br_{10}O$
Chemical Class	PBDEs
Identifier	CAS: 1163-19-5
Chemical Forms	
Physical Properties	
Molecular weight: 959.17 Boiling point: 425 °C (decomposition) Melting point: 294–296 °C Solubility: 20-30 µg/L Specific gravity:3.364 Flash Point: 241 °C	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.007 mg/kg/day (IRIS); MRL: 10 mg/kg/day (Int) (ATSDR); NOAEL: 1,120 mg/kg/day (REACH)
Toxicological Effects: not classifiable as to its carcinogenicity to humans (IARC), a possible human carcinogen (IRIS)
Exposure Limits:
Chemical Use: flame retardant
Exposure Routes: ingestion, inhalation
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (pg/m³)	<LOD	<LOD	0.77	Food - [39] (5, 50, 95%tiles); Outdoor air - [37] (5, 50, 95%tiles)	Air	27.09 (TRI 2008)	1.12% (TRI 2008)
Ground water							
Food (ng/kg)	<LOD	1.4	19		Surface Water	0.09 (TRI 2008)	0.22% (TRI 2008)
Indoor Air					Ground Water		
Surface water					Soil	60.70 (TRI 2008)	0.16% (TRI 2008)
Tap water							
Soil					Chemical Production and Use		
Dust					Production	50 to < 100 million lbs in 2006 will be reduced to zero by Dec 2012	Commitment letter to EPA from ICL – Industrial Products
Surfaces							
Biota							
Human Biomarkers				Data Source: Adipose 21% > LOD (NHATS); Human milk 70% > LOD (HSDB)			
Urine							
Adipose (pg/g lipid basis)		5 - 20					
Human milk (ng/g lipid)		up to 8.24					

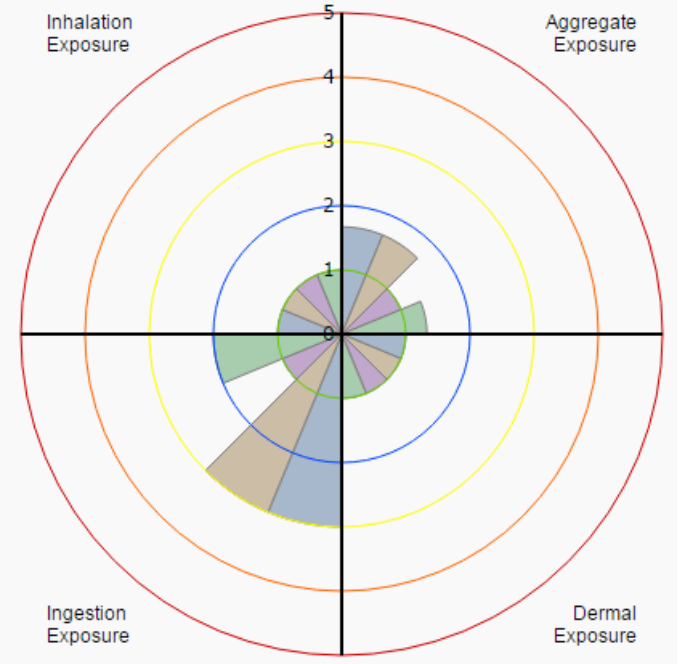
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		
	Tox Profs		□
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		
	RIVM rprts		
	IARC		●
	PSAP		
	NTP		●
	REACH		●
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		●
	ECD		●
	SRD		
Releases	TRI		●
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		
	BME		
	ERDEM		

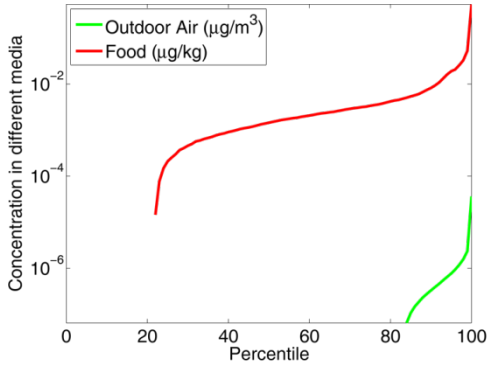
"Tier 1" Exposure Ranking for decaBDE

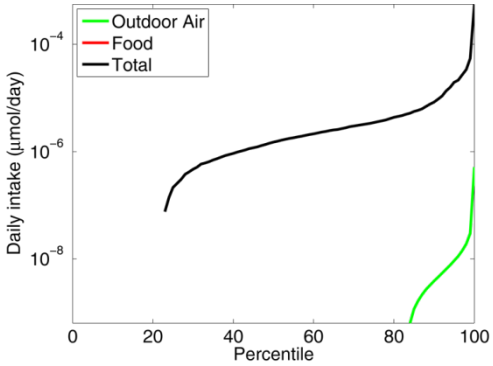
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	3	3	1	2
Dermal	1	1	1	1
Aggregate	1.66	1.66	1	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for decaBDE





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0	1.52E-06	NA	1.52E-06
90 % tile	3.92E-09	8.58E-06	NA	9.02E-06
% over 0.1 μmol/day	0	0	NA	0
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

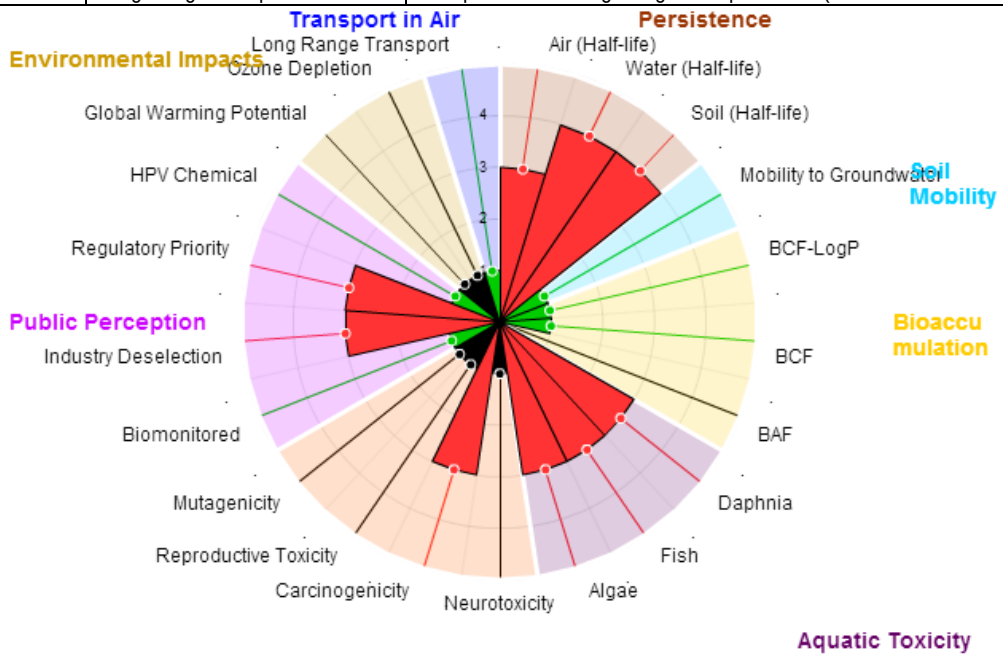
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for decaBDE

		CAS # 1163-19-5
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 476.3 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 0% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 0%, Max. BOD = 0%).
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Low mobility to groundwater based on LogKoc = 5.441
Bioaccumulation	BCF-LogP	Low bioconcentration potential based on an Estimated LogP=12.11
	BCF	Low bioconcentration potential based on Experimental LogBCF = 0.3
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) >0.0048 mg/L indicates a High toxicity to Daphnia.
	Fish	A measured LC50 (96-hr) >0.0046 mg/L indicates a High toxicity to Fish.
	Algae	A measured EC50 (72-hr) >0.0052 mg/L indicates a High toxicity to Algae.
SHR	Neurotoxicity	
	Carcinogenicity	Suggestive evidence of carcinogenic potential [2005 Guidelines] [IRIS]; Not classifiable [IARC_OE]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	2 out of 6 lists (GADSL; SINLIST)
	Regulatory Priority	2 out of 10 lists (EU_CAND; JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 358.975 km - A_TRNSPRT)



SHR

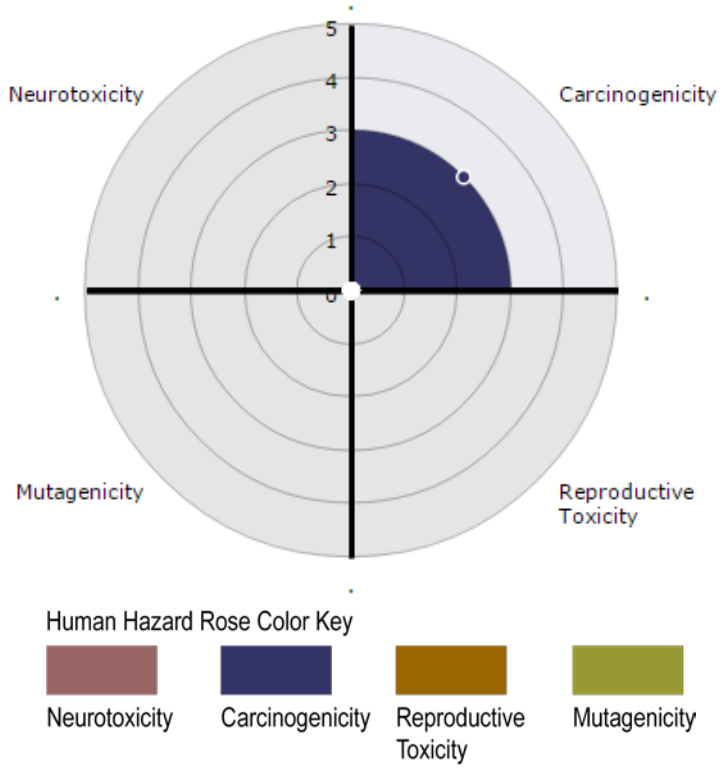
Key

- → Potential for High level of concern (**3-4**)
- → Potential for Moderate level of concern (**2**)
- → Potential for Low level of concern (**1**)

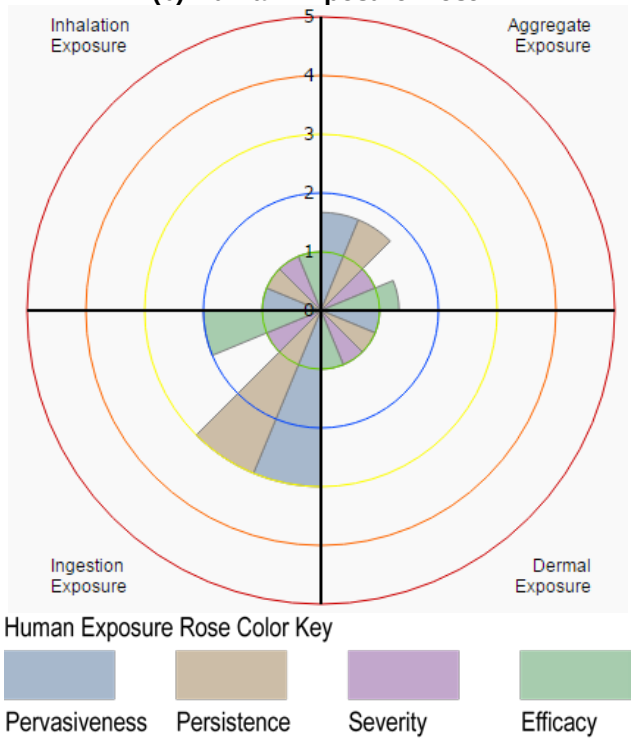
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for decaBDE

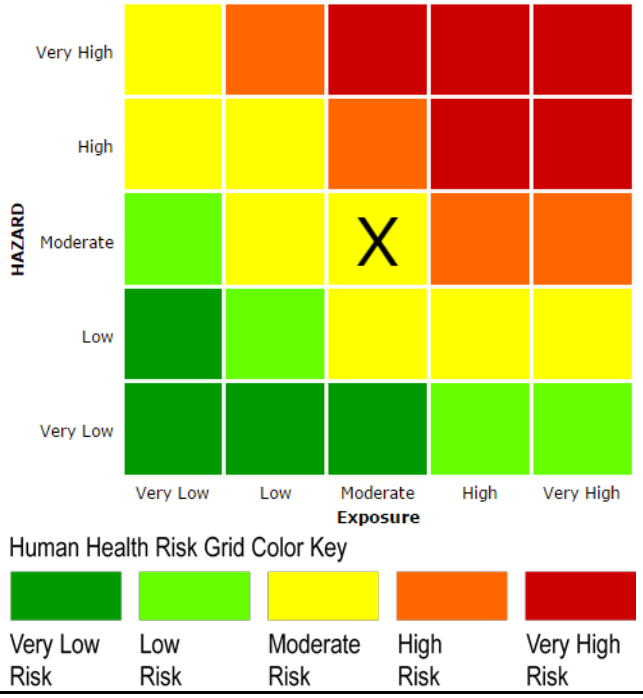
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



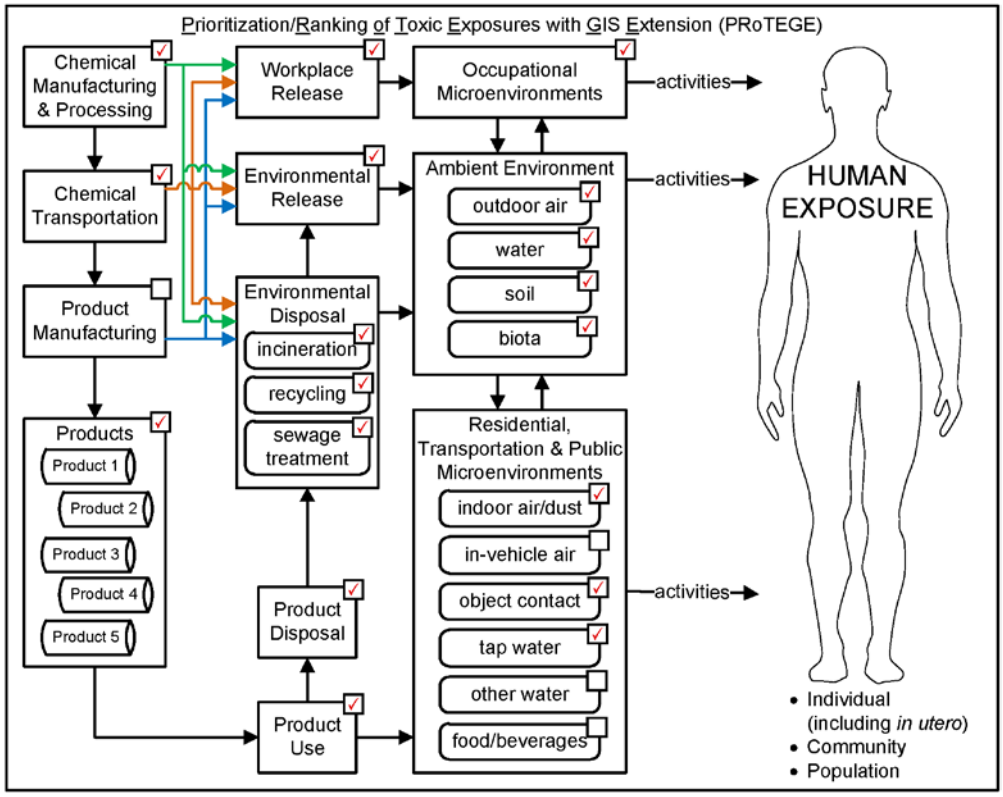
(a) Human Hazard
Estimated ranking of human hazard risk from decaBDE, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of decaBDE (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from decaBDE, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for DEHP, Di(2-ethylhexyl)phthalate



Summary Physico-Chemical Information	
Name	Di(2-ethylhexyl)phthalate
Other Names	DEHP, DOP, bis-(2-Ethylhexyl) phthalate, Octyl phthalate
Chemical Formula	$C_{24}H_{38}O_4$
Chemical Class	Plzr
Identifier	CAS: 117-81-7
Chemical Forms	
Physical Properties	
MW: 390.5 BP: 727°F FRZ: -58°F Sol: 0.00003% VP: <0.01 mmHg Sp.Gr: 0.99 Fl.P(oc): 420°F	
Additional Notes	
Colorless, oily liquid with a slight odor	

Exposure and Toxicity Information
Toxicity Limits: RfD: NA (IRIS); RfC: NA (IRIS);
Toxicological Effects: Carcinogenic classification – Group B2 probable human carcinogen (IRIS), A3 (confirmed animal carcinogen with unknown relevance to human)
Exposure Limits: NIOSH REL: Ca TWA 5 mg/m³; OSHA PEL: TWA 5 mg/m³
Chemical Use: Plasticizer for variety of plastic manufacturing processes; also used widely in insect repellant formulation
Exposure Routes: Inhalation, ingestion, skin and/or eye contact
Target Organs: Eyes, respiratory system, central nervous system, reproductive system, gastrointestinal tract

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	0.0052	0.005657	0.00828	Data Source: Outdoor air (5th, 50th, 95th %ile) – NATA county-level annual average, Groundwater– HSDB; Food – [40] (5, 50, and 95%tiles); Indoor air - [36,40] (5, 50, and 95%tiles); Tap water - [23]	Air	308.71 (NEI 2005) 79.95 (TRI 2008)	99.91% (NEI 2005) 2.7% (TRI 2008)
Ground water (ppb)		170					
Food (µg/kg)	36	132	518		Surface Water	2.08 (TRI 2008)	0.4%
Indoor Air (ng/m³)	25.8	55	116		Ground Water	NA (TRI 2008)	
Surface water					Soil	12.92 (TRI 2008)	0.06%
Tap water (µg/L)	<RL	<RL	0.255				
Soil					Chemical Production and Use		
Dust					Production	1-4 Million tons	Data source: Western EU (1997)
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

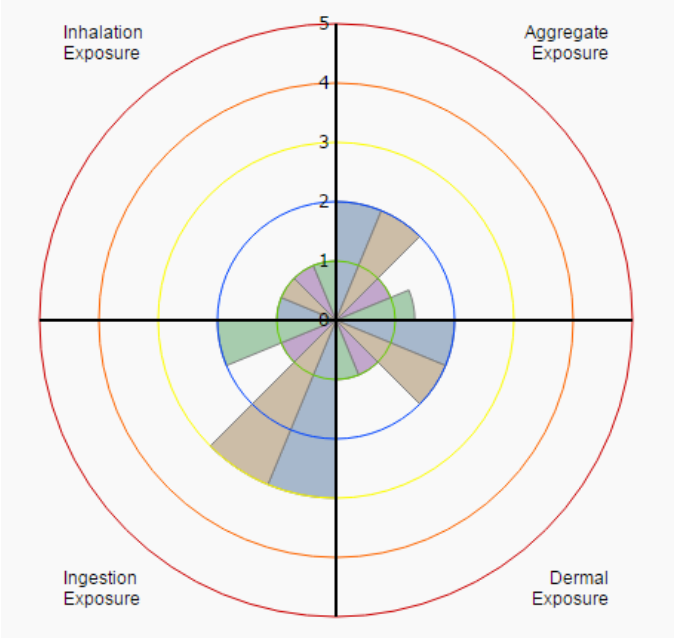
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		●
	Tox Cast	Ph I	
		Ph II	●
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		○
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		○
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [41]
	BME		
	ERDEM		

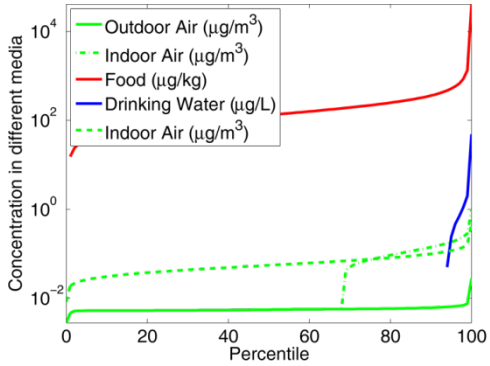
"Tier 1" Exposure Ranking for DEHP, Di(2-ethylhexyl)phthalate

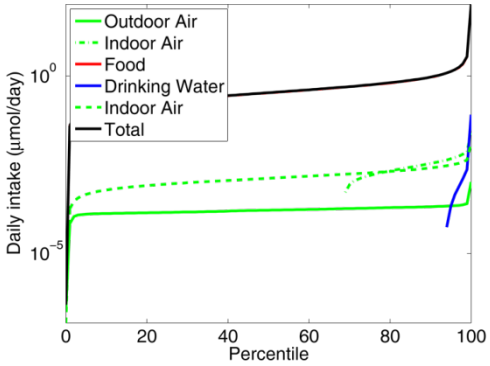
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	3	3	1	2
Dermal	2	2	1	1
Aggregate	2	2	1	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for DEHP, Di(2-ethylhexyl)phthalate





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0.00194	0.339	NA	0.341
90 % tile	0.00542	0.932	NA	0.958
% over 0.1 µmol/day	0	94.1	NA	93.7
% over 1 µmol/day	0	8.73	NA	9.25

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

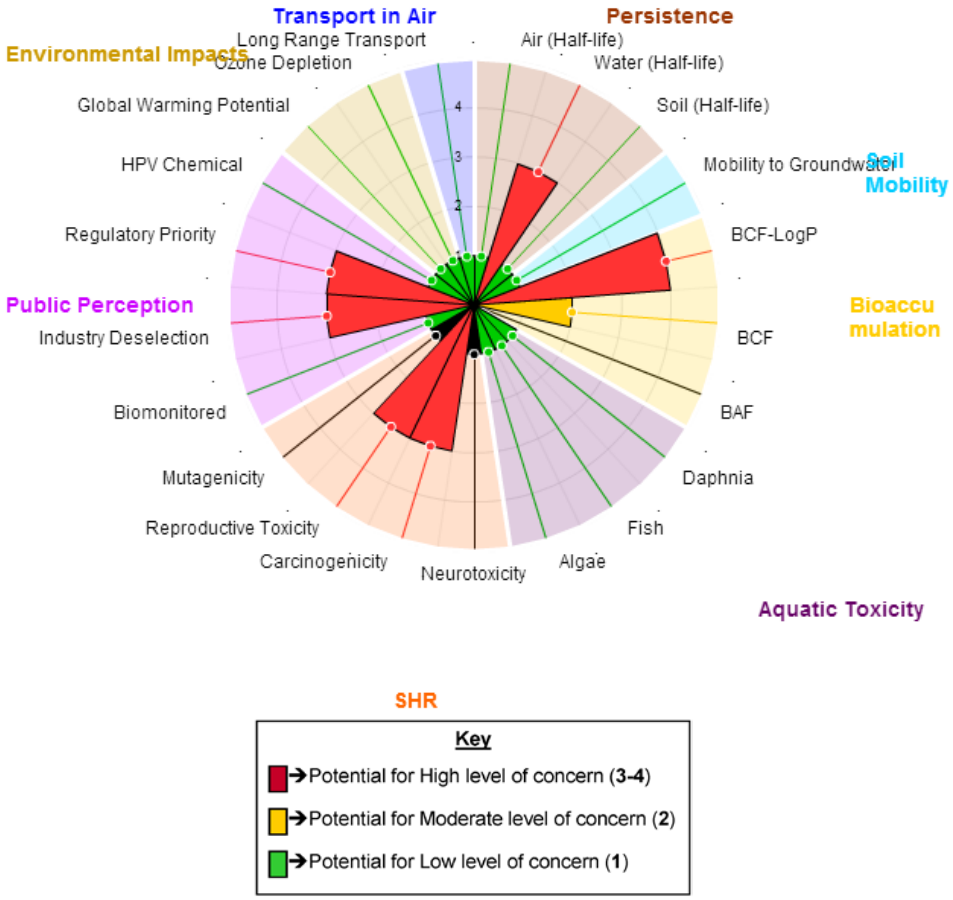
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for DEHP, Di(2-ethylhexyl)phthalate

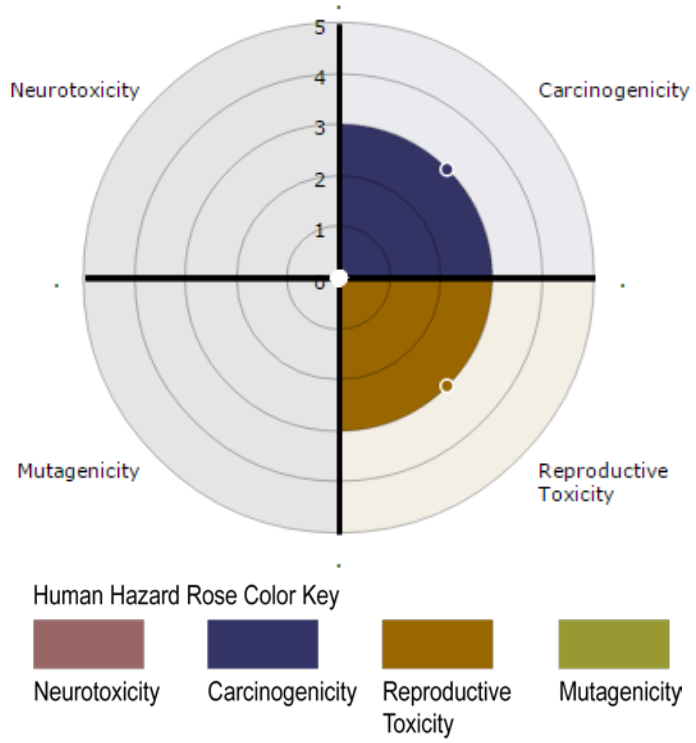
		CAS # 117-81-7
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.4872 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 29% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is persistent in water (Min. BOD = 29%, Max. BOD = 29%).
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 30 days)
Soil Mobility	Mobility to Groundwater	Low mobility to groundwater based on LogKoc = 5.219
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=7.6
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 2.93
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) >100 mg/L indicates a Low toxicity to Daphnia.
	Fish	A measured LC50 (96-hr) = 75 mg/L indicates a Low toxicity to Fish.
	Algae	A measured EC50 (72-hr) >100 mg/L indicates a Low toxicity to Algae.
SHR	Neurotoxicity	
	Carcinogenicity	Anticipated Carcinogen - there is limited evidence of carcinogenicity in humans or sufficient evidence of carcinogenicity in animals [NTP] [NTPLIST]; Possibly carcinogenic to humans [IARC_OE]; B2 (Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals) [1986 Guidelines] [IRIS]; CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]; [EU_GHS]
	Reproductive Toxicity	Toxic to reproduction - Category 1B/2A [EU_RA17_5]
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	3 out of 6 lists (GADSL; EUC2; SINLIST)
	Regulatory Priority	3 out of 10 lists (EU_CAND; EU_RA14; JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 181.181 km - A_TRNSPRT)



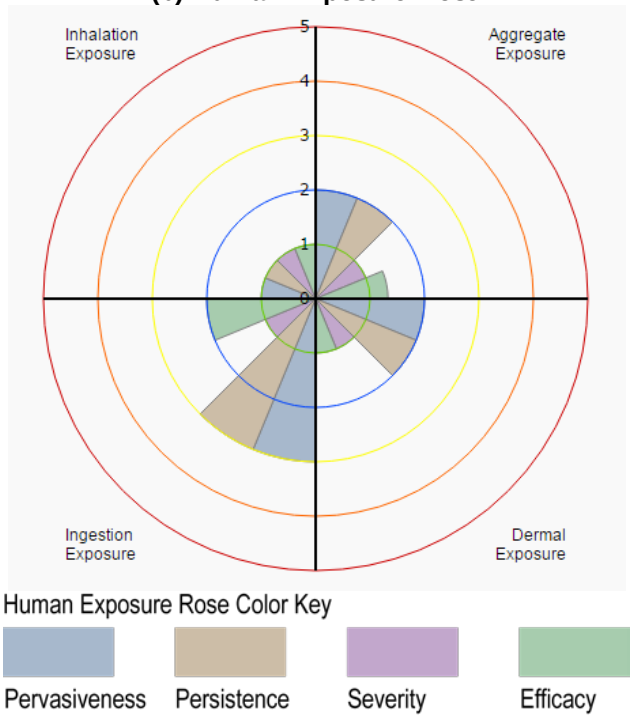
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for DEHP, Di(2-ethylhexyl)phthalate

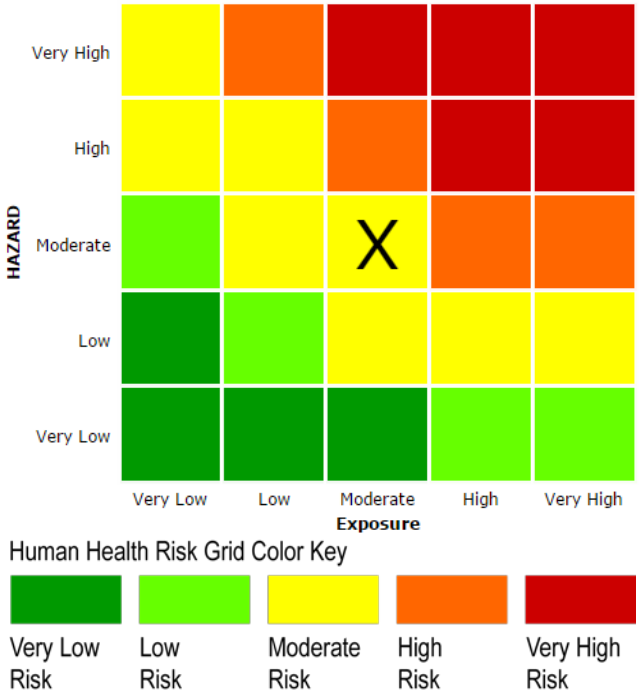
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



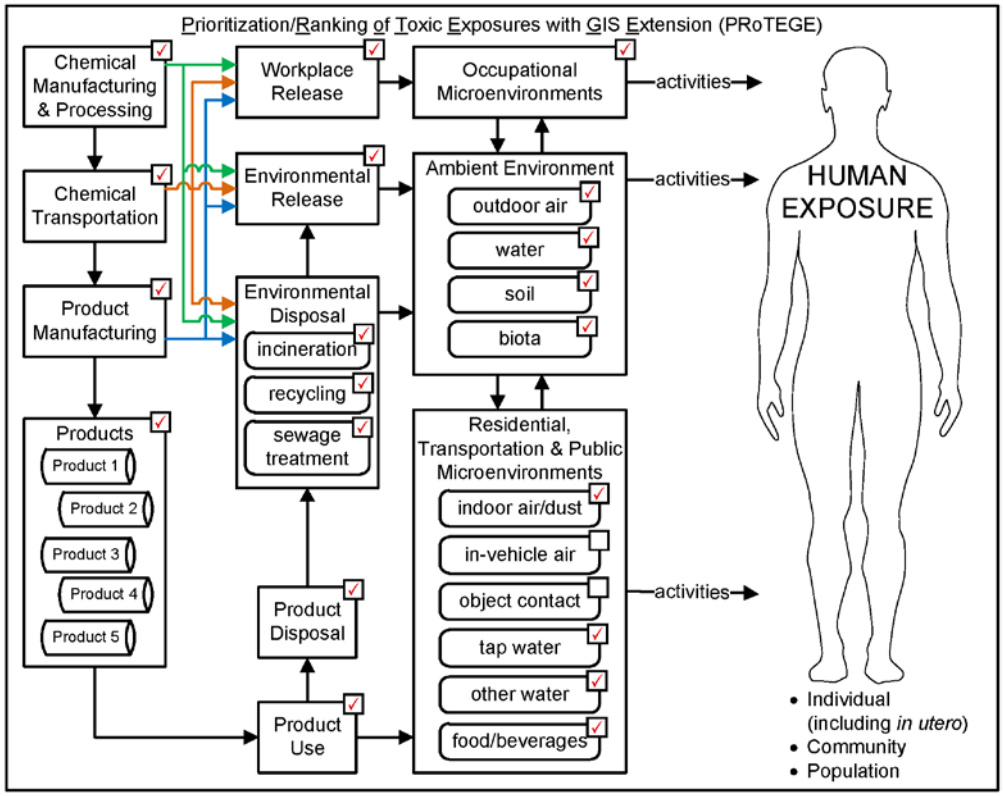
(a) Human Hazard
Estimated ranking of human hazard risk from DEHP, Di(2-ethylhexyl)phthalate, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of DEHP, Di(2-ethylhexyl)phthalate (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from DEHP, Di(2-ethylhexyl)phthalate, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Diethyl Phthalate



Summary Physico-Chemical Information	
Name	Diethyl Phthalate
Other Names	DEP, Diethyl ester of phthalic acid, Ethyl Phthalate
Chemical Formula	$C_6H_4(COOC_2H_5)_2$
Chemical Class	Plzr
Identifier	CAS:84-66-2
Chemical Forms	
Physical Properties	
Molecular Weight: 222.3 BP: 563°F FRZ: -41 °F Sol(86°F): 0.1% VP: 0.002 mmHg Sp. Gr: 1.12 Fl.P: 322°F	
Additional Notes	
Colorless to water-white, oily liquid with a very slight, aromatic odor	

Exposure and Toxicity Information
Toxicity Limits: RfD: NA (IRIS); RfC: NA (IRIS)
Toxicological Effects: Group D not classifiable as to human carcinogenicity; slightly irritating to the eyes and skin
Exposure Limits: NIOSH REL:TWA 5mg/m³; TEEL-0: 5mg/m³
Chemical Use: Pesticide
Exposure Routes: Inhalation, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, respiratory system, central nervous system, peripheral nervous system, reproductive system

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)		0.40-0.52		Data source: Outdoor (medium, high), Ground water (medium), Tap Water – [40]; Indoor air - [36]; Food - [40] (5, 50, 95%tile)	Air		
Ground water (ppb)		4.1					
Food (µg/kg)	1.18	12.0	25.2		Surface Water		
Indoor Air (µg/m³)	0.330	0.795	1.929		Ground Water		
Surface water					Soil		
Tap water (ng/L)	0.019	0.10	0.52				
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

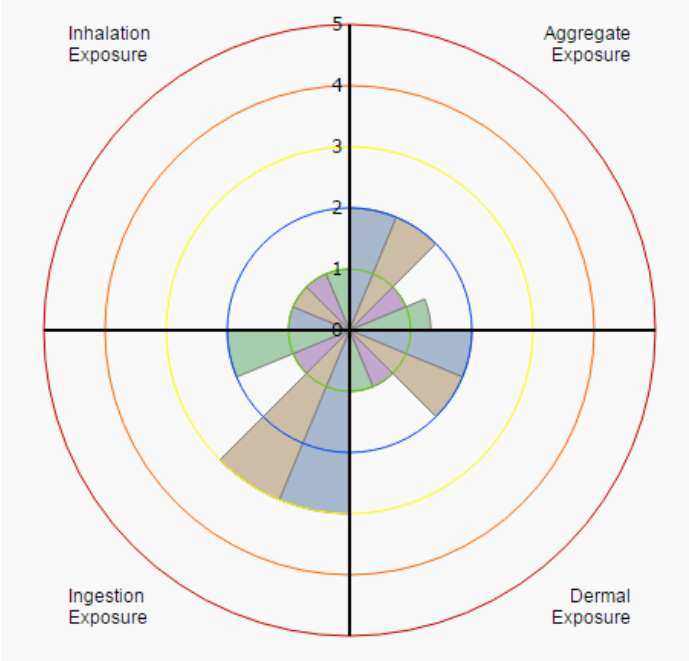
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		●
	Tox Cast	Ph I	
		Ph II	●
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		□
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [41]
	BME		
	ERDEM		

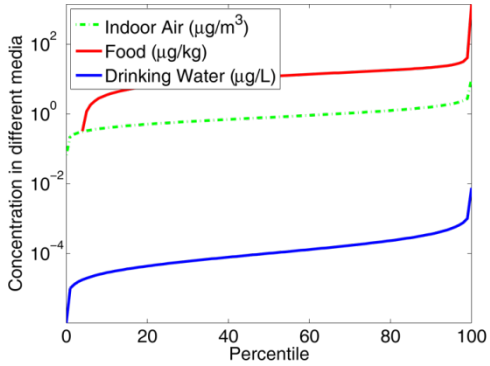
"Tier 1" Exposure Ranking for Diethyl Phthalate

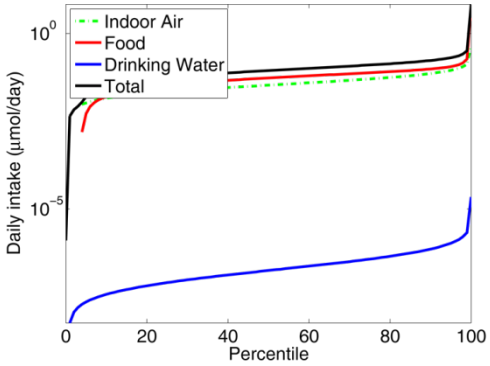
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	3	3	1	2
Dermal	2	2	1	1
Aggregate	2	2	1	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Diethyl Phthalate





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.0335	0.054	NA	0.0875
90 % tile	0.0722	0.097	NA	0.171
% over 0.1 μmol/day	3.31	8.77	NA	40.9
% over 1 μmol/day	0	0.867	NA	1.78

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

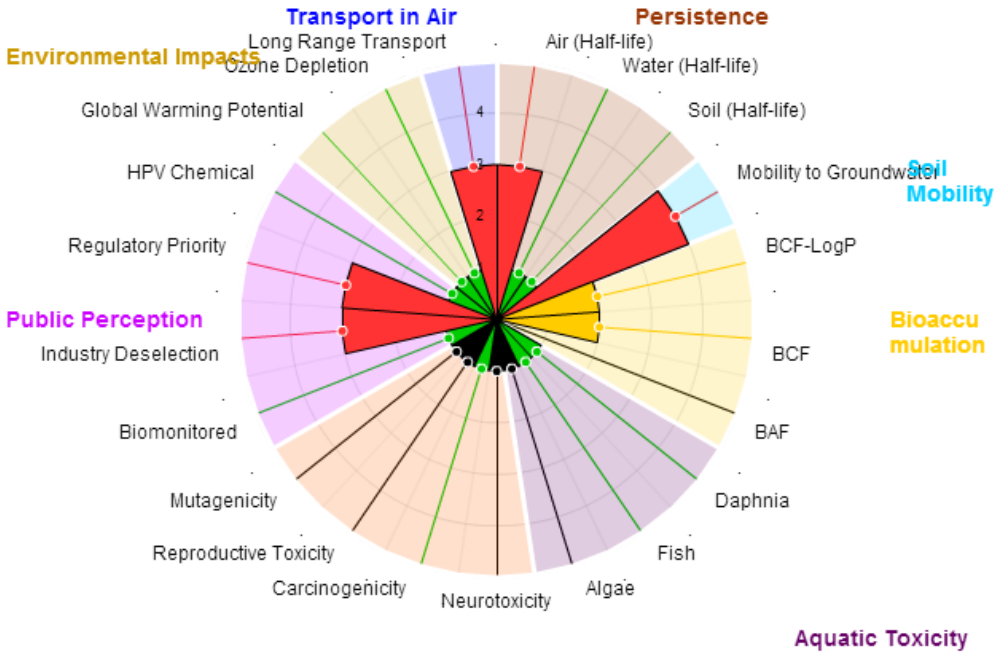
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Diethyl Phthalate

		CAS # 84-66-2
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 3.086 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 88% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is not persistent in water (Min. BOD = 86%, Max. BOD = 89%).
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 30 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 2.101
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=2.42
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 2.07
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 45.220 mg/L indicates a Low toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 15.103 mg/L indicates a Low toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	
	Carcinogenicity	CLASS A4 - Not Classifiable as a Human Carcinogen [ACGIH]; D (Not classifiable as to human carcinogenicity) [1986 Guidelines] [IRIS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (SINLIST)
	Regulatory Priority	1 out of 10 lists (EU_RRAP)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 599.789 km - A_TRNSPRT)



SHR

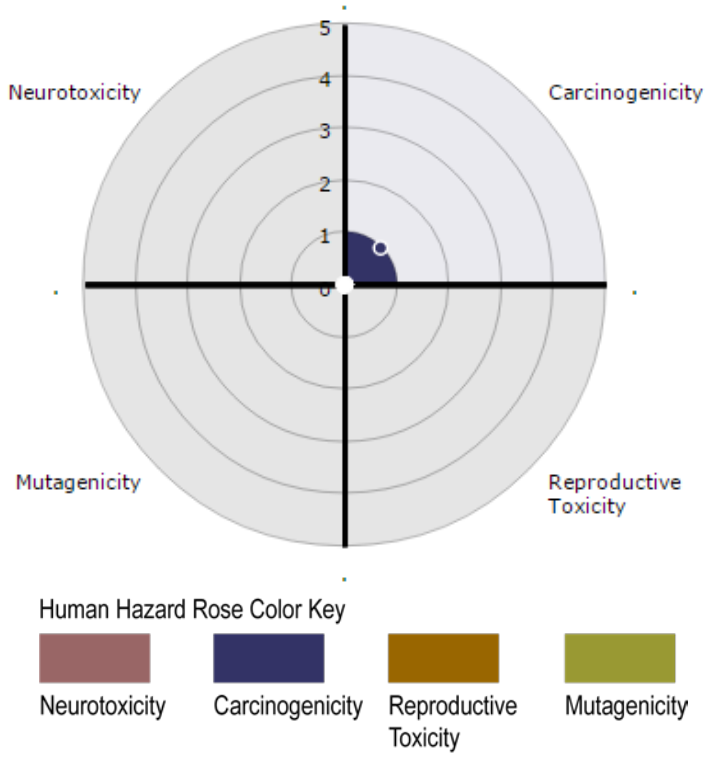
Key

- Potential for High level of concern (**3-4**)
- Potential for Moderate level of concern (**2**)
- Potential for Low level of concern (**1**)

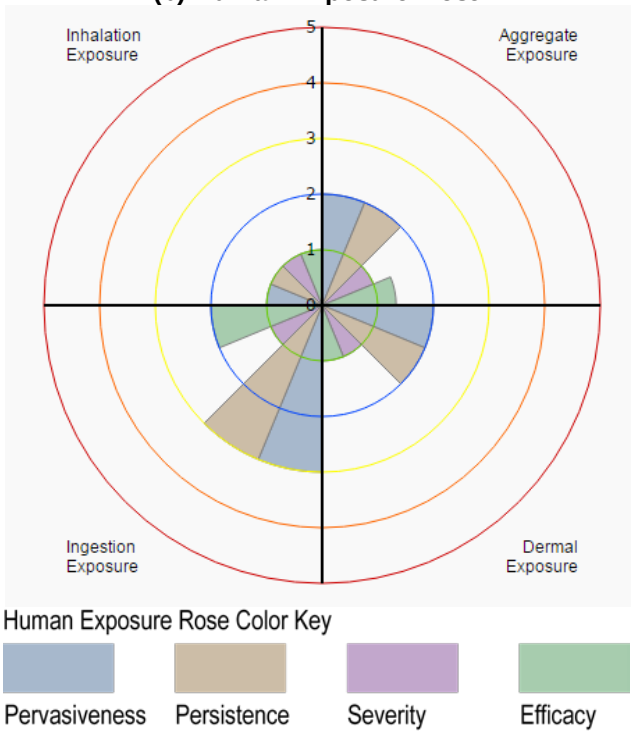
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Diethyl Phthalate

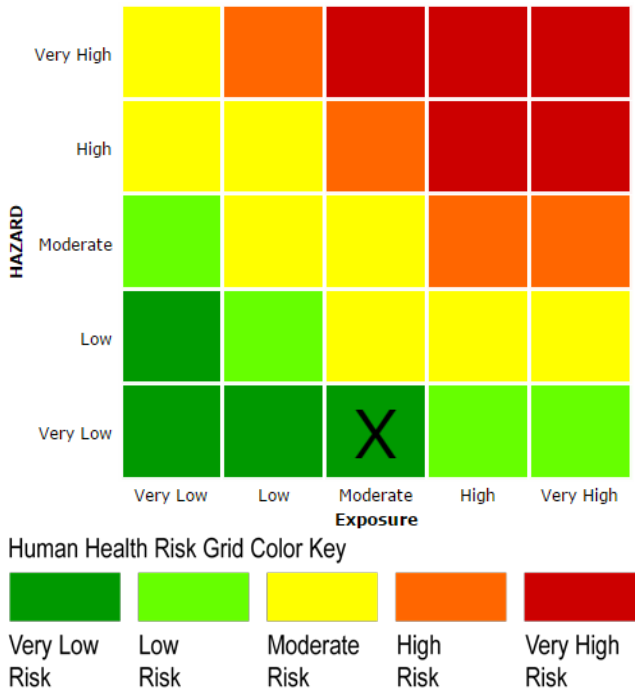
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



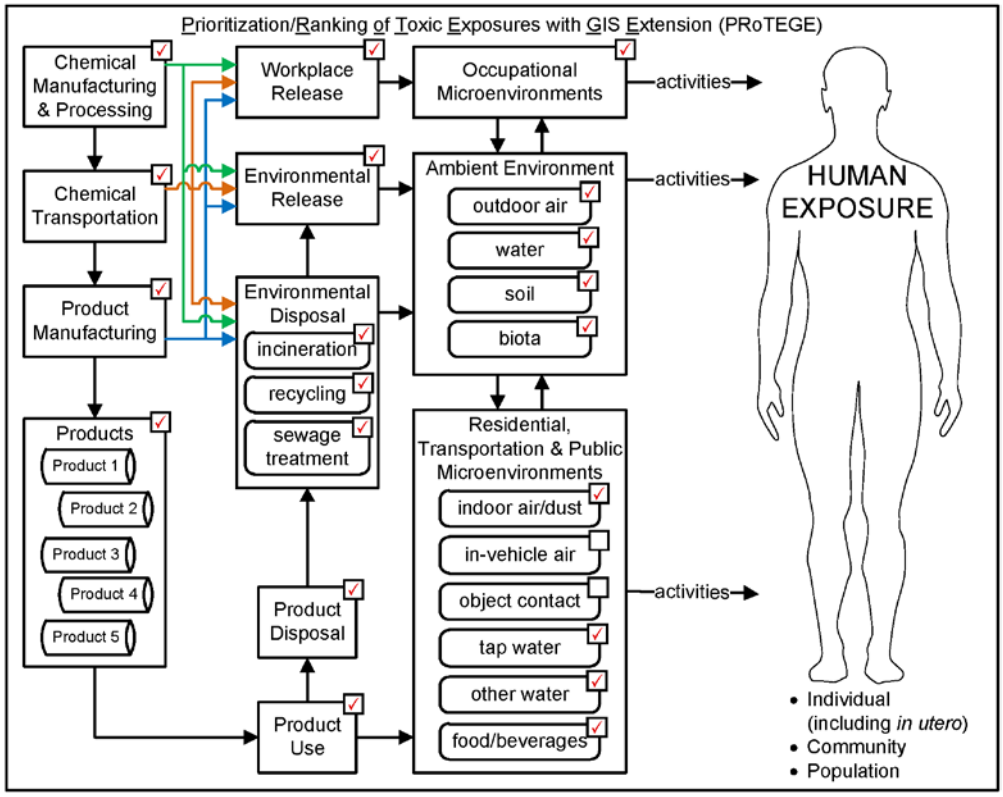
(a) Human Hazard
Estimated ranking of human hazard risk from Diethyl Phthalate, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Diethyl Phthalate (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Diethyl Phthalate, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Di-n-butylphthalate



Summary Physico-Chemical Information	
Name	Di-n-butylphthalate
Other Names	DBP; Dibutyl-1,2-benzene-dicarboxylate
Chemical Formula	$C_6H_4(COOC_4H_9)_2$
Chemical Class	Plzr
Identifier	CAS: 84-74-2
Chemical Forms	
Physical Properties	
MW: 278.34 BP: 340°C FRZ: -35°C Sol: 0.001% VP: 0.00007 mmHg Sp.Gr: 1.05 Fl.P(oc): 159°C	
Additional Notes	
Colorless to faint-yellow, oily liquid with a slight, aromatic odor academic	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.1 mg/kg/day; ; RfC: NA (IRIS)
Toxicological Effects: Group D not classifiable as to human carcinogenicity
Exposure Limits: NIOSH REL: TWA 5 mg/m^3; OSHA PEL: TWA 5 mg/m^3; TEEL-0: 5 mg/m^3
Chemical Use: Plasticizer
Exposure Routes: Inhalation, ingestion, skin and/or eye contact
Target Organs: Eyes, respiratory system, gastrointestinal tract

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m^3)	1.68*10^{-7}	1.25*10^{-5}	0.0052	Data source: Outdoor air (5th, 50th, 95th %ile) – NATA county-level annual average; Food – [40] (5, 50, 95%tiles); Indoor air - [36]; Tap water - [40]	Air	2453.93 (NEI 2005) 16.65 (TRI 2008)	97.43% (NEI 2005) 1.36% (TRI 2008)
Ground water							
Food (µg/kg)	13.9	69	464		Surface Water	0.29 (TRI 2008)	0.09%
Indoor Air (µg/m^3)	0.124	0.250	0.500		Ground Water	78.67 (TRI 2008)	0.03%
Surface water					Soil	7.89 (TRI 2008)	0.06%
Tap water (ng/L)	0.021	0.10	0.466				
Soil					Chemical Production and Use		
Dust					Production	26,000 tons/yr	Data Source: EU (1998)
Surfaces							
Biota							
Human Biomarkers							
Urine (µg/L)							
Blood							
Other							

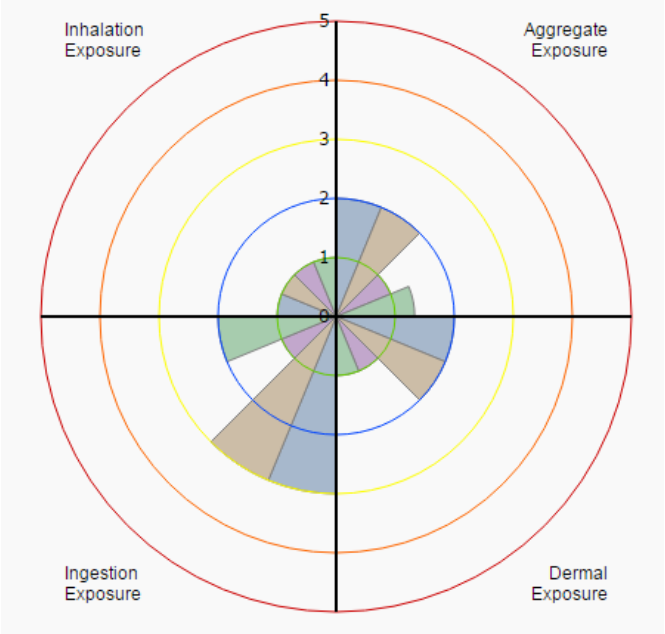
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		
	PSAP		●
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		●
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		●
	IUR		
	ECD		●
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		
	AQS		○
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PKd (H) [42]
	BME		●[43]
	ERDEM		●

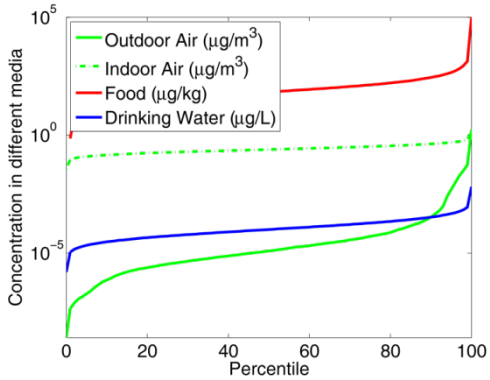
"Tier 1" Exposure Ranking for Di-n-butylphthalate

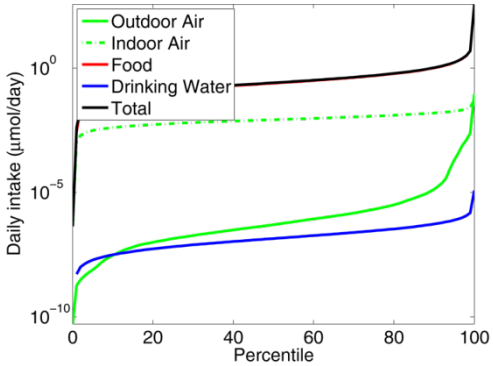
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	3	3	1	2
Dermal	2	2	1	1
Aggregate	2	2	1	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Di-n-butylphthalate





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.00849	0.248	NA	0.257
90 % tile	0.016	1.02	NA	1.07
% over 0.1 μmol/day	0.1	84.1	NA	85.1
% over 1 μmol/day	0	10.3	NA	11

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

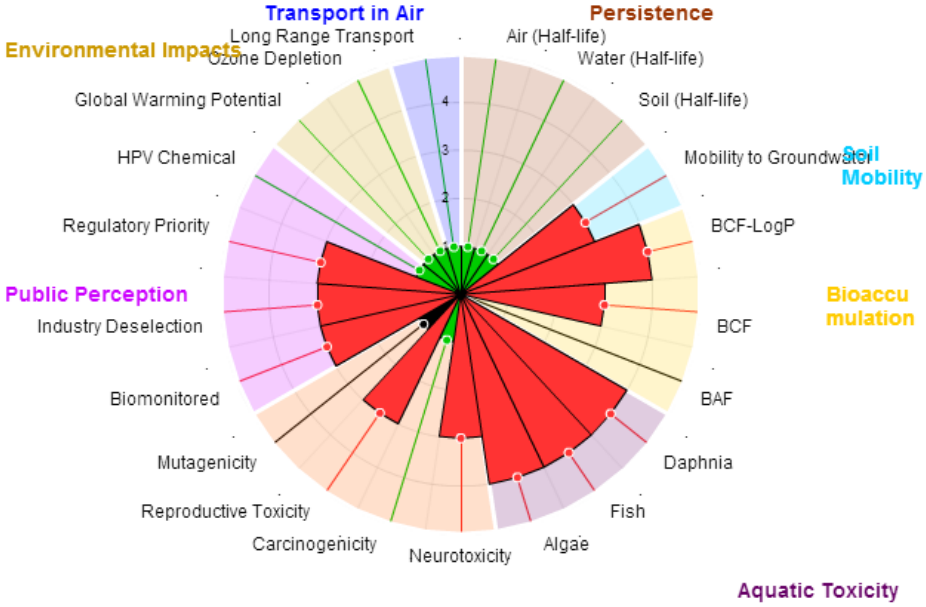
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Di-n-butylphthalate

		CAS # 84-74-2
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 1.153 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 69% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is not persistent in water (Min. BOD = 69%, Max. BOD = 69%).
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 17.34 days)
Soil Mobility	Mobility to Groundwater	High mobility to groundwater based on LogKoc = 3.164
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=4.5
	BCF	High bioconcentration potential based on Experimental LogBCF = 3.33
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) = 4.8 mg/L indicates a Moderate toxicity to Daphnia. However, this compound is classified as R50 (Very toxic to aquatic organisms.).
	Fish	A measured LC50 (96-hr) = 2.8 mg/L indicates a Moderate toxicity to Fish. However, this compound is classified as R50 (Very toxic to aquatic organisms.).
	Algae	A measured EC50 (72-hr) = 2.7 mg/L indicates a Moderate toxicity to Algae. However, this compound is classified as R50 (Very toxic to aquatic organisms.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	D (Not classifiable as to human carcinogenicity) [1986 Guidelines] [IRIS]; [ACGIH]; [EU_GHS]
	Reproductive Toxicity	Toxic to reproduction - Category 1B/2A [EU_RA17_5]; TOXIC TO REPRODUCTION - Hazard category 1B [EU_GHS]
	Mutagenicity	
Public Perception	Biomonitored	1 out of 2 lists (NHANES)
	Industry Deselection	3 out of 6 lists (GADSL; EUC2; SINLIST)
	Regulatory Priority	3 out of 10 lists (EU_CAND; EU_RA14; JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 387.901 km - A_TRNSPRT)



SHR

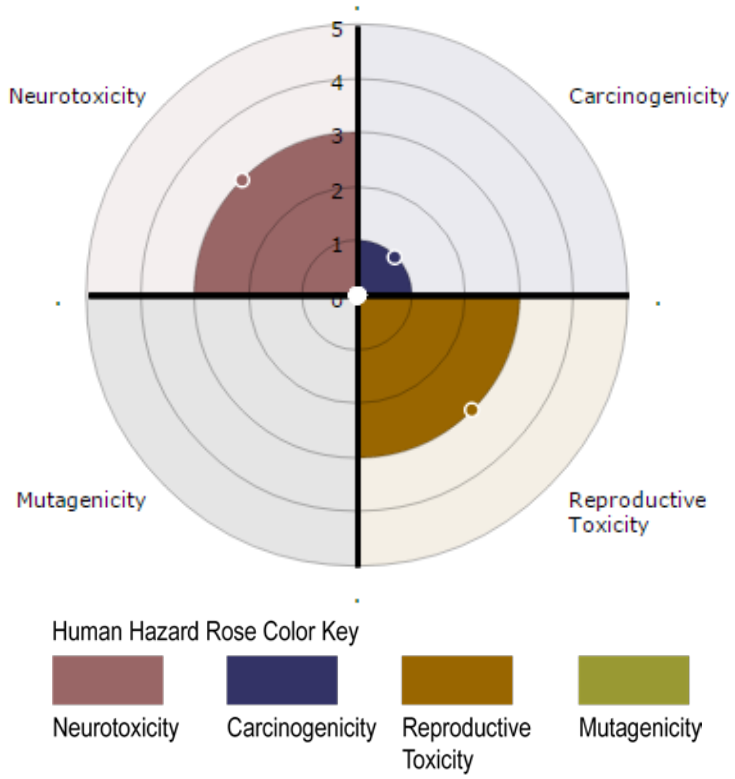
Key

- → Potential for High level of concern (**3-4**)
- → Potential for Moderate level of concern (**2**)
- → Potential for Low level of concern (**1**)

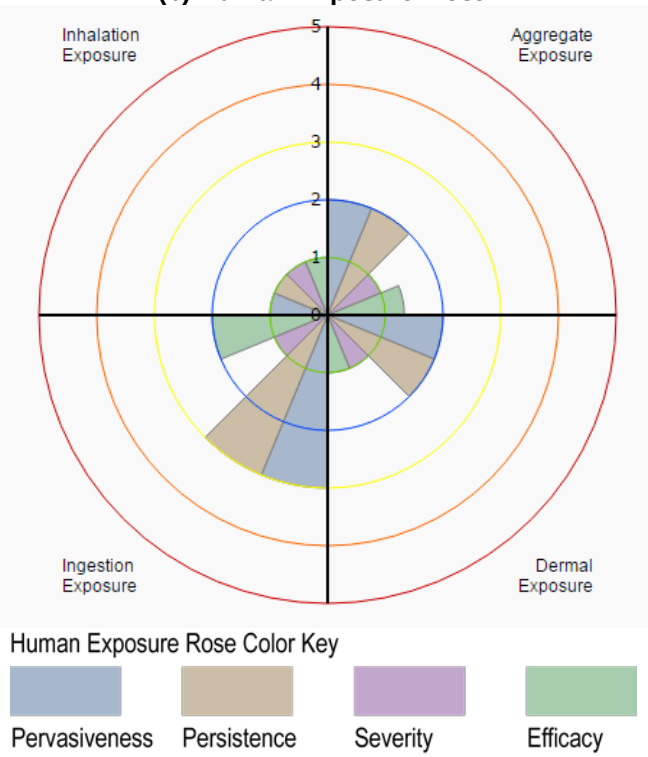
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Di-n-butylphthalate

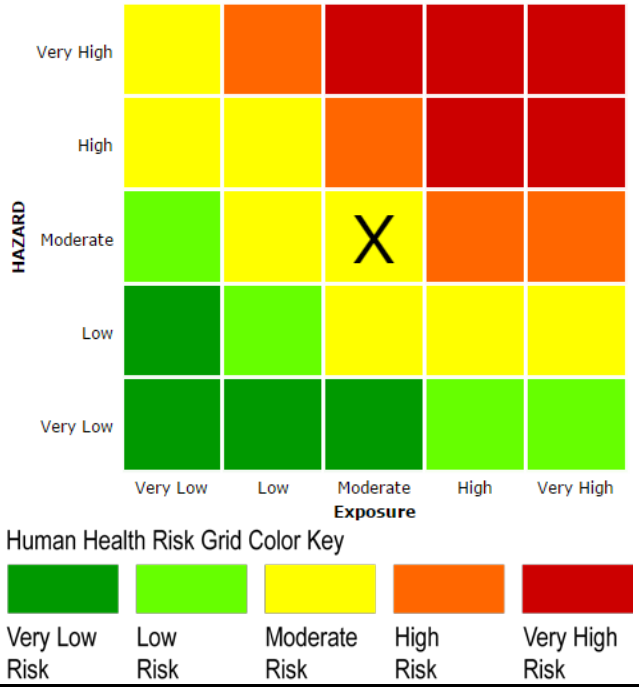
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



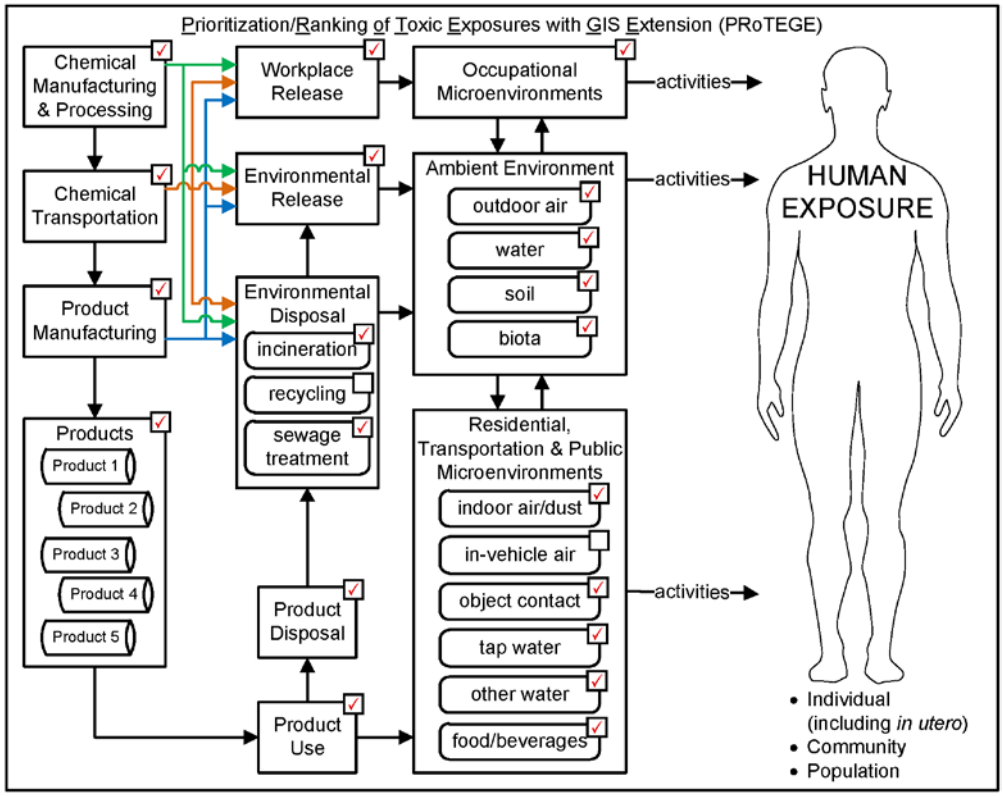
(a) Human Hazard
Estimated ranking of human hazard risk from Di-n-butylphthalate, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Di-n-butylphthalate (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Di-n-butylphthalate, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Ethane 1,1,2,2-tetrachloro-



Summary Physico-Chemical Information	
Name	Ethane, 1,1,2,2-tetrachloro-
Other Names	Acetylene tetrachloride, symmetrical tetrachloroethane
Chemical Formula	$CHCl_2CHCl_2$
Chemical Class	VOC
Identifier	CAS:79-34-5
Chemical Forms	
Physical Properties	
MW: 167.9 BP: 296°F MLT: -33°F Sol: 0.3% VP: 5 mmHg Sp. Gr: 1.59	
Additional Notes	
Colorless liquid with a mild, chloroform-like odor	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.02 mg/kg/day (IRIS) RfC: NA (IRIS)
Toxicological Effects: Carcinogenic classification: L (IRIS)
Exposure Limits: NIOSH REL: Ca TWA 1 ppm (7 mg/m³) [skin] OSHA PEL†: TWA 5 ppm (35 mg/m³) [skin]
Chemical Use: as intermediate in the synthesis of other chlorinated hydrocarbons
Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, respiratory system, liver, kidneys, central nervous system

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	0.002606	0.002875	0.004275	Data source: Outdoor air (5th, 50th, and 95th %iles – '08 annual means @ AQS; Food – not detected in TDS; Surface water – HSDB; Indoor air – [44]; Tap water - [23]	Air	Air	290.59 (NEI2005); 1.67 (TRI 2008)
Ground water							
Food (µg/g)	<LOD				Surface Water	Surface Water	0.14 (TRI 2008)
Indoor Air (ng/m³)	16	70	298		Ground Water		
Surface water (µg/L)		1	3		Soil		
Tap water (µg/L)	<RL		0.037 (99% tile)				
Soil					Chemical Production and Use		
Dust					Production	<10 million lbs/yr	Data Source: IUR
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

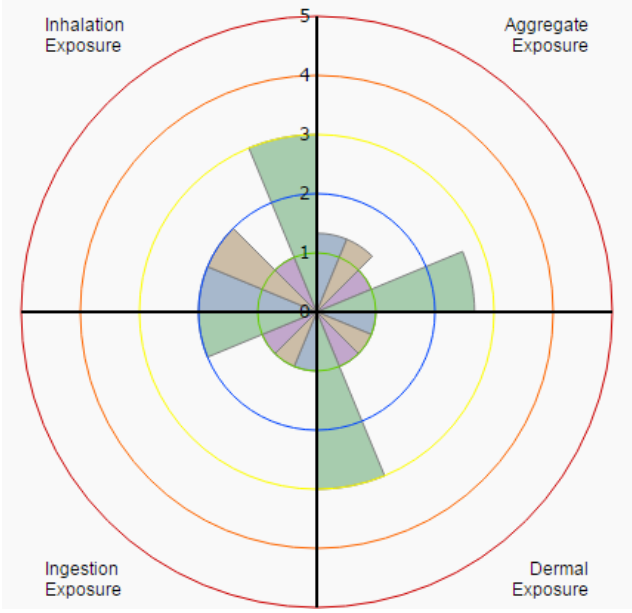
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		
	IARC		●
	PSAP		●
	NTP		●
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		●
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		●
	ECD		●
	SRD		
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PKd (R) [45]
	BME		● [46]
	ERDEM		

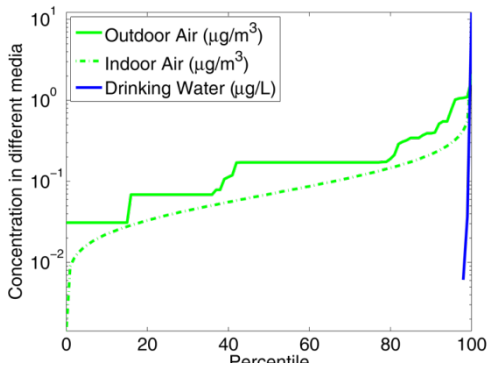
"Tier 1" Exposure Ranking for Ethane 1,1,2,2-tetrachloro-

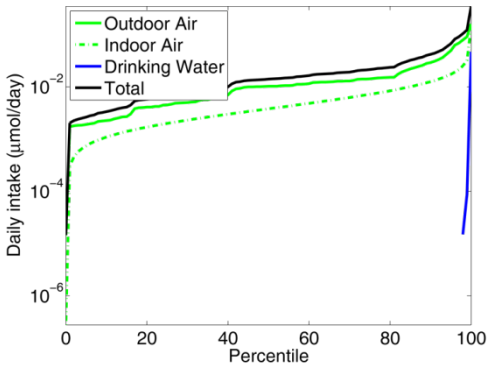
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	2	2	1	3
Ingestion	1	1	1	2
Dermal	1	1	1	3
Aggregate	1.33	1.3	1	2.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Ethane 1,1,2,2-tetrachloro-





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.0148	0	NA	0.0148
90 % tile	0.0383	0	NA	0.0393
% over 0.1 μmol/day	0.984	0	NA	1.9
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

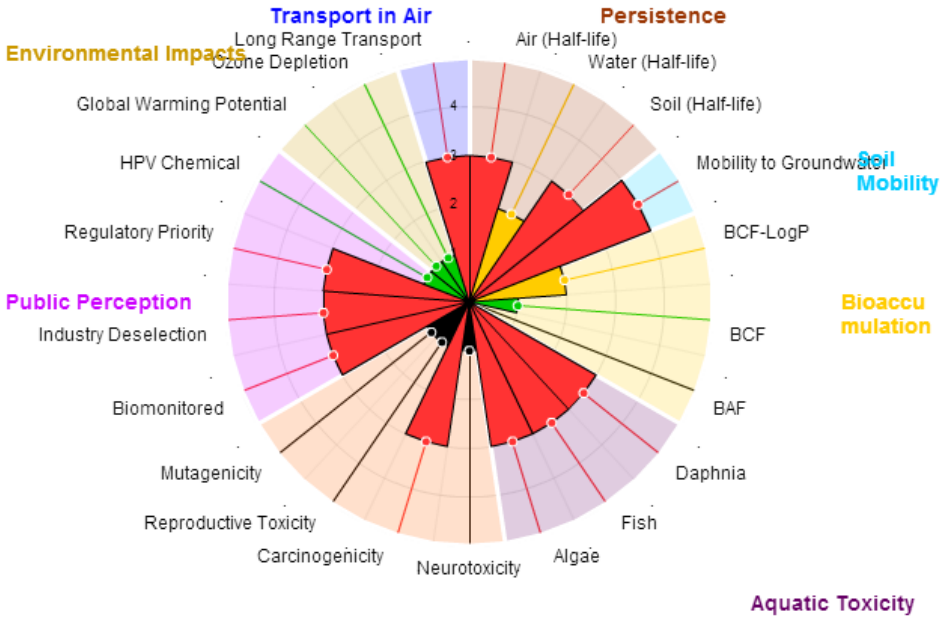
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Ethane 1,1,2,2-tetrachloro-

		CAS # 79-34-5
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 53.03 days)
	Water (Half-life)	Moderate persistence in Water (Estimated Half-life = 60 days)
	Soil (Half-life)	High persistence in Soil (Estimated Half-life = 120 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 2.029
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=2.39
	BCF	Low bioconcentration potential based on Experimental LogBCF = 0.91
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 89.541 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 82.475 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	Possibly carcinogenic to humans [IARC_OE]; Likely to be carcinogenic to humans [2005 Guidelines] [IRIS]; CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	1 out of 2 lists (NHANES IV)
	Industry Deselection	1 out of 6 lists (GADSL)
	Regulatory Priority	1 out of 10 lists (JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 1356.79 km - A_TRNSPRT)



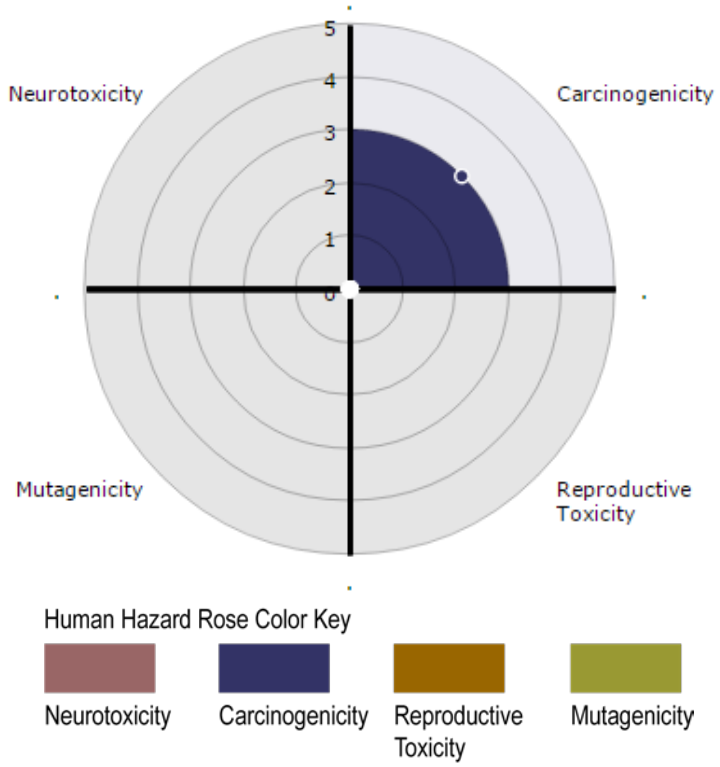
Key

- Potential for High level of concern (**3-4**)
- Potential for Moderate level of concern (**2**)
- Potential for Low level of concern (**1**)

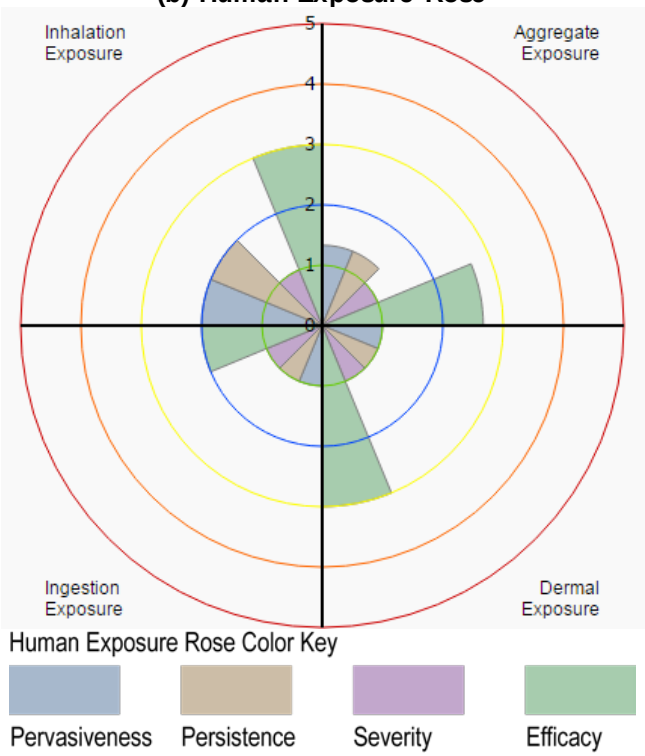
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Ethane 1,1,2,2-tetrachloro-

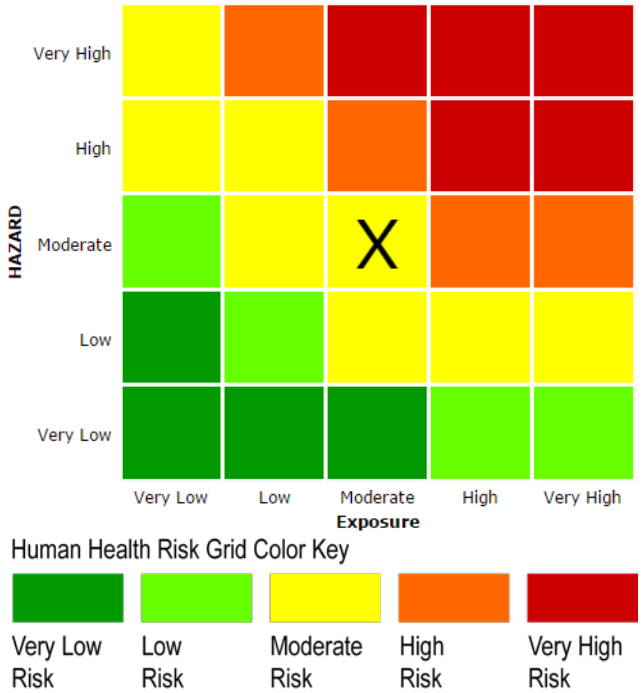
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



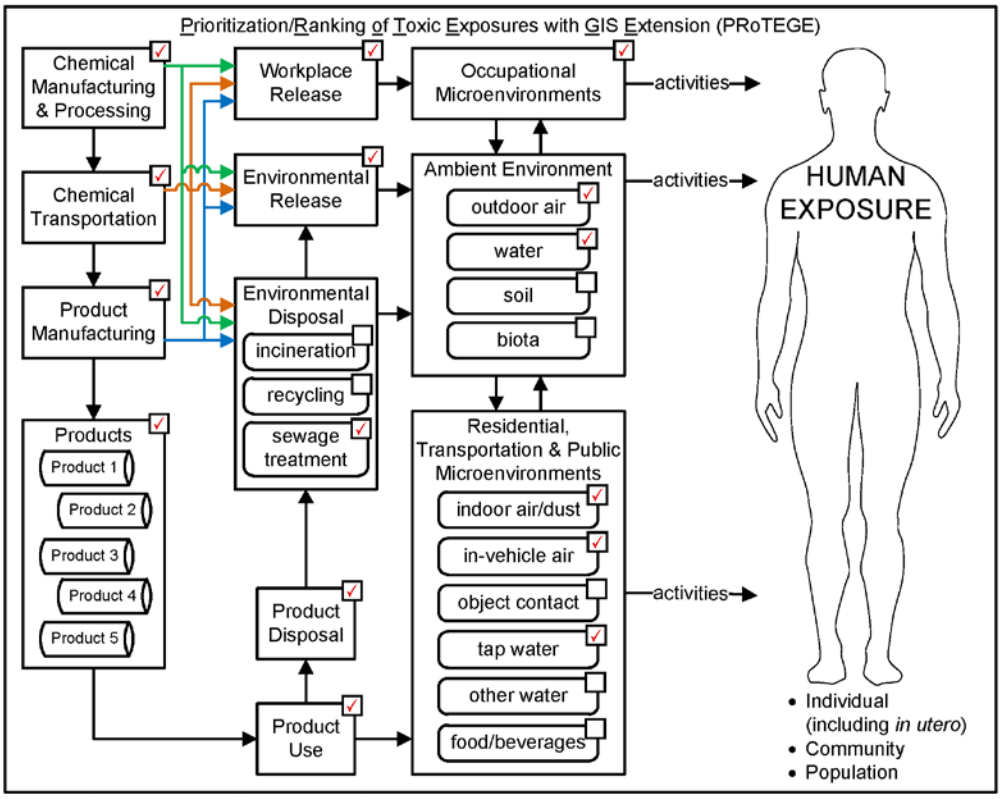
(a) Human Hazard
Estimated ranking of human hazard risk from Ethane 1,1,2,2-tetrachloro-, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Ethane 1,1,2,2-tetrachloro- (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Ethane 1,1,2,2-tetrachloro-, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Perchlorethylene



Summary Physico-Chemical Information	
Name	Ethene, 1,1,2,2-tetrachloro
Other Names	Perchloroethylene, Perc
Chemical Formula	C2Cl4 / Cl2C=CCl2
Chemical Class	VOC
Identifier	CAS: 127-18-4; NIOSH/RTECS: KX3850000; ICSC: 0076; UN: 1897; EC: 602-028-00-4
Chemical Forms	
Physical Properties	
Molecular weight: 165.8 Boiling point: 121 °C Melting point: -22 °C Solubility in water: 0.15 g/L at 20 °C Relative density (water): 1.6 Vapor pressure (kPa at 20 °C): 1.9 Relative vapor density (air): 5.8 Octanol/water partition coefficient as log Pow: 2.9	
Additional Notes	
Colorless liquid with a mild, chloroform-like odor. Noncombustible Liquid, but decomposes in a fire to hydrogen chloride and phosgene.	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.01 mg/kg/day (IRIS); RfC: NA (IRIS); LD50 (oral-rat): 8850 mg/kg; LD50 (ipr-mouse): 4700 mg/kg
Toxicological Effects: Carcinogenic Classification – NA (IRIS), 3B (DFG 2004), A3 (confirmed animal carcinogen with unknown relevance to humans)
Exposure Limits: NIOSH REL Ca. Minimize workplace exposure concentrations; OSHA PEL: TWA 100 ppm; C 200 ppm (for 5 minutes in any 3-hour period), with a maximum peak of 300 ppm. TLV: 25 ppm as TWA, 100 ppm as STEL
Chemical Use: Dry cleaning agent, degreasing agent and as a chemical intermediate in the production of fluorocarbons
Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, respiratory system, liver, kidneys, central nervous system

Environmental Concentrations				
	Low	Medium	High	Notes
Outdoor air (ppb)	0.008	0.025	0.116	Data sources: Outdoor air (5th, 50th, and 95th %iles) - '08 annual means @ AQS monitors; corresponding 2002 NATA county-level annual averages - 0.003, 0.006 and 0.028. Indoor air – 57% > LOD (5th, 50th, and 95th %iles) - NHEXAS (non-smoking residences). Ground water, food and tap water - HSDB. Soil - STORET.
Ground water (ppb)	0.07	0.60	130.00	
Food (µg/kg)	0.60	9.70	13.00	
Indoor Air (ppb)	0.05	0.28	1.46	
Surfaces				
Tap water (ppb)	0.30	3.00	21.00	
Soil (µg/kg)	0.20	1.00	19,000.00	
Dust				
Biota				
Outdoor air (ppb)	0.008	0.025	0.116	
Human Biomarkers				
Urine (µg/L)	0.049	0.0835	0.18	Blood: 16.6% > LD (NHANES '03-'04)
Blood				
Other				

Environmental Releases		
	Emissions Tons/yr	% Counties Reporting Emissions
Air	31752 (NEI 2005); 985 (TRI 2008)	99.94 (NEI 2005); 4.81% (TRI 2008)
Surface Water	0.35 (TRI 2008)	0.65 %
Ground Water	22.93 (TRI 2008)	0.19 %
Soil	27.13 (TRI 2008)	0.22 %
Chemical Production and Use		
Production	500 million to 1 billion lbs/yr	Data Source: IUR

Historical measured outdoor concentrations: 0.2 to 9.75 ppb [from HSDB]; Soil concentrations data from STORET are used without filtering unusually large values found at waste disposal sites; Exposures to perc for general populations from ingestion (food, drinking water, and non-dietary ingestion) are assumed to be negligible in this analysis.

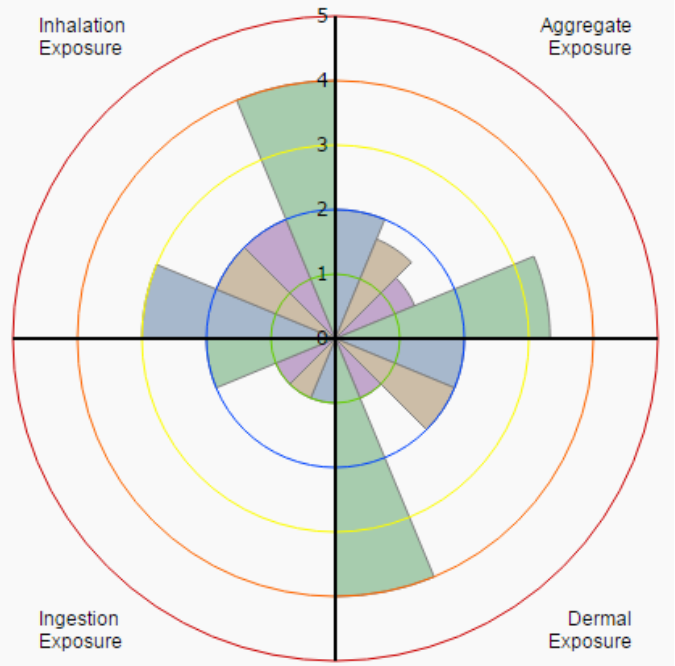
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		
	PSAP		●
	NTP		●
	REACH		●
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		●
	ECD		○
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	b
		05-06	(b)
		07-08	(b)
		09-10	(b)
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		RM[47]
	BME		● [46]
	ERDEM		

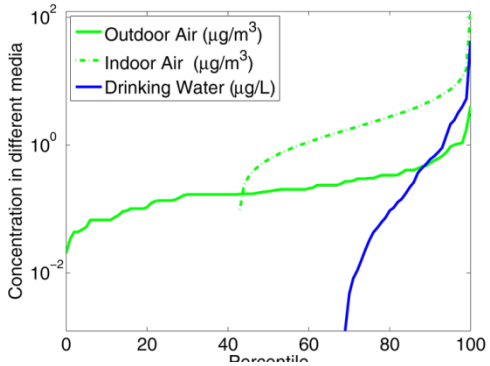
"Tier 1" Exposure Ranking for Perchlorethylene

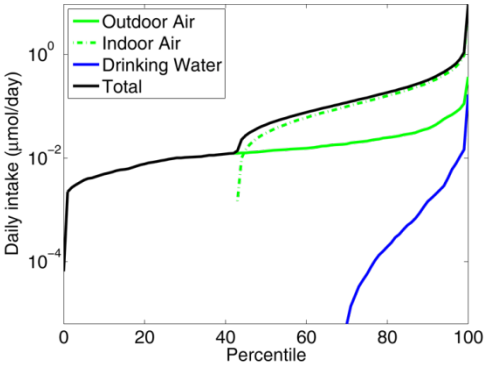
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	3	2	2	4
Ingestion	1	1	1	2
Dermal	2	2	1	4
Aggregate	2.00	1.66	1.33	3.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Perchlorethylene





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.0546	0	NA	0.0546
90 % tile	0.305	0.00146	NA	0.315
% over 0.1 μmol/day	34.8	0.449	NA	35
% over 1 μmol/day	0.985	0	NA	1.92

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

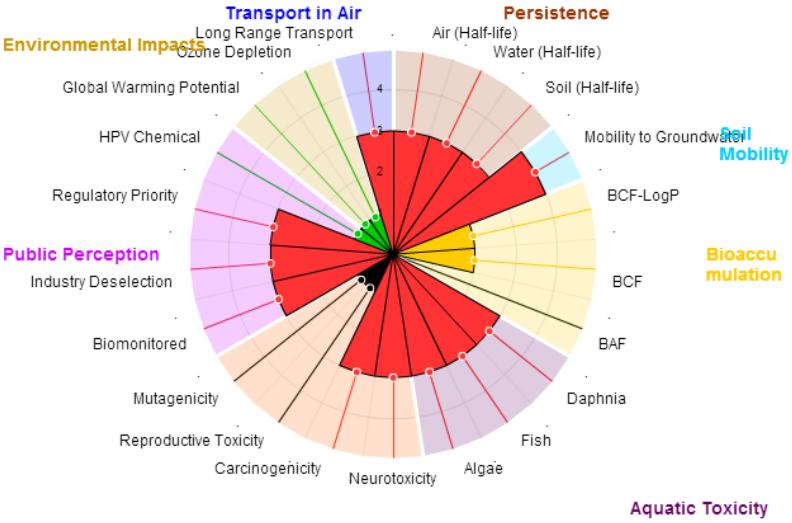
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Perchlorethylene

		CAS # 127-18-4
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 50 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 11% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is persistent in water (Min. BOD = 11%, Max. BOD = 11%).
	Soil (Half-life)	High persistence in Soil (Estimated Half-life = 120 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 2.029
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=3.4
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 1.69
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) = 1.3 mg/L indicates a Moderate toxicity to Daphnia. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	A measured LC50 (96-hr) = 14 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	A measured EC50 (72-hr) = 27 mg/L indicates a Low toxicity to Algae. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	Anticipated Carcinogen - there is limited evidence of carcinogenicity in humans or sufficient evidence of carcinogenicity in animals [NTP] [NTPLIST]; Probably carcinogenic to humans [IARC_OE]; Carc. 2: [EU_GHS]; Likely to be carcinogenic to humans [2005 Guidelines] [IRIS]; CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	1 out of 2 lists (NHANES IV)
	Industry Deselection	3 out of 6 lists (GADSL; EUC2; SINLIST)
	Regulatory Priority	2 out of 10 lists (EU_RRAP; JCL2_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP = 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 1371.34 km - A_TRNSPRT)



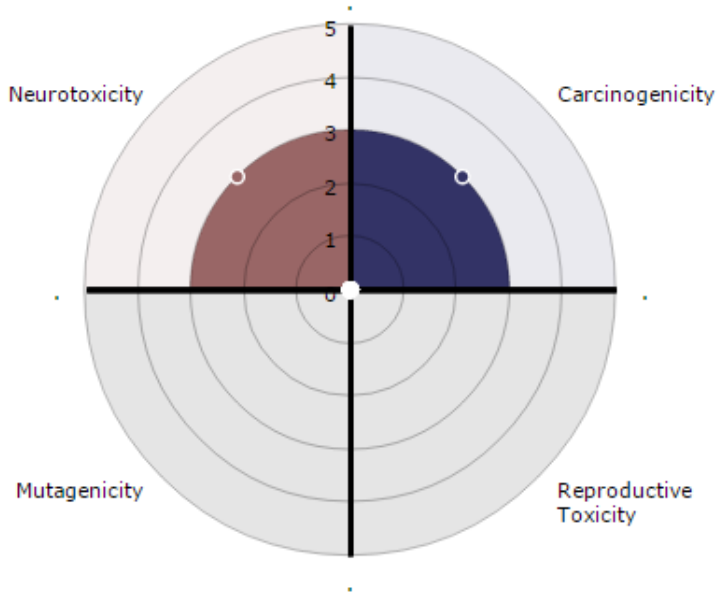
Key

- → Potential for High level of concern (**3-4**)
- → Potential for Moderate level of concern (**2**)
- → Potential for Low level of concern (**1**)

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Perchlorethylene

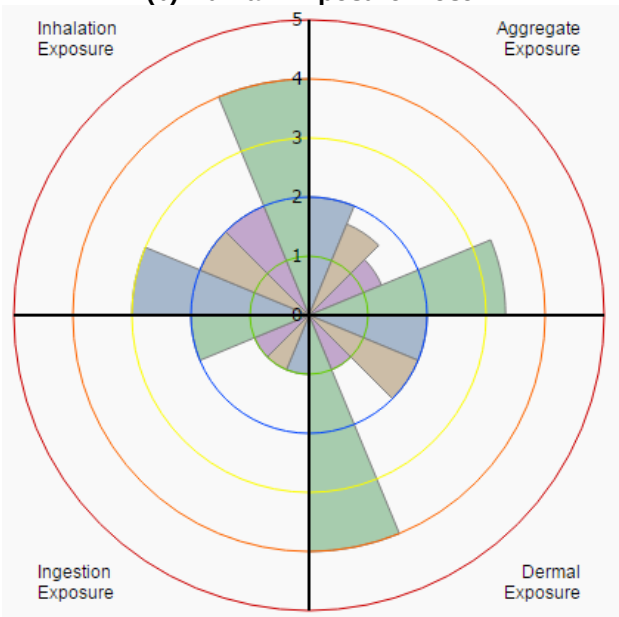
(a) Human Hazard Rose



Human Hazard Rose Color Key

Neurotoxicity | Carcinogenicity | Reproductive Toxicity | Mutagenicity

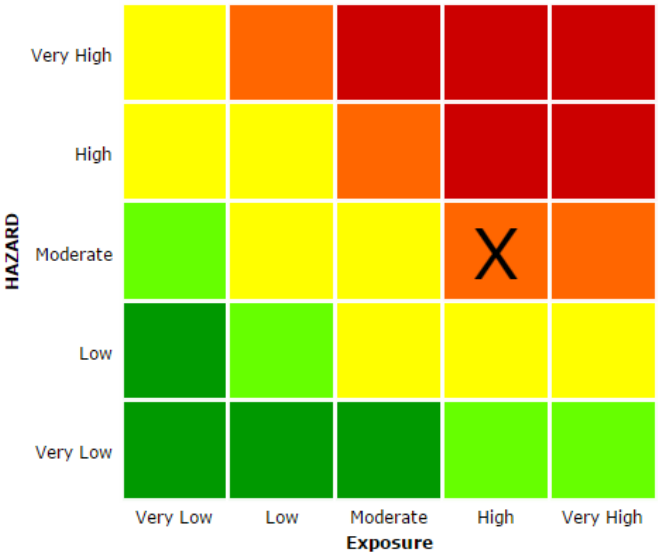
(b) Human Exposure Rose



Human Exposure Rose Color Key

Pervasiveness | Persistence | Severity | Efficacy

(c) Human Health Risk Grid



Human Health Risk Grid Color Key

Very Low Risk | Low Risk | Moderate Risk | High Risk | Very High Risk

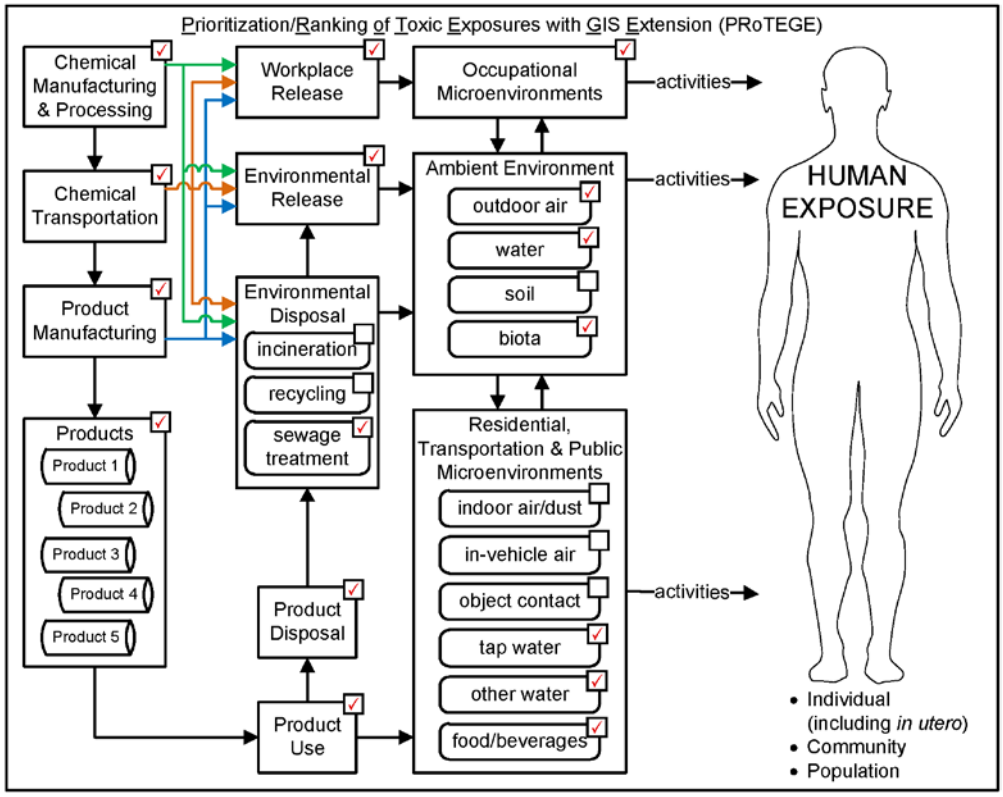
(a) Human Hazard
Estimated ranking of human hazard risk from Perchlorethylene, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Perchlorethylene (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Perchlorethylene, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Ethylene Thiourea



Summary Physico-Chemical Information	
Name	Ethylene Thiourea
Other Names	1,3-Ethylene-2-thiourea; N,N-Ethylenethiourea; ETU; 2-Imidazolidine-2-thione
Chemical Formula	$C_3H_6N_2S$
Chemical Class	Fung
Identifier	CAS:96-45-7
Chemical Forms	
Physical Properties	
Molecular Weight: 102.2 BP: 446-595°F MLT: 392°F Sol(86°F): 2% VP: 16 mmHg IP: 8.15 eV Fl.P: 486°F	
Additional Notes	
White to pale-green, crystalline solid with a faint, amine odor	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.00008mg/kg-day (IRIS)
Toxicological Effects: No classifiable as to human carcinogenicity (IARC); reasonably anticipated to be a human carcinogen (NTP)
Exposure Limits: TEEL -0: 0.75 mg/m³
Chemical Use: Fungicide
Exposure Routes: Inhalation, ingestion, skin and/ or eye contact
Target Organs: Eyes, skin, thyroid, reproductive system

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	0	0	1.37*10-6	Data Source: Outdoor air (5th, 50th, 95th %ile) – NATA 2002 county-level annual average, Food (5th, 50th, 95th %iles)-TDS '94 –'02	Air		
Ground water							
Food (µg/g)	0.003	0.008	0.0216		Surface Water		
Indoor Air					Ground Water		
Surface water					Soil		
Tap water							
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

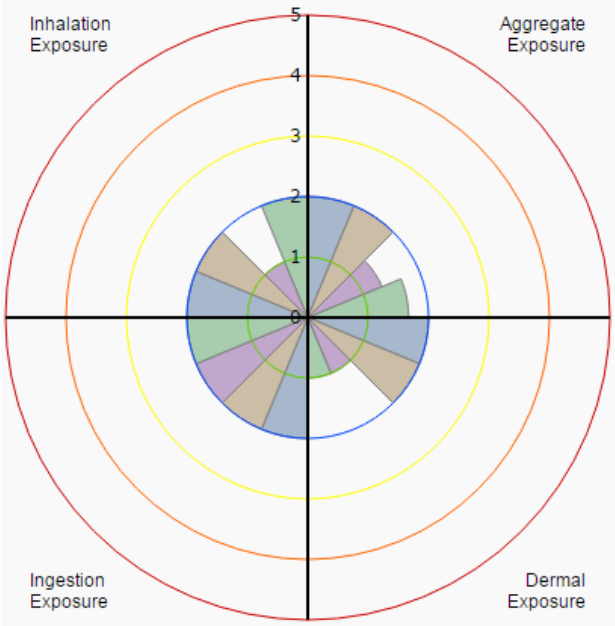
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		●
	Tox Cast	Ph I	
		Ph II	●
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		○
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		○
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [41]
	BME		
	ERDEM		

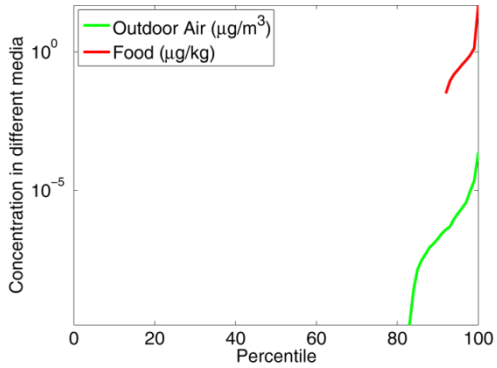
"Tier 1" Exposure Ranking for Ethylene Thiourea

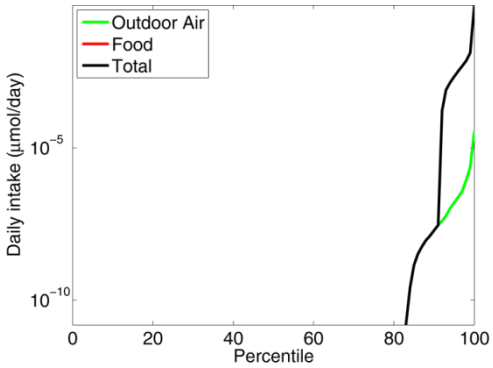
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	2	2	1	2
Ingestion	2	2	2	2
Dermal	2	2	1	1
Aggregate	2	2	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Ethylene Thiourea





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	2.04E-08	0	NA	2.42E-08
% over 0.1 µmol/day	0	0.814	NA	1.61
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

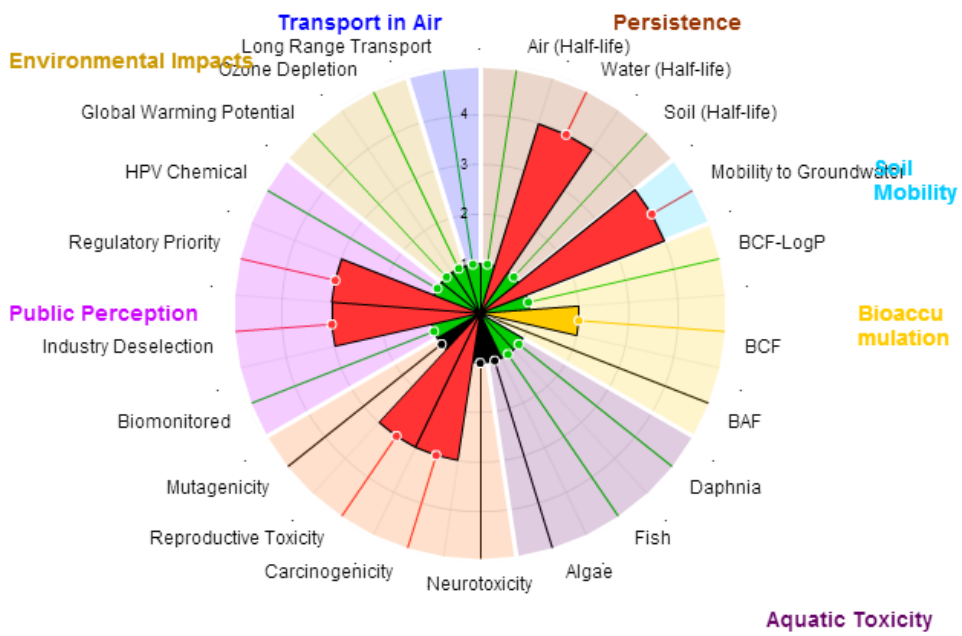
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Ethylene Thiourea

		CAS # 96-45-7
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.07658 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 0% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 0%, Max. BOD = 0%).
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 30 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 0.814
Bioaccumulation	BCF-LogP	Low bioconcentration potential based on an Experimental LogP=-0.66
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 1
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 14967.815 mg/L indicates a Low toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 16590.457 mg/L indicates a Low toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	
	Carcinogenicity	Anticipated Carcinogen - there is limited evidence of carcinogenicity in humans or sufficient evidence of carcinogenicity in animals [NTP] [NTPLIST]; Not classifiable [IARC_OE]; [EU_GHS]
	Reproductive Toxicity	Toxic to reproduction - Category 1B/2A [EU_RA17_5]
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	2 out of 6 lists (EUC2; SINLIST)
	Regulatory Priority	2 out of 10 lists (EU_CAND; JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 34.2835 km - A_TRNSPRT)



SHR

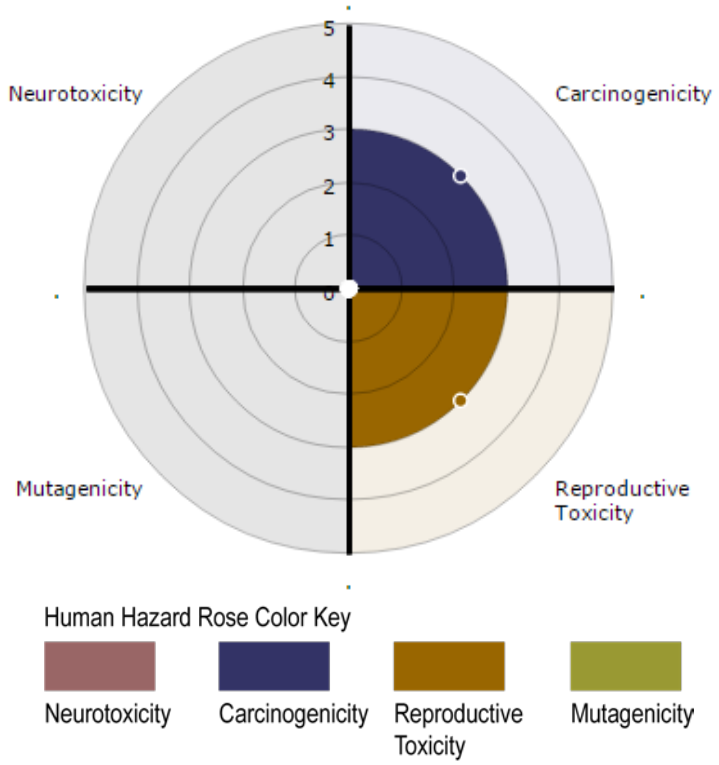
Key

- → Potential for High level of concern (**3-4**)
- → Potential for Moderate level of concern (**2**)
- → Potential for Low level of concern (**1**)

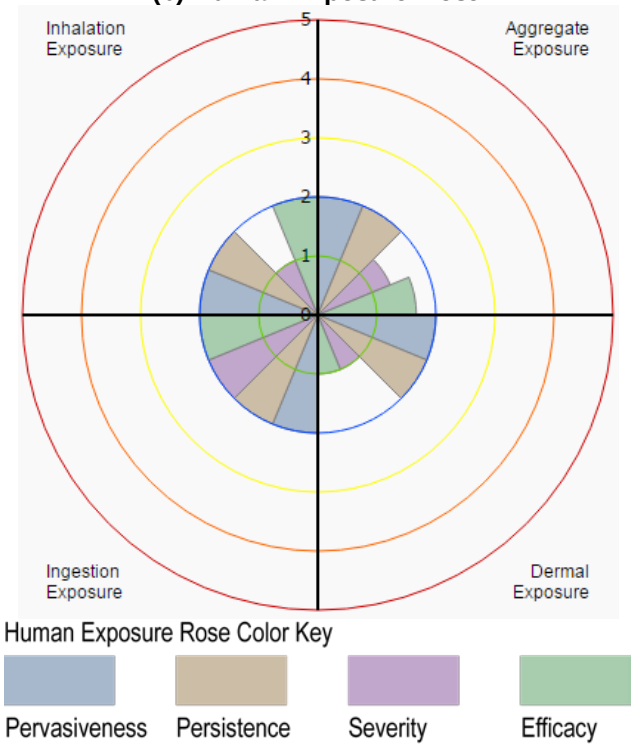
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Ethylene Thiourea

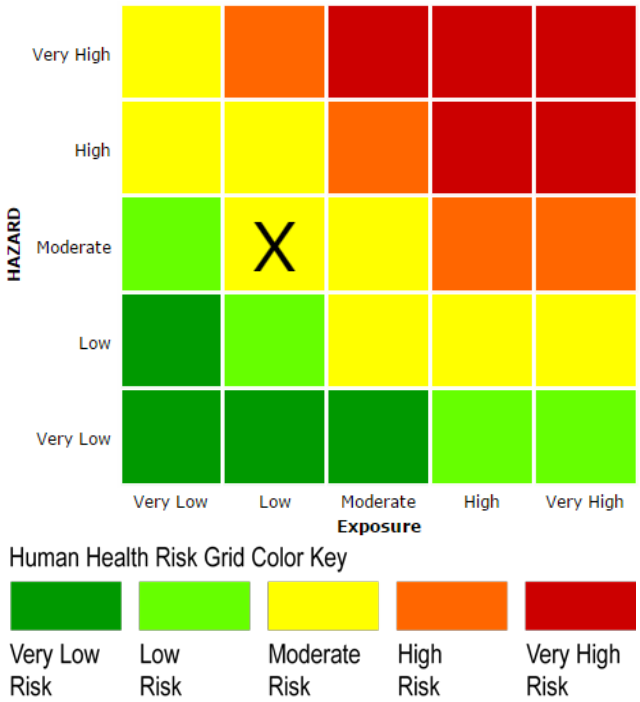
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



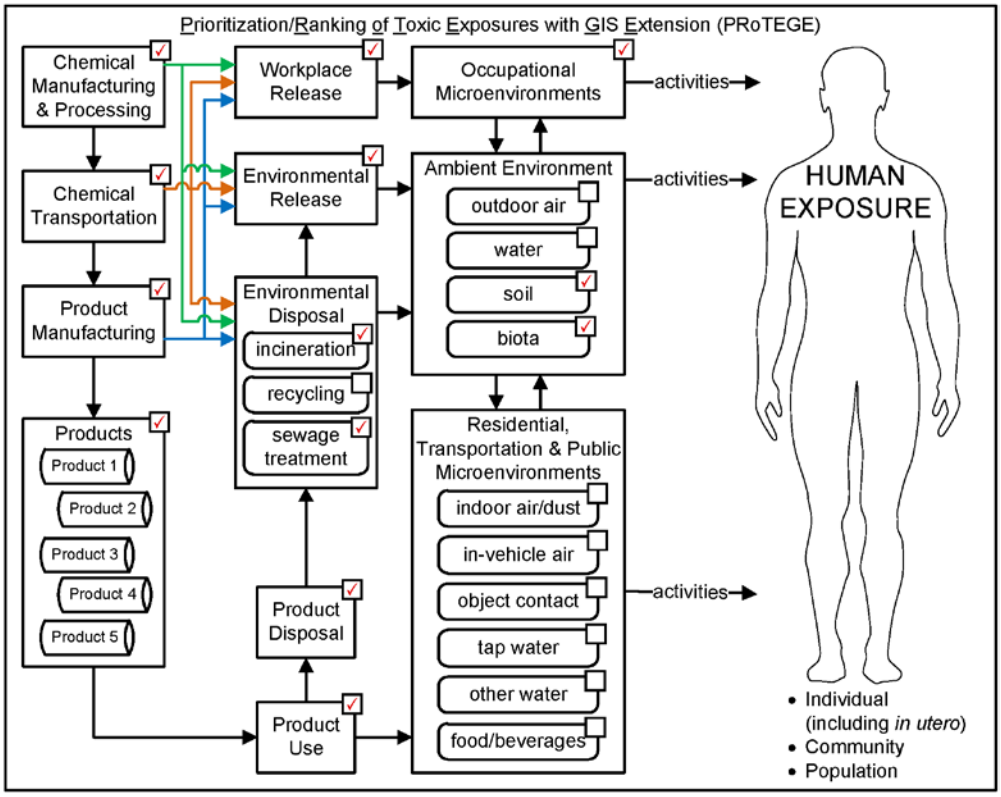
(a) Human Hazard
Estimated ranking of human hazard risk from Ethylene Thiourea, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Ethylene Thiourea (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Ethylene Thiourea, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Ranking for Ethylparaben



Summary Physico-Chemical Information	
Name	Ethylparaben
Other Names	Ethyl 4-hydroxybenzoate
Chemical Formula	$C_9H_{10}O_3$
Chemical Class	FP
Identifier	CAS: 120-47-8
Chemical Forms	
Physical Properties	
MW: 166.17 MP: 115–118 °C BP: 297–298 °C FP: 248 °C Sp.Gr: 0.946	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD: NA
Toxicological Effects: Contact dermatitis and estrogenic effect in estrogen-dependent human breast cancer cells (HSBD)
Exposure Limits: TEEL-0: 250mg/m³
Chemical Use: an antifungal preservative
Exposure Routes: Ingestion of food and skin contact
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air				Data sources: Soil - [82]; Indoor air - [77] (97% of samples <LOD)	Air		
Ground water							
Food					Surface Water		
Indoor Air (ng/m³)	<LOD		4.0		Ground Water		
Surface water					Soil		
Tap water							
Soil (ppm)	0.00054	0.0012	0.0051		Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

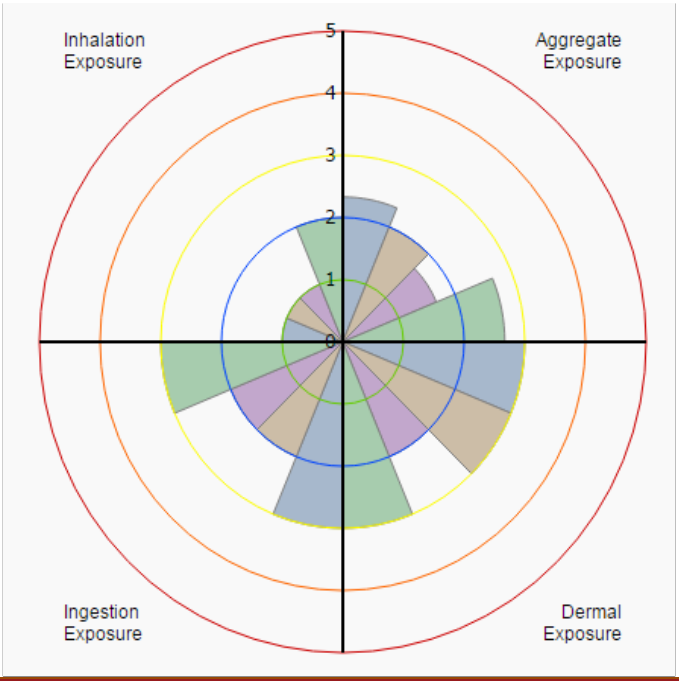
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		
	ICSC		
	Tox Profs		
	IRIS		
	HSDB		●
	ITER		
	McKay		
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		
	HPVIS		
	Tox Cast	Ph I	
		Ph II	●
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	u
		09-10	(u)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PKm (H) [38]
	BME		
	ERDEM		

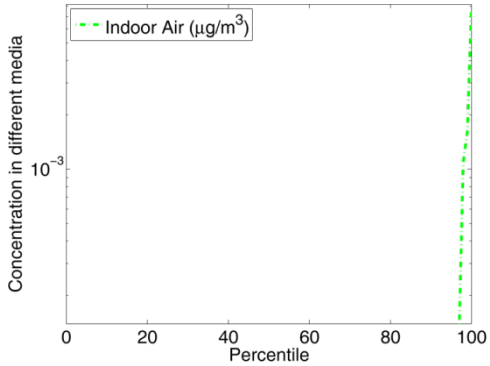
"Tier 1" Exposure Ranking for Ethylparaben

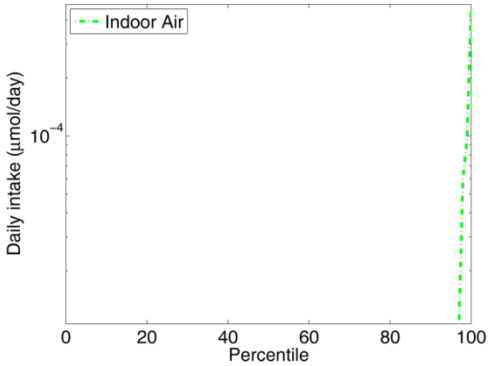
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	2
Ingestion	3	2	2	3
Dermal	3	3	2	3
Aggregate	2.33	2	1.66	2.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Ethylparaben





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0	0	NA	0
90 % tile	0	0	NA	0
% over 0.1 μmol/day	0	0	NA	0
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

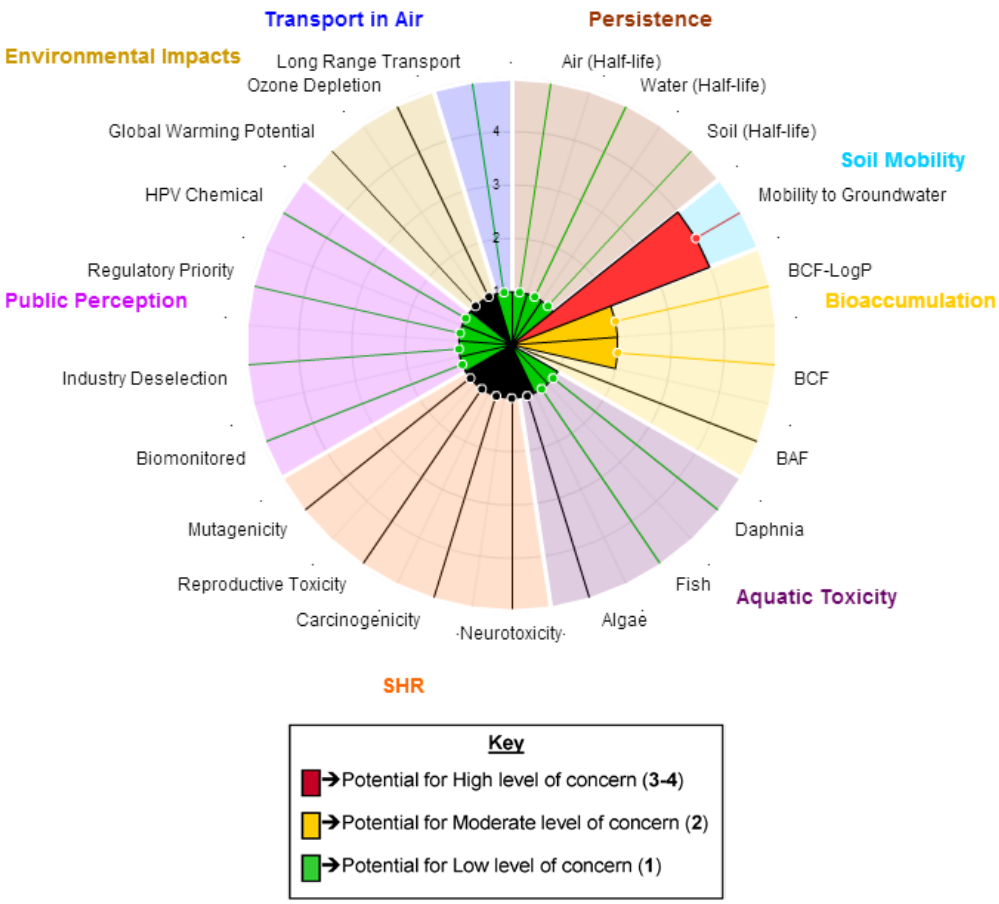
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Ethylparaben

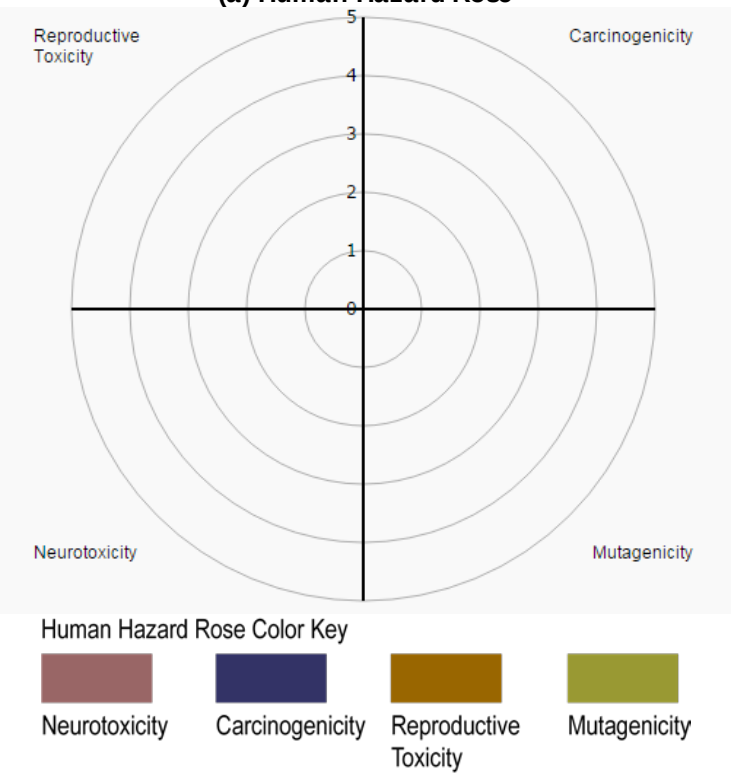
		CAS # 120-47-8
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.8506 days)
	Water (Half-life)	Low persistence in Water (Estimated Half-life = 15 days)
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 30 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 2.365
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=2.47
	BCF	Moderate bioconcentration potential based on Estimated LogBCF = 1.202
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 47.280 mg/L indicates a Low toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 13.754 mg/L indicates a Low toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	
	Carcinogenicity	
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	0 out of 6 lists
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 16.7772 km - A_TRNSPRT)



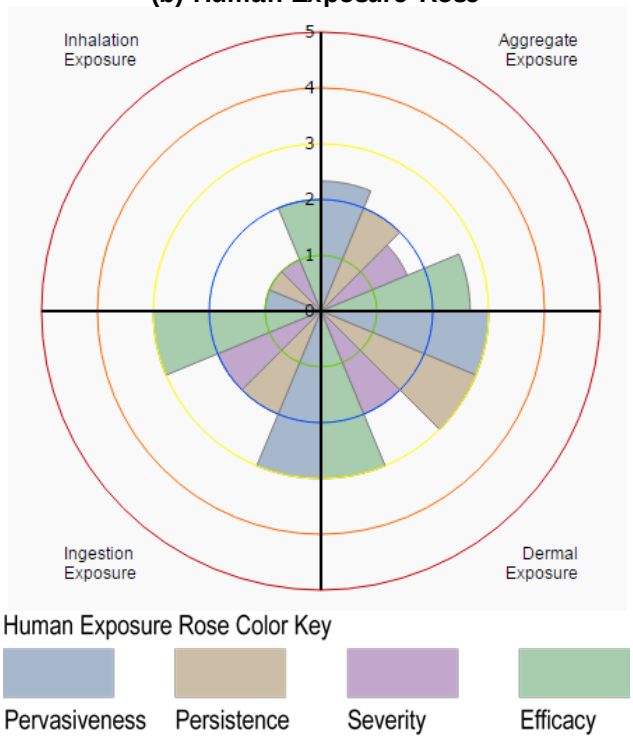
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Ethylparaben

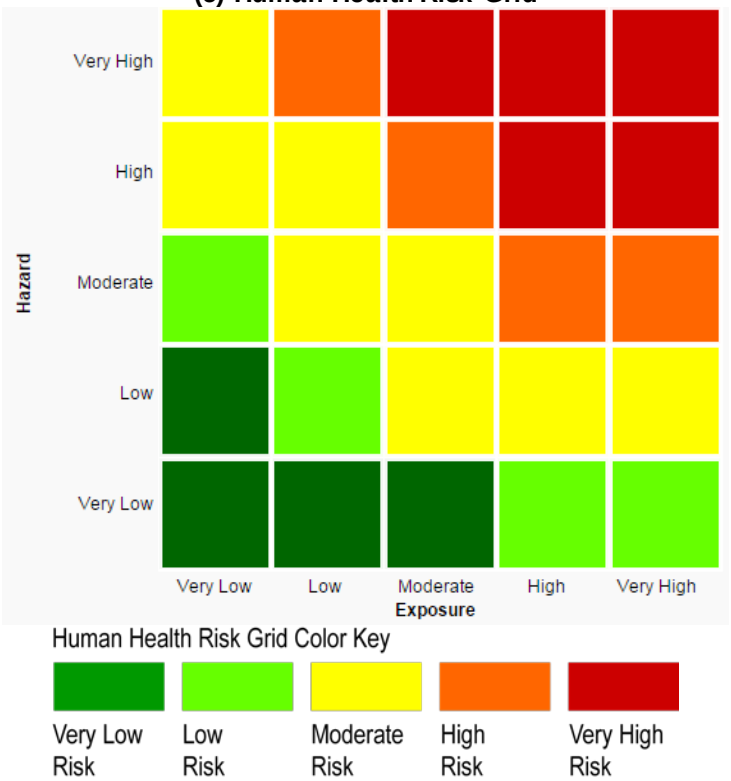
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



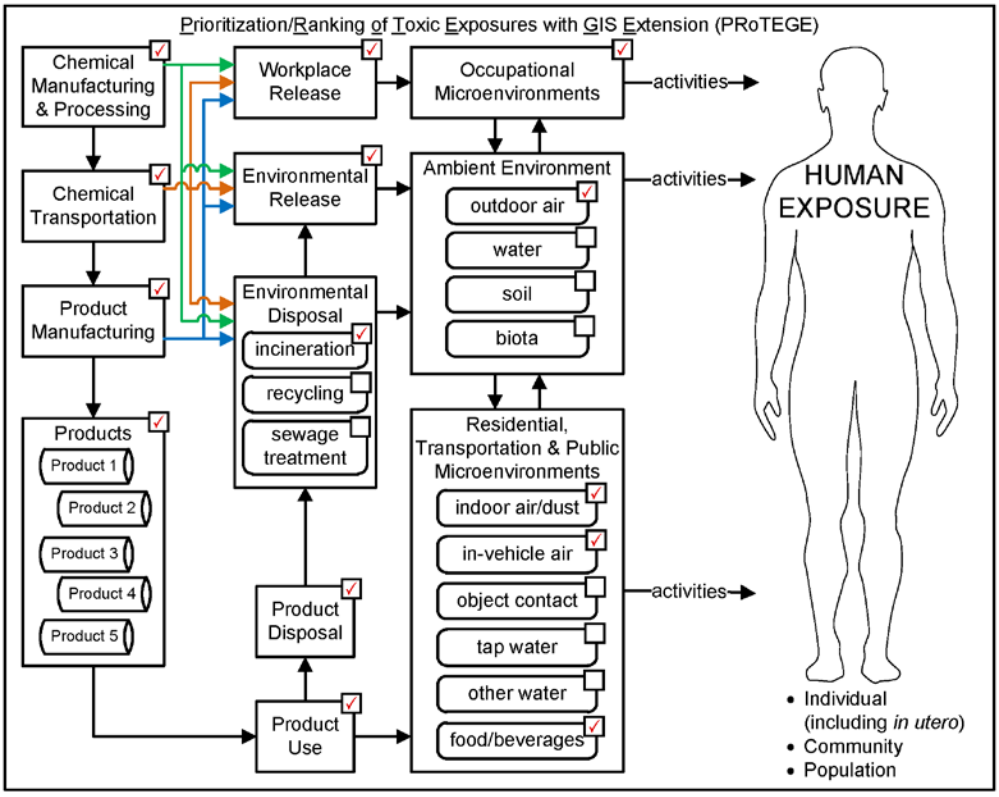
(a) Human Hazard
Estimated ranking of human hazard risk from Ethylparaben, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Ethylparaben (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Ethylparaben, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Formaldehyde



Summary Physico-Chemical Information	
Name	Formaldehyde
Other Names	Methanal, Methyl aldehyde
Chemical Formula	CH_2O/ HCHO
Chemical Class	VOC
Identifier	CAS: 50-00-0; NIOSH/RTECS: LP8925000; ICSC: 0695; UN: 2209; EC: 605-001-00-5
Chemical Forms	
Physical Properties	
Molecular weight: 30.0 Boiling point: -21 °C Melting point: -92 °C Solubility: Miscible Vapor pressure: > 1 atm (at 20 °C) Relative vapor density (air): 1.08 Octanol/water partition coefficient as log Pow: -0.65	
Additional Notes	
Nearly colorless gas with a pungent, suffocating odor. [Note: Often used in an aqueous solution.]	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.2 mg/kg-day (IRIS); RfC: NA (IRIS)
Toxicological Effects: Carcinogenic Classification – B1 (IRIS), A2; potential to produce significant sensitization (ACGIH 2004), Category 4 (DFG 2004)
Exposure Limits: NIOSH REL: Ca TWA 0.016 ppm C 0.1 ppm [15-minute]. OSHA PEL: [1910.1048] TWA 0.75 ppm ST 2 ppm. TLV: 0.3 ppm (Ceiling value); MAK: 0.3 ppm, 0.37 mg/m³; Sh
Chemical Use: Manufacture of resins, disinfectants, preservatives, and other chemicals
Exposure Routes: Inhalation, skin and/or eye contact
Target Organs: Eyes, respiratory system

Environmental Concentrations				
	Low	Medium	High	Notes
Outdoor air (ppb)	0.533	1.83	6.28	Data sources: Outdoor air (5th, 50th, and 95th % iles) '08 annual means @ AQS monitors; corresponding 2002 NATA county-level annual averages - 0.0205, 0.088 and 0.379. Indoor air - 69% > LOD (5th, 50th, and 95th % iles) - NHEXAS (non-smoking residences). Food - HSDB.
Ground water (ppb)				
Food (µg/kg)	0.001	0.0015	0.06	
Indoor Air (ppb)	6.26	17.1	46.7	
Surfaces				
Tap water (ppb)				
Soil (µg/kg)				
Dust				
Biota				
Human Biomarkers				
Urine (µg/L)				
Blood				
Other				

Environmental Releases		
	Emissions Tons/yr	% Counties Reporting Emissions
Air	249377(NEI 2005) 3086 (TRI 2008)	99.94 (NEI 2005) 13.05 (TRI 2008)
Surface Water	125.1 (TRI 2008)	3.78
Ground Water	4982.4 (TRI 2008)	0.22
Soil	17.0 (TRI 2008)	1.80
Chemical Production and Use		
Production	1 billion and greater lbs/yr	Data Source: IUR 2006

Exposures to formaldehyde for general populations from ingestion (food, drinking water, and non-dietary ingestion) are assumed to be negligible in this analysis.

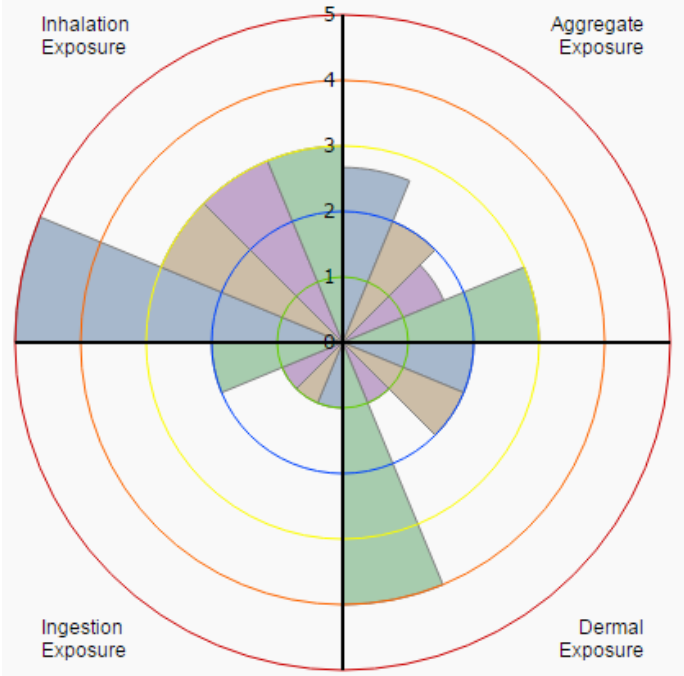
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		
	IARC		●
	PSAP		●
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		●
	IUR		●
	ECD		●
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PKm (R/Mm/H) [48]
	BME		
	ERDEM		

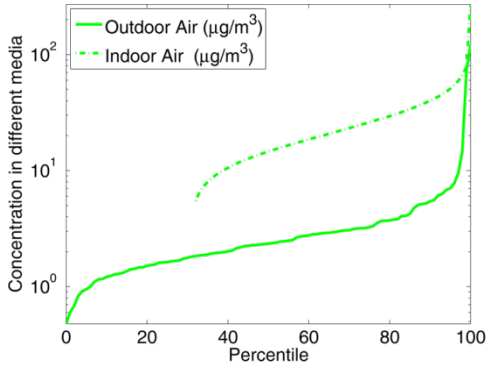
"Tier 1" Exposure Ranking for Formaldehyde

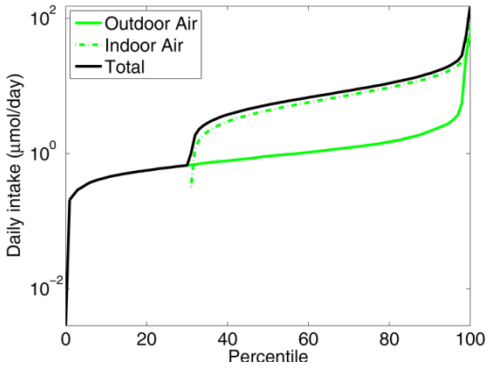
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	5	3	3	3
Ingestion	1	1	1	2
Dermal	2	2	1	4
Aggregate	2.66	2	1.66	3

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Formaldehyde





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	5.5	0	NA	5.5
90 % tile	15.2	0	NA	15.5
% over 0.1 μmol/day	99.7	0	NA	99.4
% over 1 μmol/day	82.3	0	NA	82

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

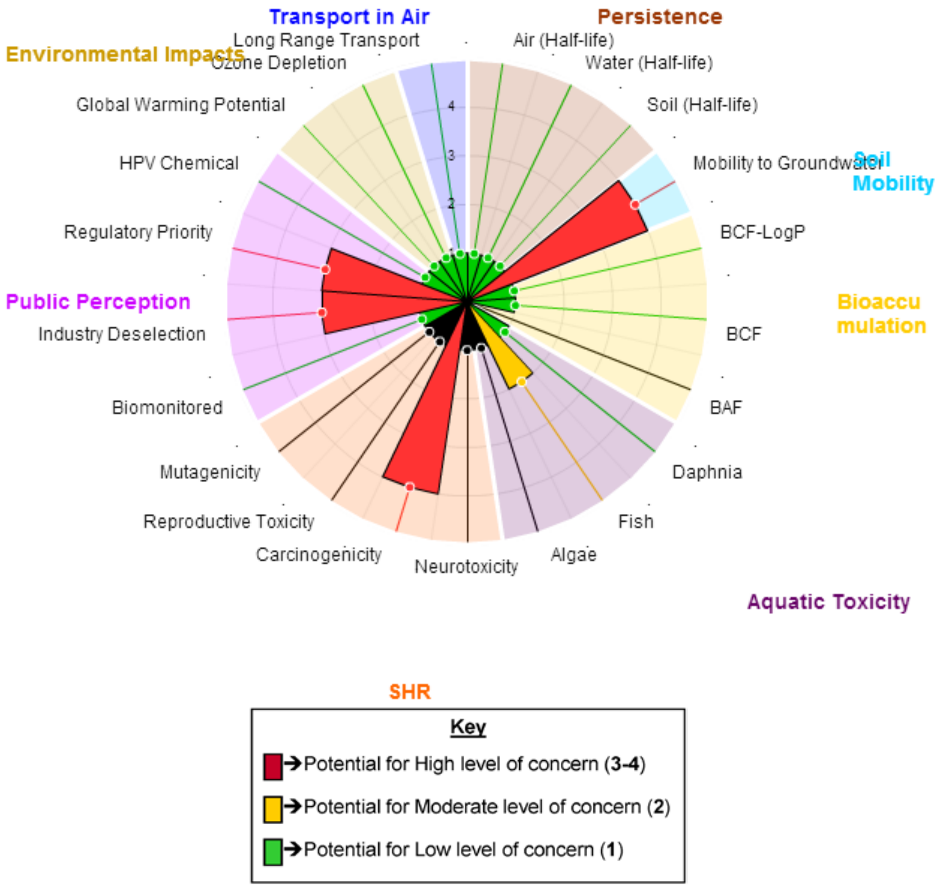
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Formaldehyde

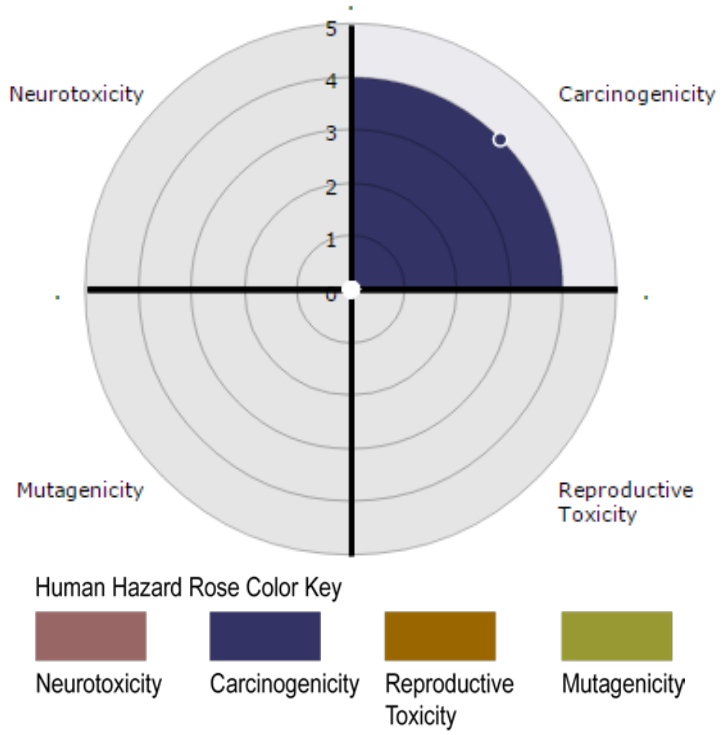
		CAS # 50-00-0
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 1.316 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 91% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is not persistent in water (Min. BOD = 87%, Max. BOD = 96%).
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 30 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 0
Bioaccumulation	BCF-LogP	Low bioconcentration potential based on an Experimental LogP=0.35
	BCF	Low bioconcentration potential based on Estimated LogBCF = 0.5
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 16.071 mg/L indicates a Low toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 8.297 mg/L indicates a Moderate toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	
	Carcinogenicity	Known Carcinogen - human studies indicate a causal relationship between exposure and human cancer [NTPLIST]; Carcinogenic to humans [IARC_OE]; Carc. 1B: [EU_GHS]; CLASS A2 - Suspected Human Carcinogen [ACGIH]; B1 (Probable human carcinogen - based on limited evidence of carcinogenicity in humans and sufficient evidence of carcinogenicity in animals) [1986 Guidelines] [IRIS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	3 out of 6 lists (GADSL; EUC3; SINLIST)
	Regulatory Priority	3 out of 10 lists (EU_RRAP; CAN_PSL; JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP = 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 333.85 km - A_TRNSPRT)



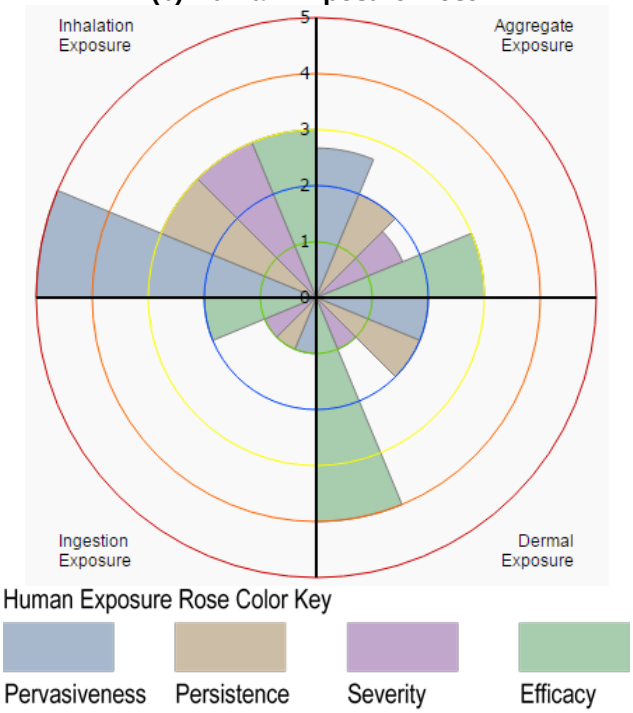
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Formaldehyde

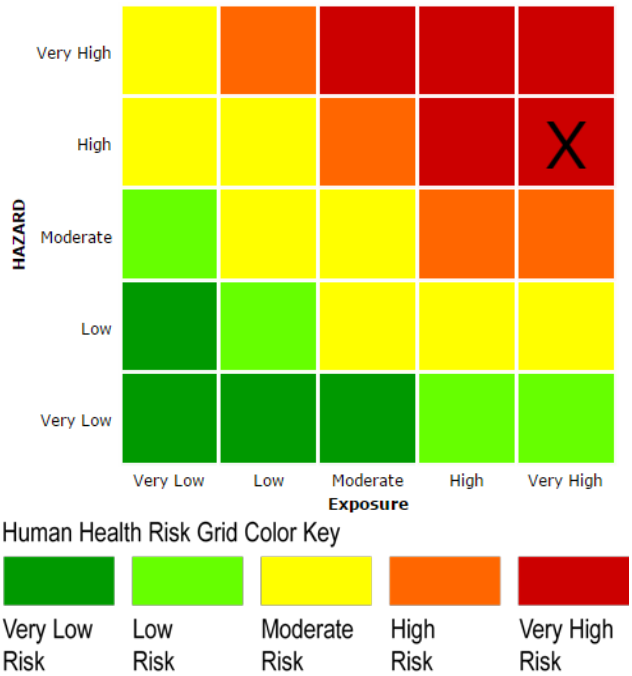
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



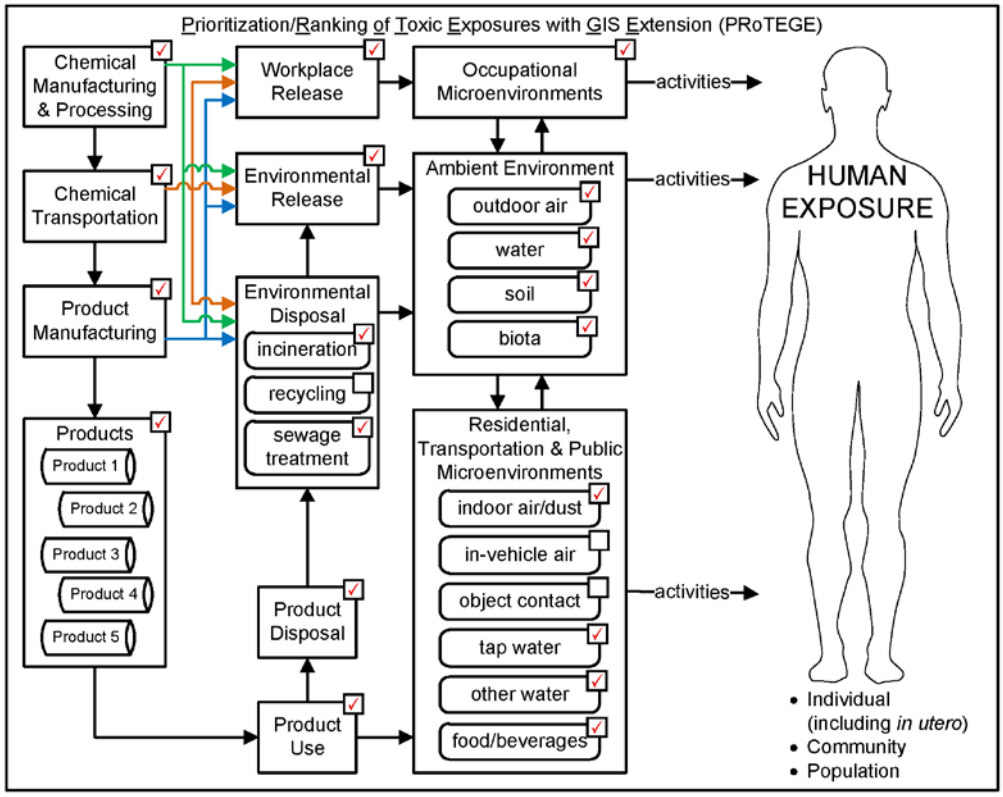
(a) Human Hazard
Estimated ranking of human hazard risk from Formaldehyde, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Formaldehyde (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Formaldehyde, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for gamma-Hexachlorocyclohexane



Summary Physico-Chemical Information	
Name	gamma-Hexachlorocyclohexane
Other Names	Lindane
Chemical Formula	$C_6H_6Cl_6$
Chemical Class	OCP
Identifier	CAS: 58-89-9
Chemical Forms	
Physical Properties	
MW: 290.8 BP: 614°F MLT: 235°F Sol: 0.001% VP: 0.00001 mmHg Sp.Gr: 1.85	
Additional Notes	
White to yellow, crystalline powder with a slight, musty odor	

Exposure and Toxicity Information
Toxicity Limits: Oral LD_{50}: 88mg/kg in rats; RfD: 0.0003 mg/kg/day
Toxicological Effects: Classified as 2B "possible" human carcinogen (IARC)
Exposure Limits: NIOSH REL: TWA 0.5 mg/m³ [skin]; OSHA PEL: TWA 0.5 mg/m³ [skin]; TEEL-0: 0.5 mg/m³
Chemical Use: Pesticide
Exposure Routes: Inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, respiratory system, central nervous system, blood, liver, kidney

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (pg/m³)	8	36	115	Data Source: Food (5th, 50th, 95th %iles) – TDS '94 -'02, Ground water, surface water – HSDB; Tap water - [23] >99% of measurements <RL; Outdoor air - [49]	Air	4.41 (NEI 2005); 0.05 (TRI 2008)	4.16% (NEI 2005); 0.16% (TRI 2008)
Ground water (ppb)	0.016	0.163	0.9				
Food (µg/g)	0.001	0.005	0.03		Surface Water		
Indoor Air					Ground Water		
Surface water (µg/L)	0.00002	0.000077	0.00016		Soil		
Tap water (µg/L)	<LOD	<LOD	0.030 (99.5% tile)				
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

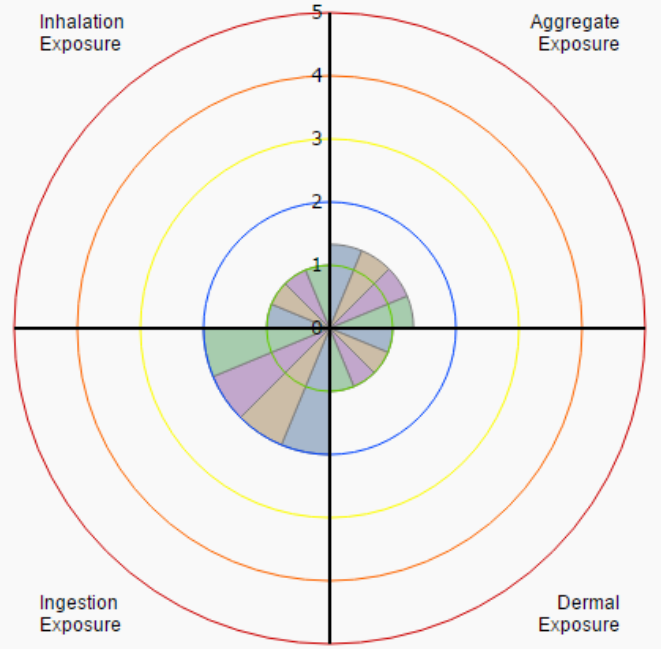
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		●
	ICSC		●
	Tox Profs		□
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		
	PSAP		
	NTP		●
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		●
Production and Use	SIDS		
	EHPV		
	HPD		
	IUR		
	ECD		○
	SRD		
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		○
	CERCLIS		●
	NATA		○
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		●
	NHANES	03-04	s
		05-06	(▯)
		07-08	(s)
		09-10	(s)
	NHEXAS		●
PK/PBPK Model (▯r Data)	ScLit		PBPKm (R) [50]
	BME		
	ERDEM		

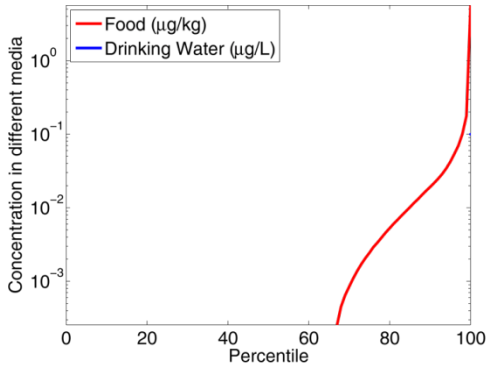
"Tier 1" Exposure Ranking for gamma-Hexachlorocyclohexane

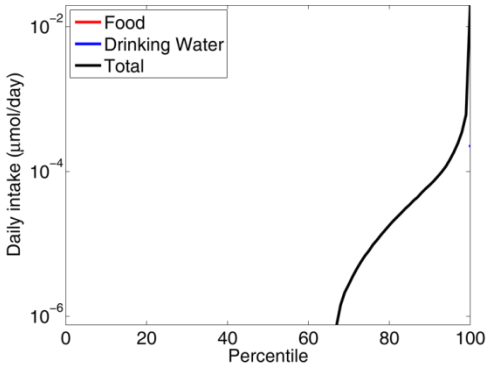
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	1
Aggregate	1.33	1.33	1.33	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for gamma-Hexachlorocyclohexane





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	9.53E-07	0	NA	9.53E-07
90 % tile	3.48E-06	6.67E-05	NA	7.37E-05
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

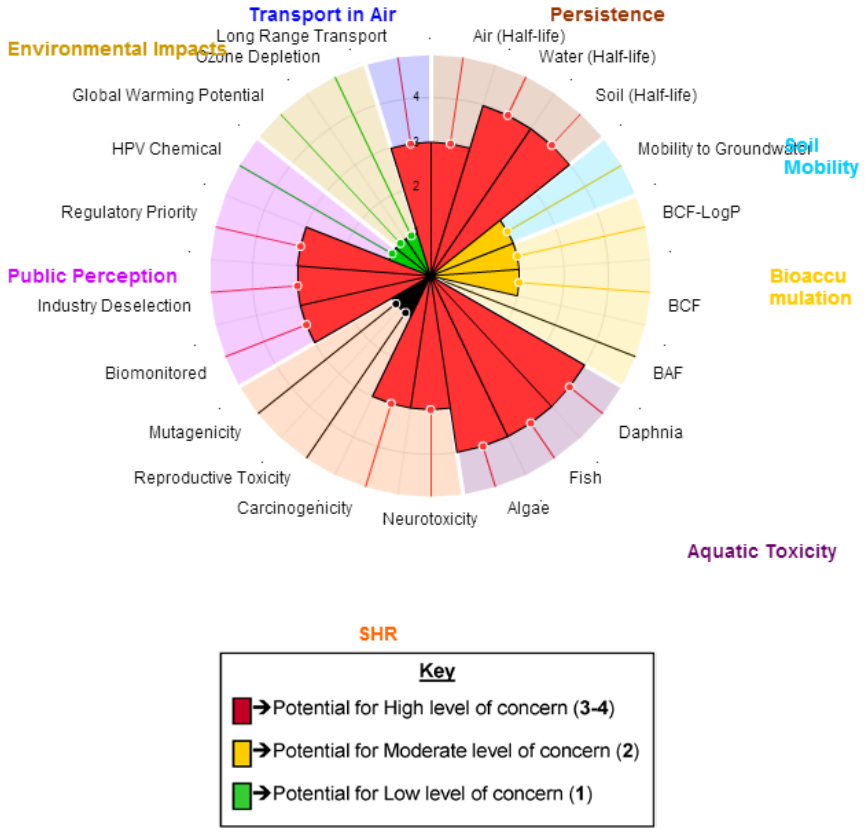
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for gamma-Hexachlorocyclohexane

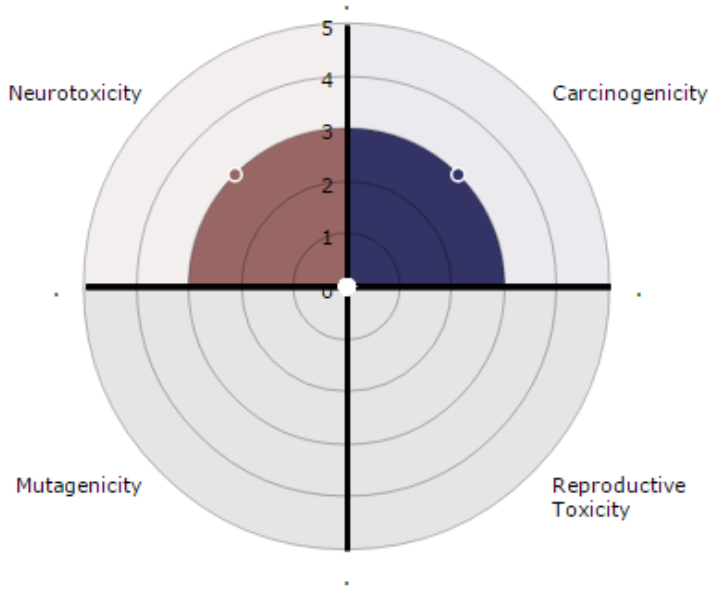
		CAS # 58-89-9
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 18.66 days)
	Water (Half-life)	Very High persistence in Water (Estimated Half-life = 180 days)
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Moderate mobility to groundwater based on LogKoc = 3.529
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=3.72
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 2.67
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 2.028 mg/L indicates a Moderate toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 1.619 mg/L indicates a Moderate toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	Anticipated Carcinogen - there is limited evidence of carcinogenicity in humans or sufficient evidence of carcinogenicity in animals [NTP] [NTPLIST]; CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	2 out of 6 lists (GADSL; RC_PIC)
	Regulatory Priority	1 out of 10 lists (JCL1_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 1268.46 km - A_TRNSPRT)



IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for gamma-Hexachlorocyclohexane

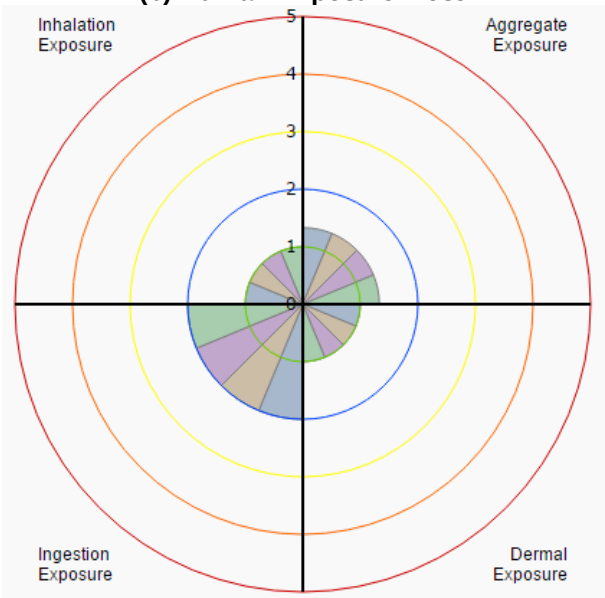
(a) Human Hazard Rose



Human Hazard Rose Color Key

Neurotoxicity | Carcinogenicity | Reproductive Toxicity | Mutagenicity

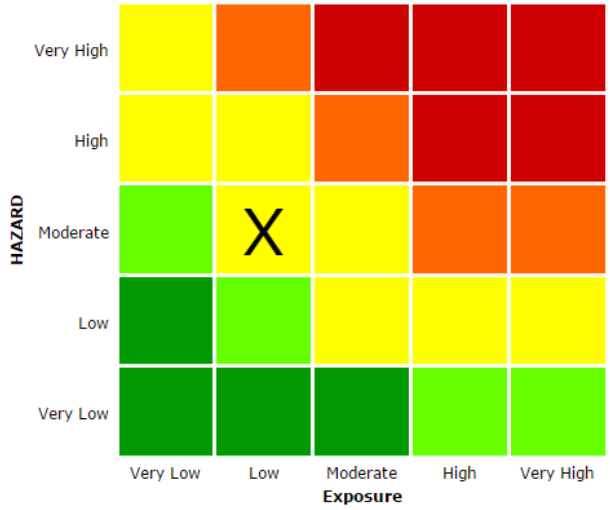
(b) Human Exposure Rose



Human Exposure Rose Color Key

Pervasiveness | Persistence | Severity | Efficacy

(c) Human Health Risk Grid



Human Health Risk Grid Color Key

Very Low Risk | Low Risk | Moderate Risk | High Risk | Very High Risk

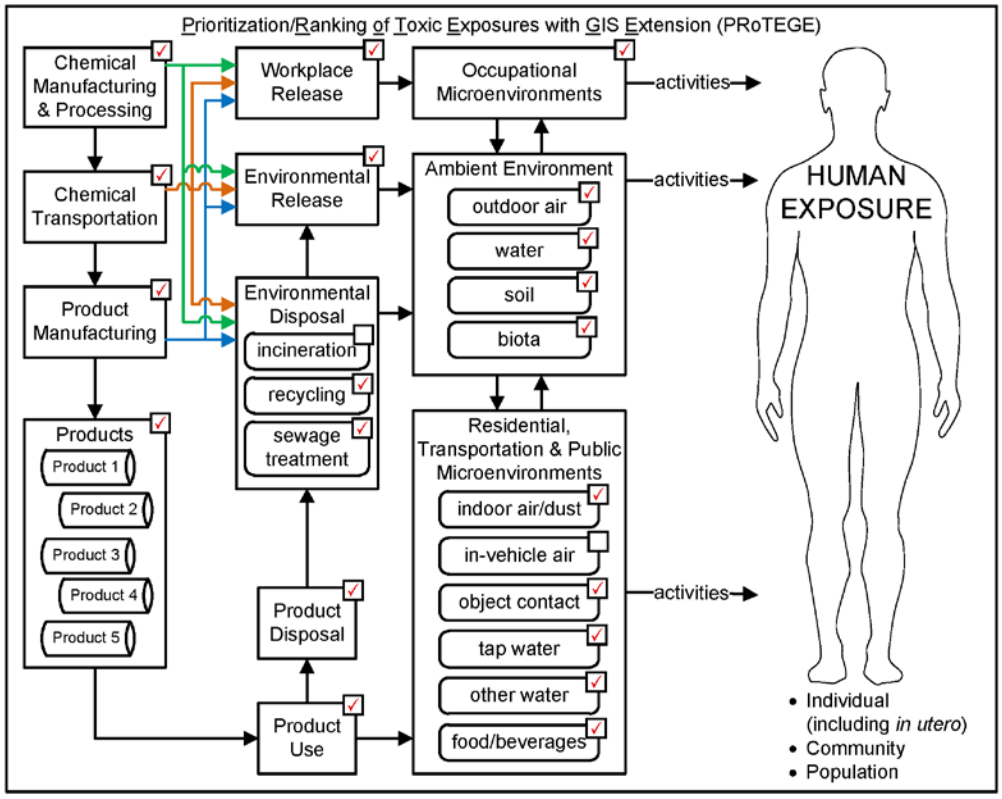
(a) Human Hazard
Estimated ranking of human hazard risk from gamma-Hexachlorocyclohexane, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of gamma-Hexachlorocyclohexane (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from gamma-Hexachlorocyclohexane, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Ranking for Lead



Summary Physico-Chemical Information	
Name	Lead
Other Names	
Chemical Formula	Pb
Chemical Class	Mt/MU
Identifier	CAS:7439-92-1; RTECS: OF7525000
Chemical Forms	Many compounds including elemental lead, tetra-ethyl lead, lead telluride, lead selenide, lead chromate lead carbonate, lead antimonide, galena (PbS), cerussite ($PbCO_3$) and anglesite ($PbSO_4$)
Physical Properties	
Molecular weight: 207.2 Boiling point: 1740°C Melting point: 327.5°C Solubility: Insoluble Vapor pressure: negligible at 20°C Density: 11.34 g/cm³	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: TDI0.0036mg/kg/day (RIVM)
Toxicological Effects: Carcinogenic Classification – B2 (IRIS), 2A (IARC), A3 (ACGIH 2004)
Exposure Limits: NIOSH REL: TWA (8-hour) 0.050 mg/m³; OSHA PEL: [1910.1025] TWA 0.050 mg/m³
Chemical Use: Batteries. Previous uses included solder, pipes, gasoline additive, paints, pigments and ammunition
Exposure Routes: Inhalation, ingestion, skin and/or eye contact (NIOSH)
Target Organs: Central nervous system, cardiovascular system, kidneys, and the immune system

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ppb)	0.002	0.01	0.04	Data sources: Outdoor air (5th, 50th, and 95th %iles) - '08 annual means @ AQS monitors; corresponding 2002 NATA county-level annual averages - 5.37e-04, 0.0020, and 0.0036. Food (5th, 50th, and 95th %iles) - TDS '94-'02. Indoor Air - 50.7% > LOD, Dust - 1-4 month accumulation (5th, 50th, and 95th %iles), Tap Water – flushed 82.6% > LOD (5th,50th, and 95th %iles) and Surfaces (50th, and 95th %iles) [71].	Air	953.07 (NEI 2005) 234.16(TRI 2008)	99.94% (NEI 2005) 30.39% (TRI 2008)
Ground water							
Food (µg/g)	0.007	0.012	0.035		Surface Water	5.63 (TRI 2008)	9.89%
Indoor Air (ng/m³)	0.77	6.56	56.1		Ground Water	46.87(TRI 2008)	0.19%
Surfaces (µg/cm²)	15	134	1176		Soil	5632.70(TRI 2008)	10.17%
Tap water (µg/L)	0.011	0.3	4.71				
Soil					Chemical Production and Use		
Dust (µg/cm²)	8.06	65.2	527		Production	1 billion and greater lbs/yr	Data Source: IUR 2006
Outdoor air (ppb)	0.002	0.01	0.04				
Biota							
Human Biomarkers				Data sources: Urine: 84.8 - 98.0% > LD (NHANES '03-'08); Blood: 99.7% > LD (NHANES '03-'04)			
Urine (µg/L)	0.14	0.56	0.94				
Blood (µg/dL)	5.0	14	23				
Other							

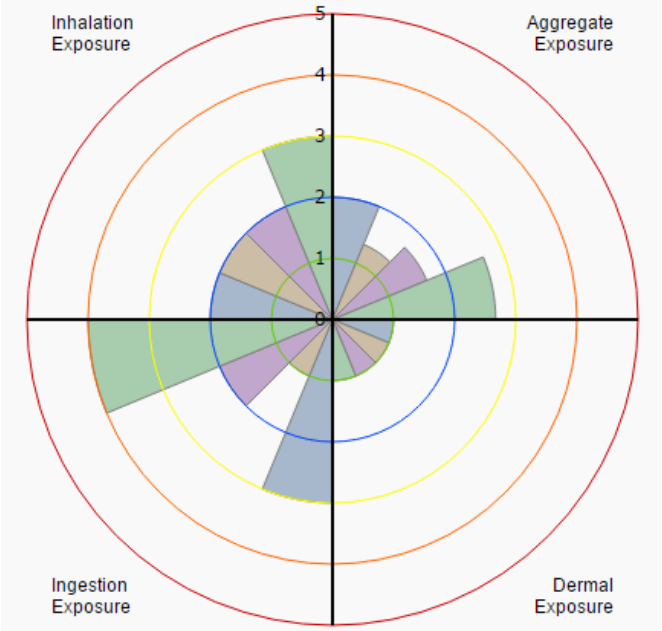
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		●
	IARC		●
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		●
	ECD		○
	SRD		
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		●
	NAWQA		●
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		●
	NHANES	03-04	b,u
		05-06	(b),u
		07-08	(b),u
		09-10	(b,u)
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PBPKm (R) [42]
	BME		
	ERDEM		

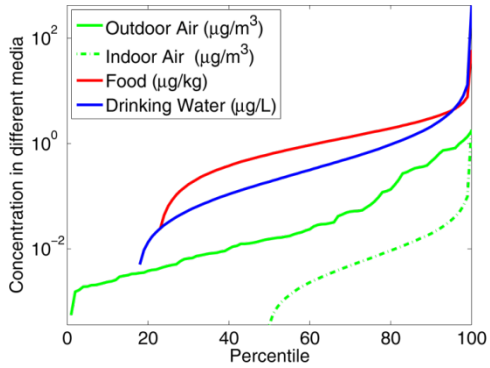
"Tier 1" Exposure Ranking for Lead

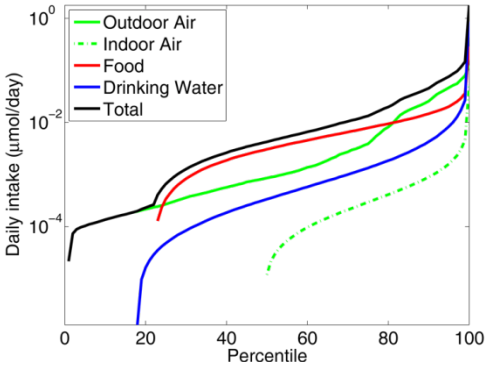
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	2	2	2	3
Ingestion	3	1	2	4
Dermal	1	1	1	1
Aggregate	2	1.33	1.66	2.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Lead





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.00119	0.0046	NA	0.00579
90 % tile	0.0258	0.0181	NA	0.0458
% over 0.1 μmol/day	0.604	0.982	NA	2.72
% over 1 μmol/day	0	0.656	NA	1.36

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

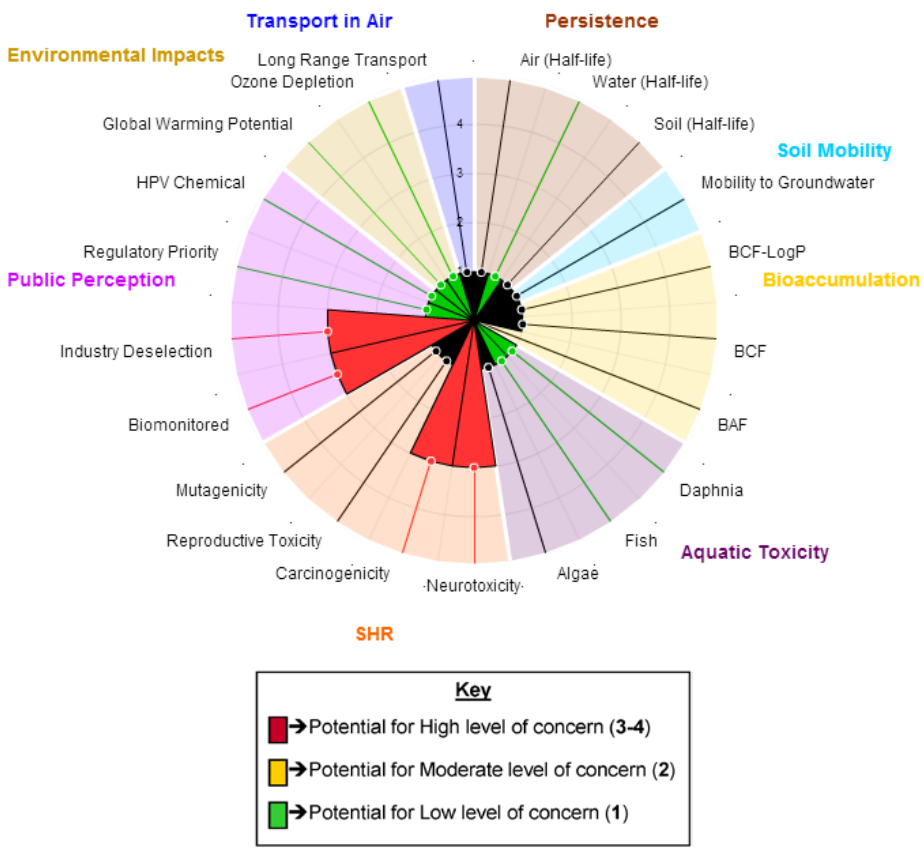
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Lead

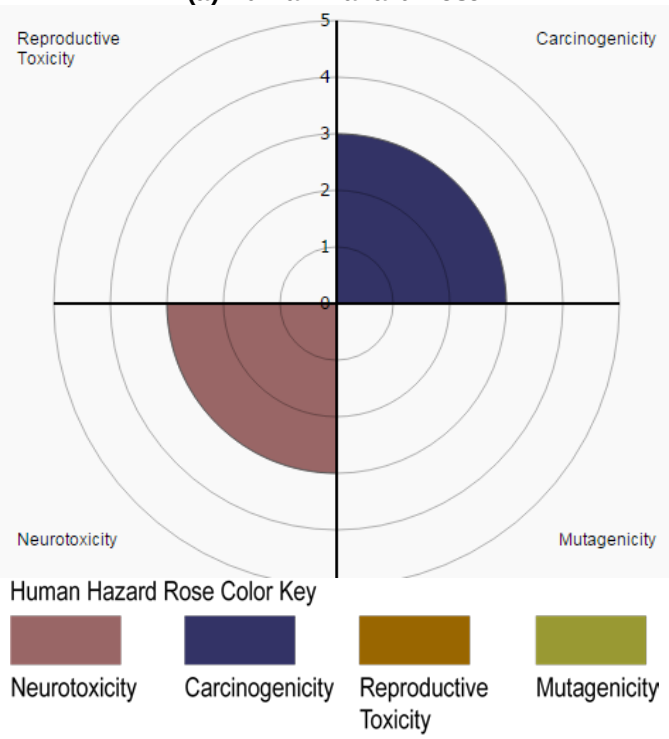
		CAS # 7439-92-1
Persistence	Air (Half-life)	Persistence in Air has not been calculated for this compound
	Water (Half-life)	Persistence in Water has not been calculated for this compound.
	Soil (Half-life)	Persistence in Soil has not been calculated for this compound.
Soil Mobility	Mobility to Groundwater	Soil mobility has not been calculated for this compound
Bioaccumulation	BCF-LogP	BCF value based on LogP has not been calculated for this compound
	BCF	BCF value has not been calculated for this compound
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 2355.536 mg/L indicates a Low toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 2399.881 mg/L indicates a Low toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	Known Neurotoxin [Grandjean et al]
	Carcinogenicity	Anticipated Carcinogen - there is limited evidence of carcinogenicity in humans or sufficient evidence of carcinogenicity in animals [NTP] [NTPLIST]; Possibly carcinogenic to humans [IARC_OE]; B2 (Probable human carcinogen - based on sufficient evidence of carcinogenicity in animals) [1986 Guidelines] [IRIS]; CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	2 out of 6 lists (GADSL; EUC2)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Long Range Transport in Air has not been calculated for this compound



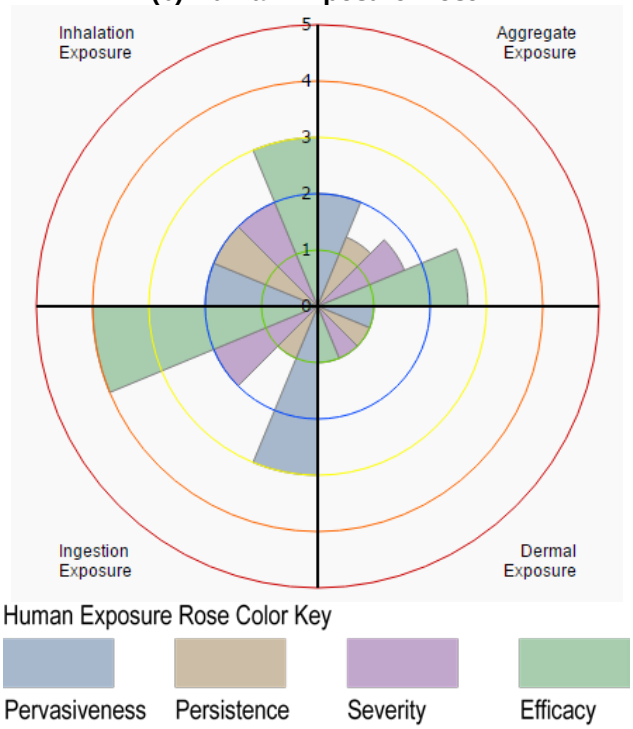
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Lead

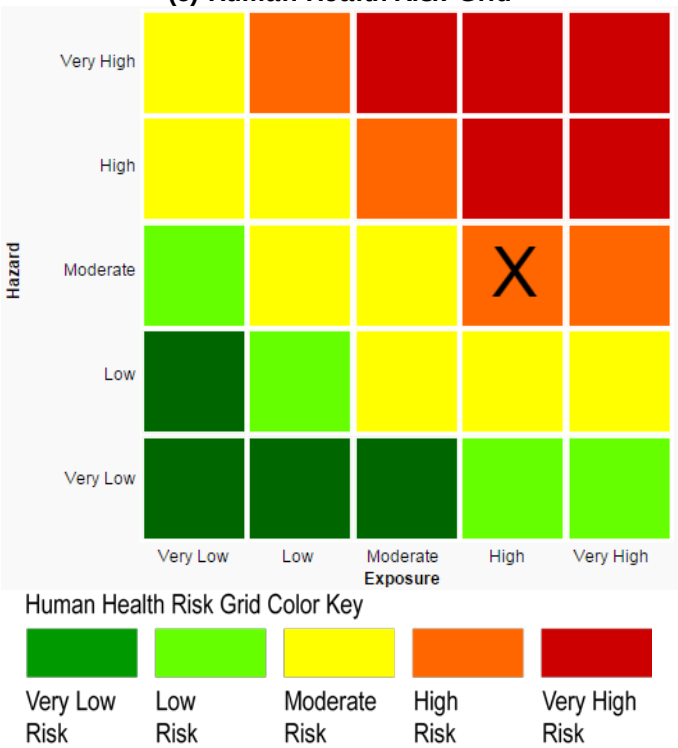
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



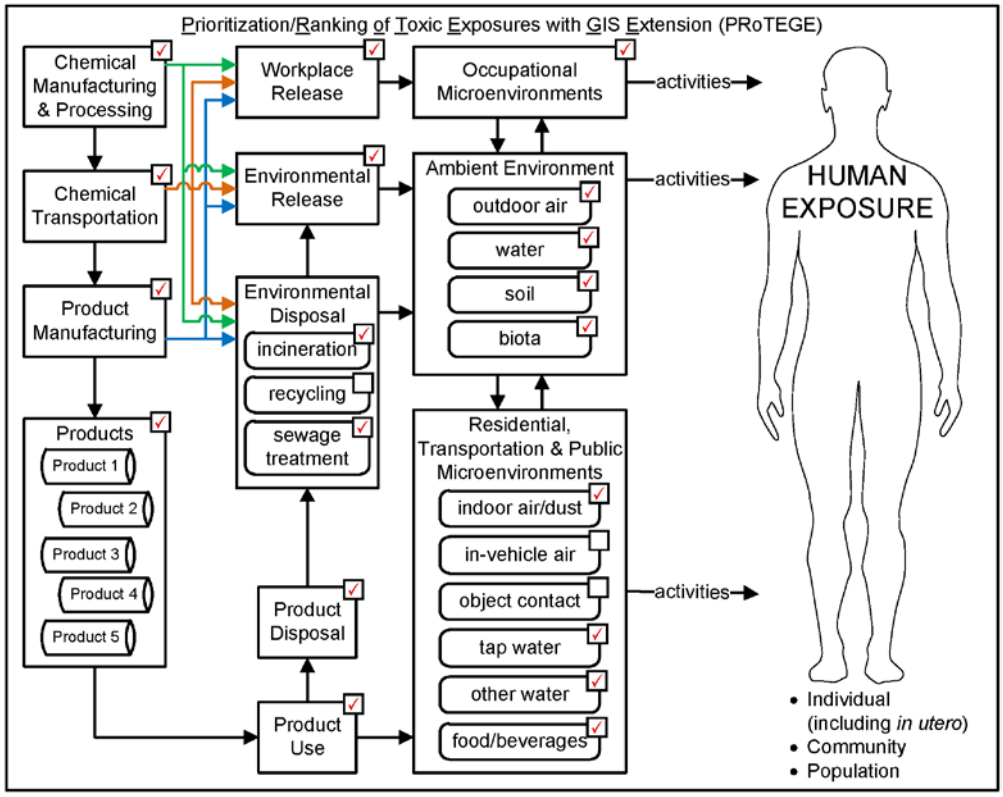
(a) Human Hazard
Estimated ranking of human hazard risk from Lead, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Lead (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Lead, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Malathion



Summary Physico-Chemical Information	
Name	Malathion
Other Names	Diethyl ester; Carbofos; Mecaptothion; 2-(dimethoxyphophinothiolthio) butanedioic acid
Chemical Formula	$C_{10}H_{19}O_6PS_2$
Chemical Class	OPP
Identifier	CAS: 121-75-5
Chemical Forms	
Physical Properties	
MW: 330.4 BP: 140°F (Decomposes) FRZ: 37°F Sol: 0.02% VP: 0.00004 mmHg Sp.Gr: 1.21 Fl.P(oc): >325°F	
Additional Notes	
Deep-brown to yellow liquid with a garlic-like odor	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.02 mg/kg/day (IRIS); RfC: NA (IRIS)
Toxicological Effects: Suggestive evidence of carcinogenicity but not sufficient to assess human carcinogenic potential (EPA OPP)
Exposure Limits: OSHA PEL: TWA 15 mg/m³ [skin]; TEEL-0: 1mg/m³
Chemical Use: Organophosphate insecticide
Exposure Routes: Inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, respiratory system, liver, blood cholinesterase, central nervous system, cardiovascular system, gastrointestinal tract

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air				Data source: Food (5th, 50th, 95th %iles) – TDS '94 -'02; Soil (low, high) - HSDB, Surface water - STORET	Air	1.87 (TRI 2008)	0.22% (TRI 2008)
Ground water							
Food (µg/g)	0.001	0.004	0.02		Surface Water	0.0025 (TRI 2008)	0.03% (TRI 2008)
Indoor Air					Ground Water		
Surface water (µg/L)	0	0.048	50		Soil		
Tap water (µg/L)							
Soil (ppm)	1.4		14.1		Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

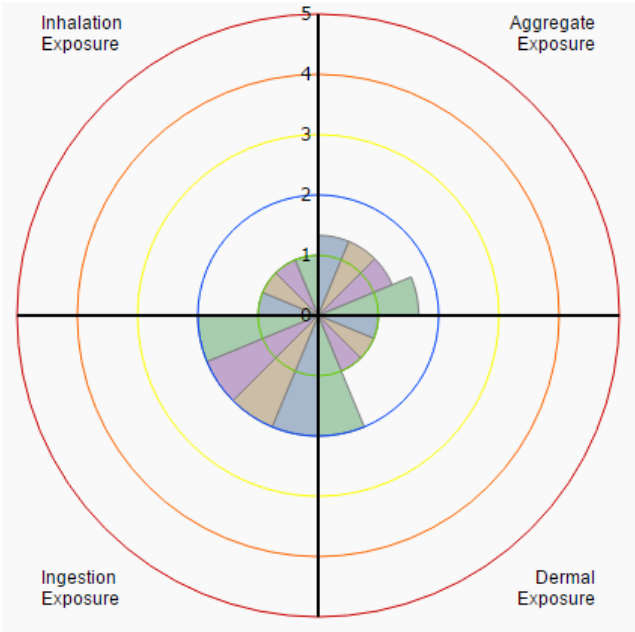
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		
	IARC		
	PSAP		
	NTP		●
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		●
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		□
	SRD		●
Releases	TRI		●
	NEI		
Environmental Quality	NGA		
	NAWQA		●
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [24]
	BME		
	ERDEM		● PKd

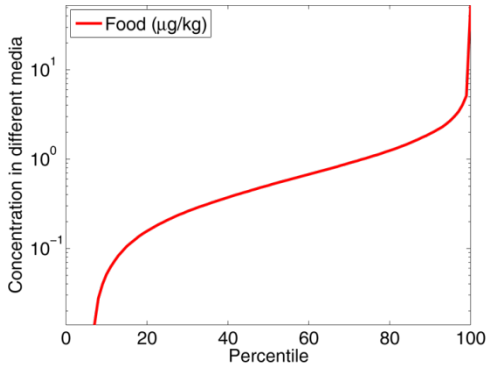
"Tier 1" Exposure Ranking for Malathion

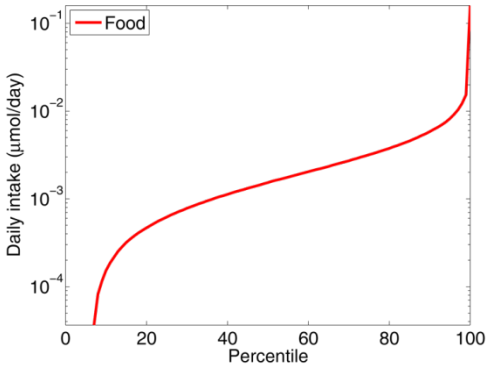
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Malathion





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0.00155	NA	0.00155
90 % tile	0	0.00584	NA	0.00597
% over 0.1 µmol/day	0	0.414	NA	0.812
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

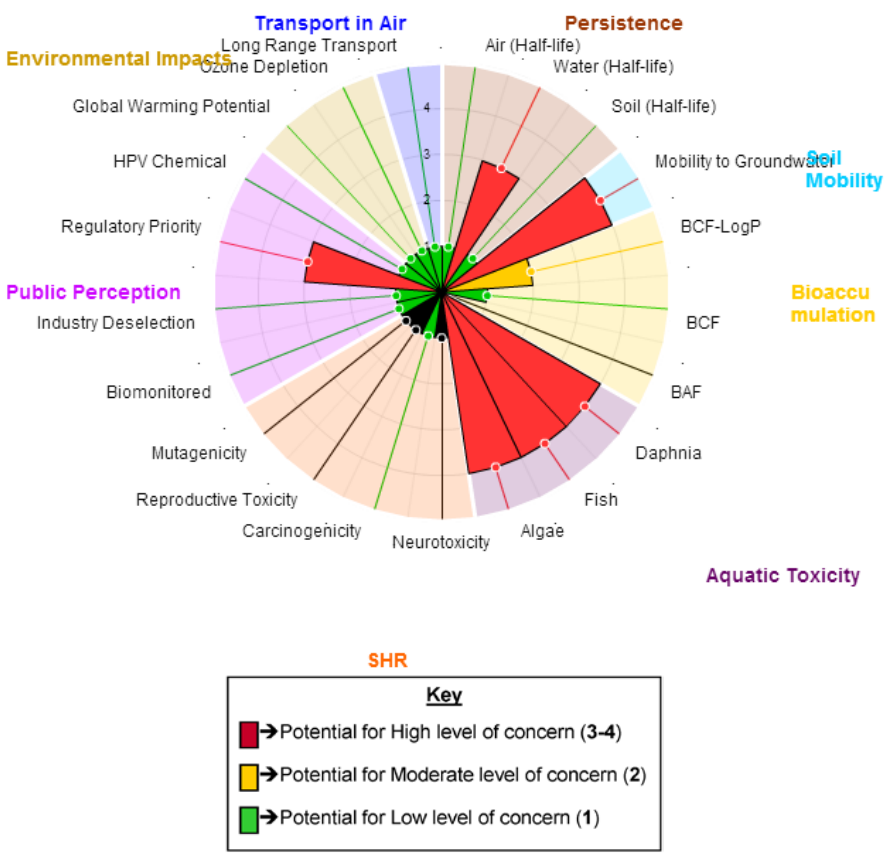
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Malathion

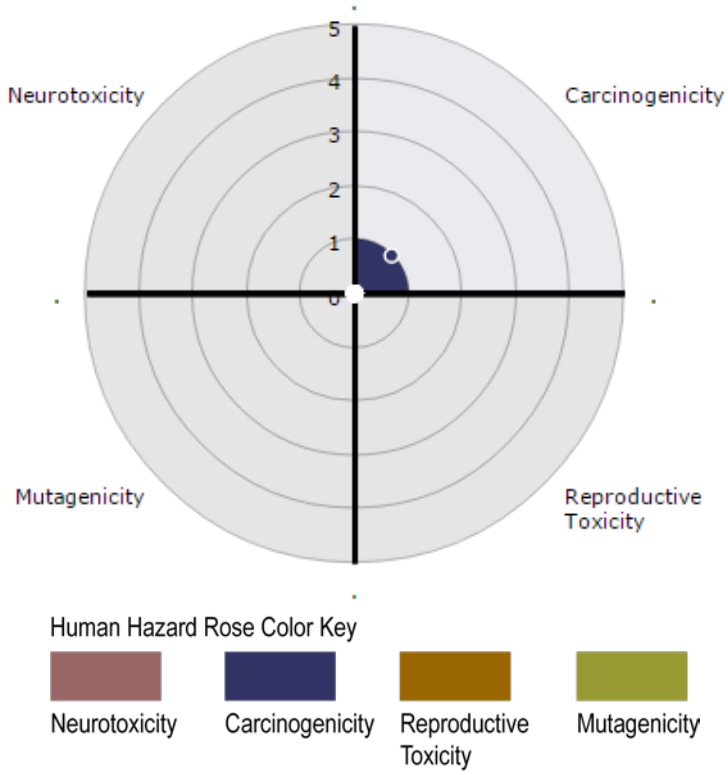
		CAS # 121-75-5
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.1382 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 22% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is persistent in water (Min. BOD = 20%, Max. BOD = 23%).
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 30 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 1.484
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=2.36
	BCF	Low bioconcentration potential based on Experimental LogBCF = 0.54
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 142.915 mg/L indicates a Low toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 34.981 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	CLASS A4 - Not Classifiable as a Human Carcinogen [ACGIH]; Not classifiable [IARC_OE]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	0 out of 6 lists
	Regulatory Priority	1 out of 10 lists (JMON3)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 20.0569 km - A_TRNSPRT)



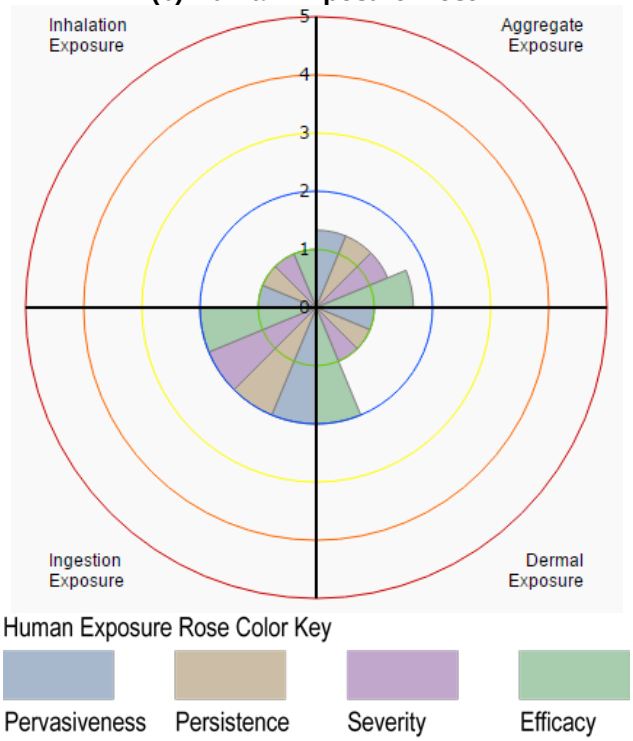
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Malathion

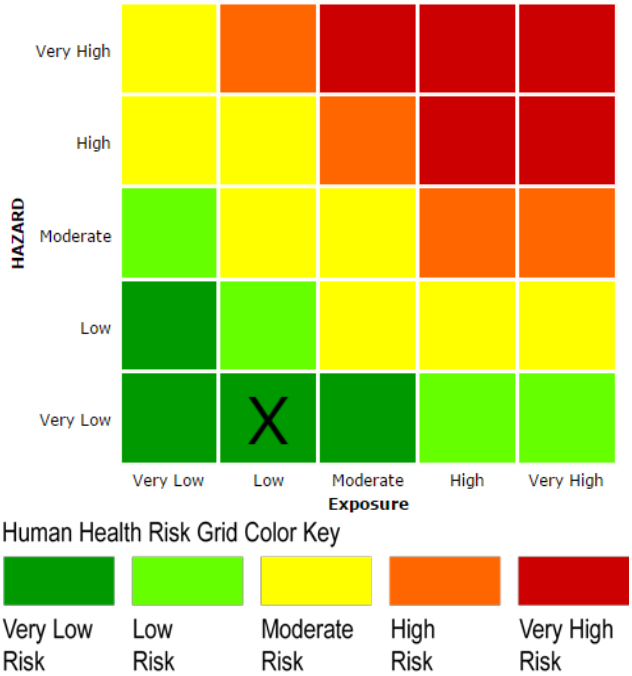
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



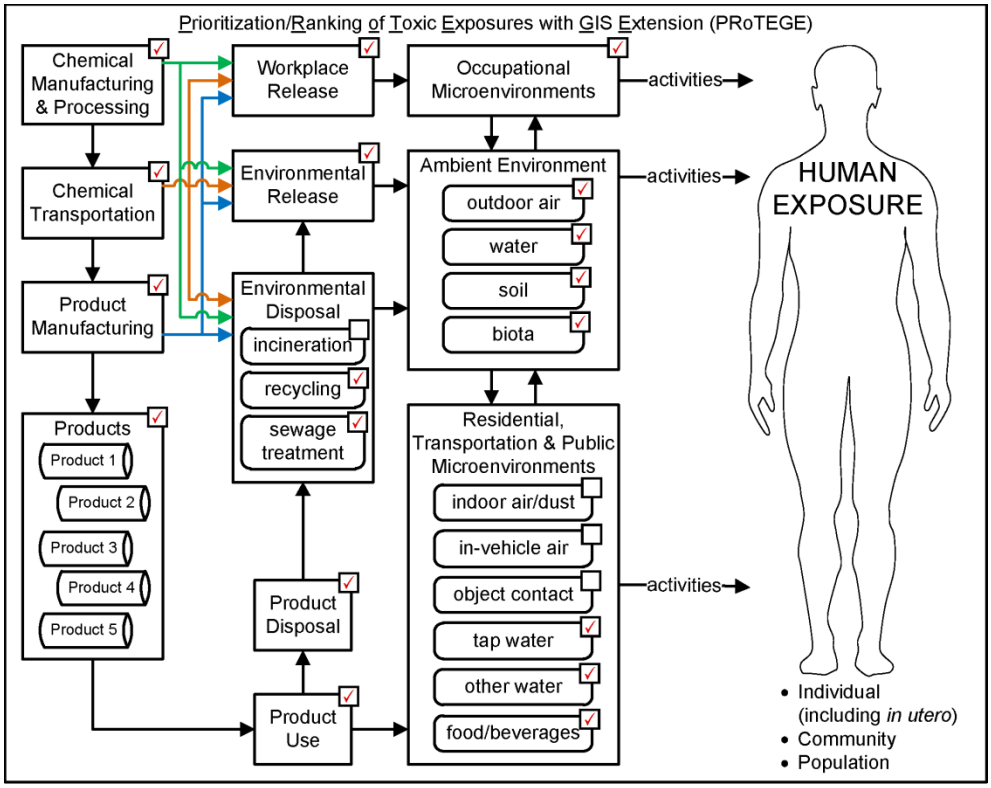
(a) Human Hazard
Estimated ranking of human hazard risk from Malathion, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Malathion (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Malathion, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Manganese



Summary Physico-Chemical Information	
Name	Manganese
Other Names	
Chemical Formula	Mn
Chemical Class	Mt/MU
Identifier	CAS: 7439-96-5
Chemical Forms	
Physical Properties	
MW: 54.9 BP: 3564°F MLT: 2271°F Sol: Insoluble VP: 0 mmHg (approx) Sp.Gr: 7.20 (metal)	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD (mg/kg/day): 0.14 (IRIS)
Toxicological Effects:
Exposure Limits: NIOSH REL: TWA 1 mg/m³ ST 3 mg/m³, OSHA PEL: C 5 mg/m³
Chemical Use: Steel production, dry cell batteries, plant fertilizers, animal feed, brick colorant
Exposure Routes: inhalation, ingestion (NIOSH)
Target Organs: respiratory system, central nervous system, blood, kidneys

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	0.005	0.0211	0.128	Data sources: Outdoor air '08 annual means @ AQS monitors, Manganese (TSP) STP; Food (5th, 50th, and 95th %iles) - TDS 94-02; Tap water - [51] (5, 50, 95%tiles); Surface water data - STORET.	Air	1546.53 (NEI 2005) 1835.87 (TRI 2008)	99.94% (NEI 2005) 5.02% (TRI 2008)
Food (ppb)	12.7	141	546				
Indoor Air					Surface Water	58.55 (TRI 2008)	5.02% (TRI 2008)
Tap water(mg/L)	<LOD	<LOD	0.24		Ground Water	0.01 (TRI 2008)	0.06% (TRI 2008)
Surface water (µg/L)	0.001	37	18604000.0		Soil	5055.30 (TRI 2008)	2.29% (TRI 2008)
Soil							
Dust					Chemical Production and Use		
Surfaces					Production	500 million to < 1 billion lbs/yr	Data Sources: IUR
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

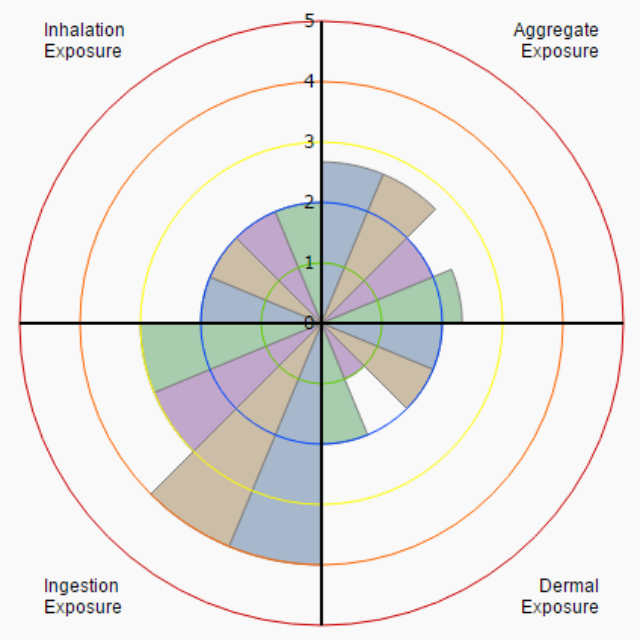
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		●
	ECD		□
	SRD		
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		●
PK/PBPK Model (or Data)	ScLit		PBPKm (R) [52]
	BME		
	ERDEM		

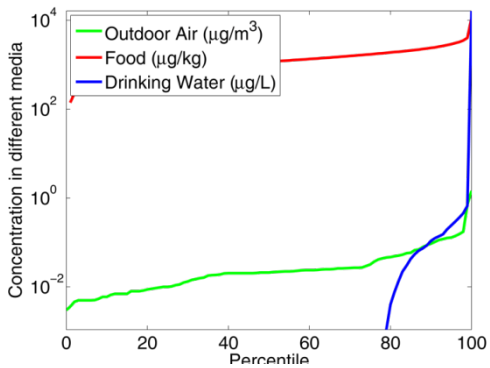
"Tier 1" Exposure Ranking for Manganese

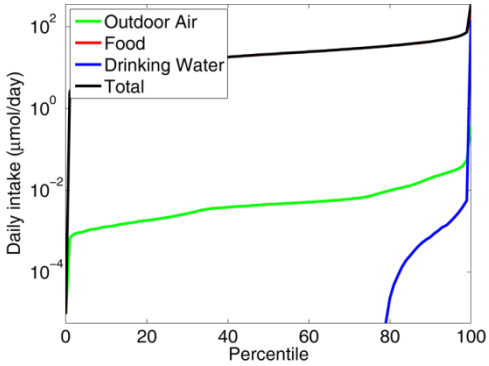
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	2	2	2	2
Ingestion	4	4	3	3
Dermal	2	2	1	2
Aggregate	2.66	2.66	2	2.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Manganese





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.00451	21.2	NA	21.2
90 % tile	0.02	43.6	NA	44.2
% over 0.1 μmol/day	0.869		NA	99.9
% over 1 μmol/day	0		NA	99.2

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

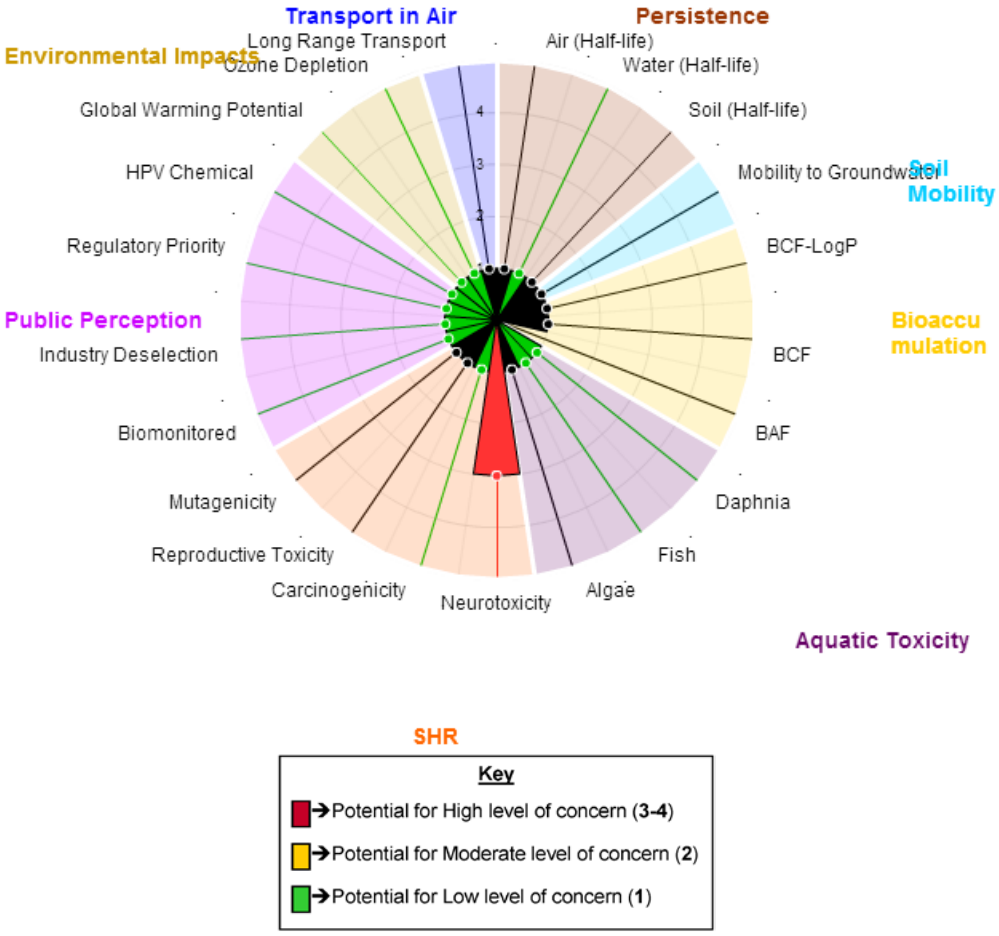
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Manganese

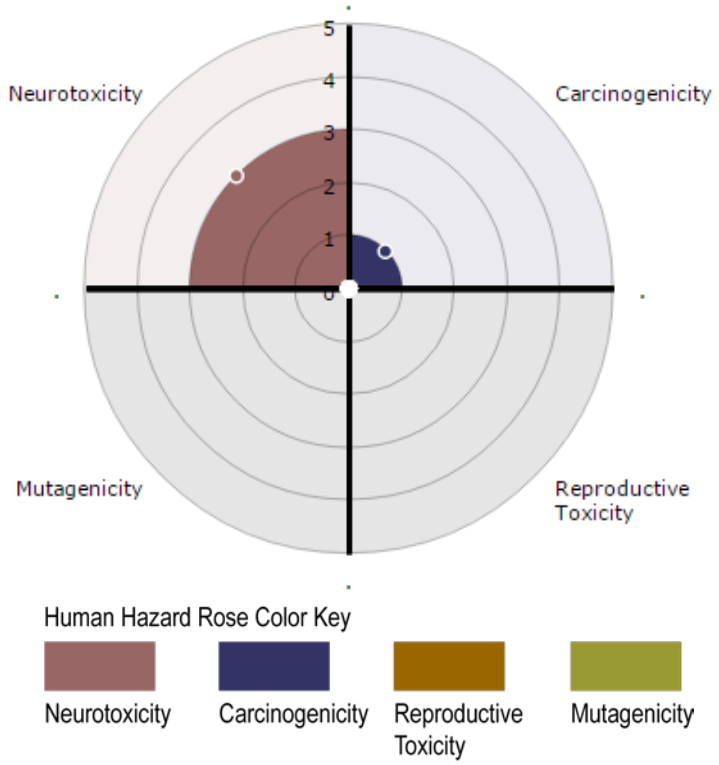
		CAS # 7439-96-5
Persistence	Air (Half-life)	Persistence in Air has not been calculated for this compound
	Water (Half-life)	Persistence in Water has not been calculated for this compound.
	Soil (Half-life)	Persistence in Soil has not been calculated for this compound.
Soil Mobility	Mobility to Groundwater	Soil mobility has not been calculated for this compound
Bioaccumulation	BCF-LogP	BCF value based on LogP has not been calculated for this compound
	BCF	BCF value has not been calculated for this compound
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 1780.628 mg/L indicates a Low toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 1877.903 mg/L indicates a Low toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	D (Not classifiable as to human carcinogenicity) [1986 Guidelines] [IRIS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	0 out of 6 lists
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Long Range Transport in Air has not been calculated for this compound



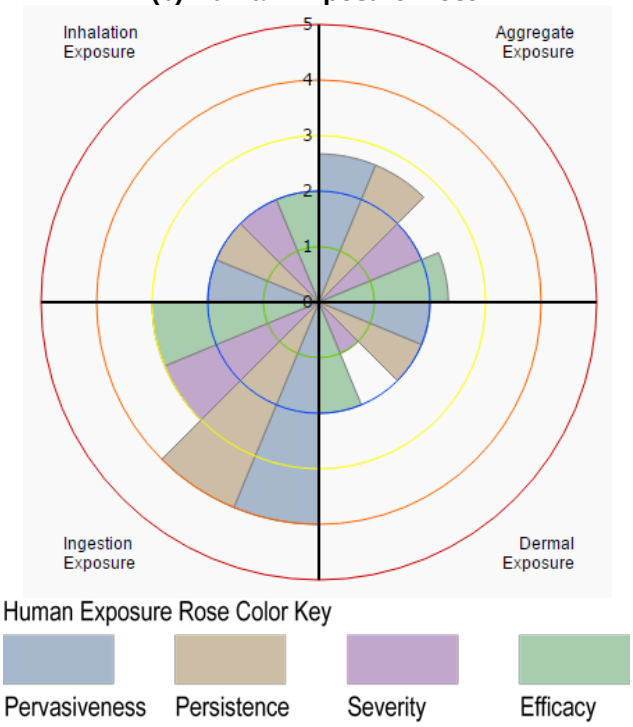
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Manganese

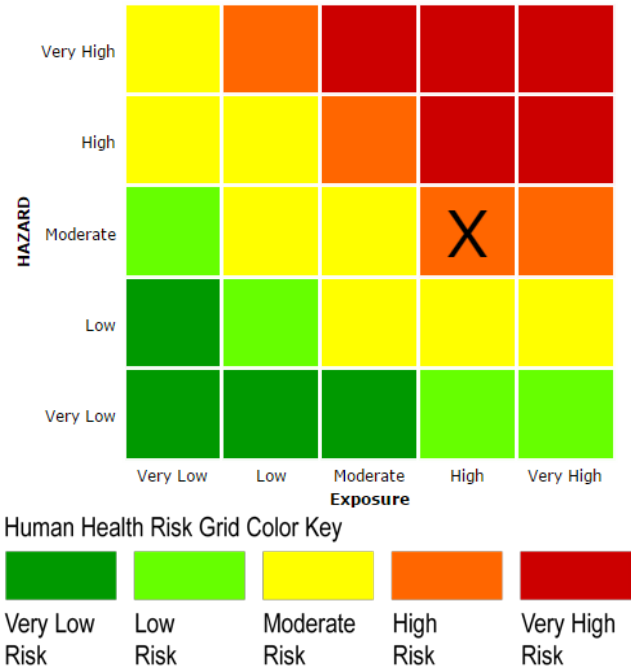
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



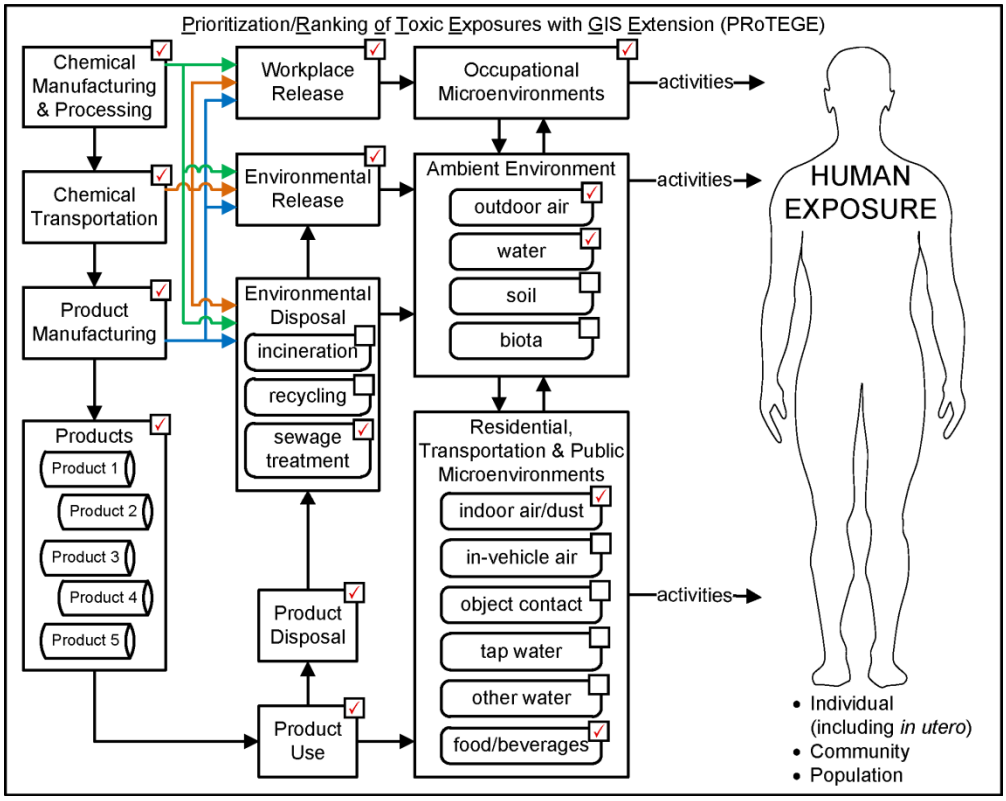
(a) Human Hazard
Estimated ranking of human hazard risk from Manganese, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Manganese (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Manganese, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Methoxychlor



Summary Physico-Chemical Information	
Name	Methoxychlor
Other Names	p,p'-Dimethoxydiphenyltrichloroethane; DMDT; Methoxy-DDT; 2,2-bis(p-Methoxyphenyl)-1,1,1-trichloroethane; 1,1,1-Trichloro-2,2-bis-(p-methoxyphenyl)ethane
Chemical Formula	$(C_6H_4OCH_3)_2CHCCl_3$
Chemical Class	OCP
Identifier	CAS 72-43-5
Chemical Forms	
Physical Properties	
MW: 345.7 BP: Decomposes MLT: 171°F Sol: 0.00001% VP: Very low	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD 0.005 mg/kg/day (IRIS)
Toxicological Effects: Not classifiable as to human carcinogenicity (IRIS)
Exposure Limits: OSHA PEL: TWA 15 mg/m³
Chemical Use: insecticide
Exposure Routes: inhalation, ingestion
Target Organs: central nervous system, liver, kidneys

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ng/m³)		0.25		Data sources: Outdoor air '08 annual mean @ one AQS monitor; Food (5th, 50th, and 95th %iles) - TDS 91-03; Tap water - [23] (>99% of measurements <RL)	Air	0.0018	0.16
Ground water							
Food (ppb)	0.2	0.4	1.69		Surface Water	NA	NA
Indoor Air					Ground Water	NA	NA
Surface water					Soil	0.93	0.06
Tap water (µg/L)	<RL	<RL	0.020 (99.9% tile)				
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

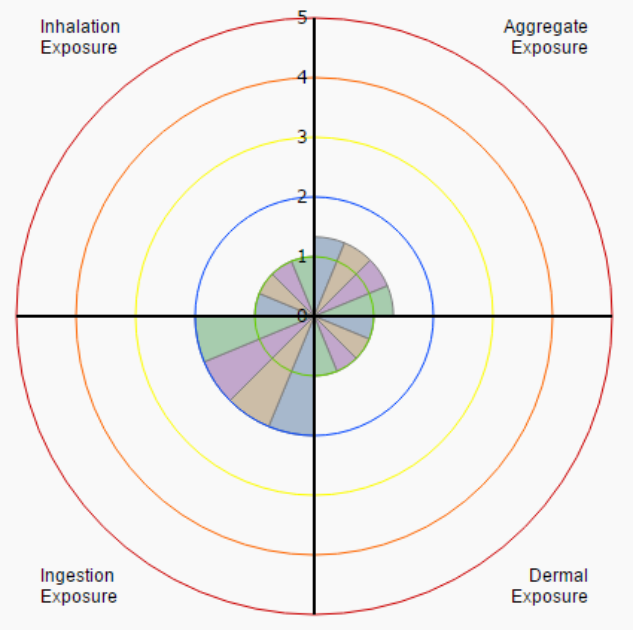
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		
	IARC		
	PSAP		
	NTP		●
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		●
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		
	BME		
	ERDEM		

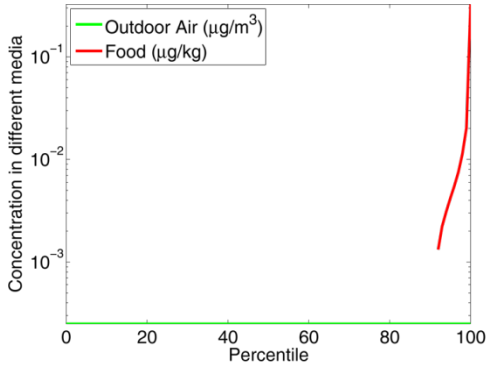
"Tier 1" Exposure Ranking for Methoxychlor

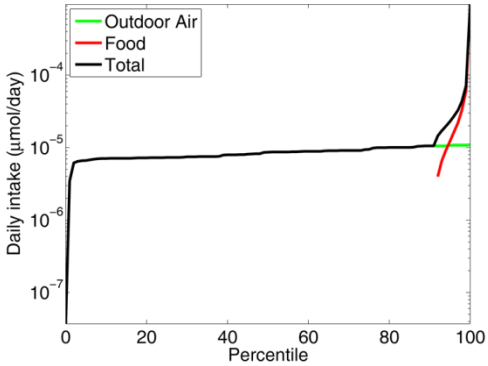
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	1
Aggregate	1.33	1.33	1.33	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Methoxychlor





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	8.63E-06	0	NA	8.63E-06
90 % tile	1.06E-05	0	NA	1.06E-05
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

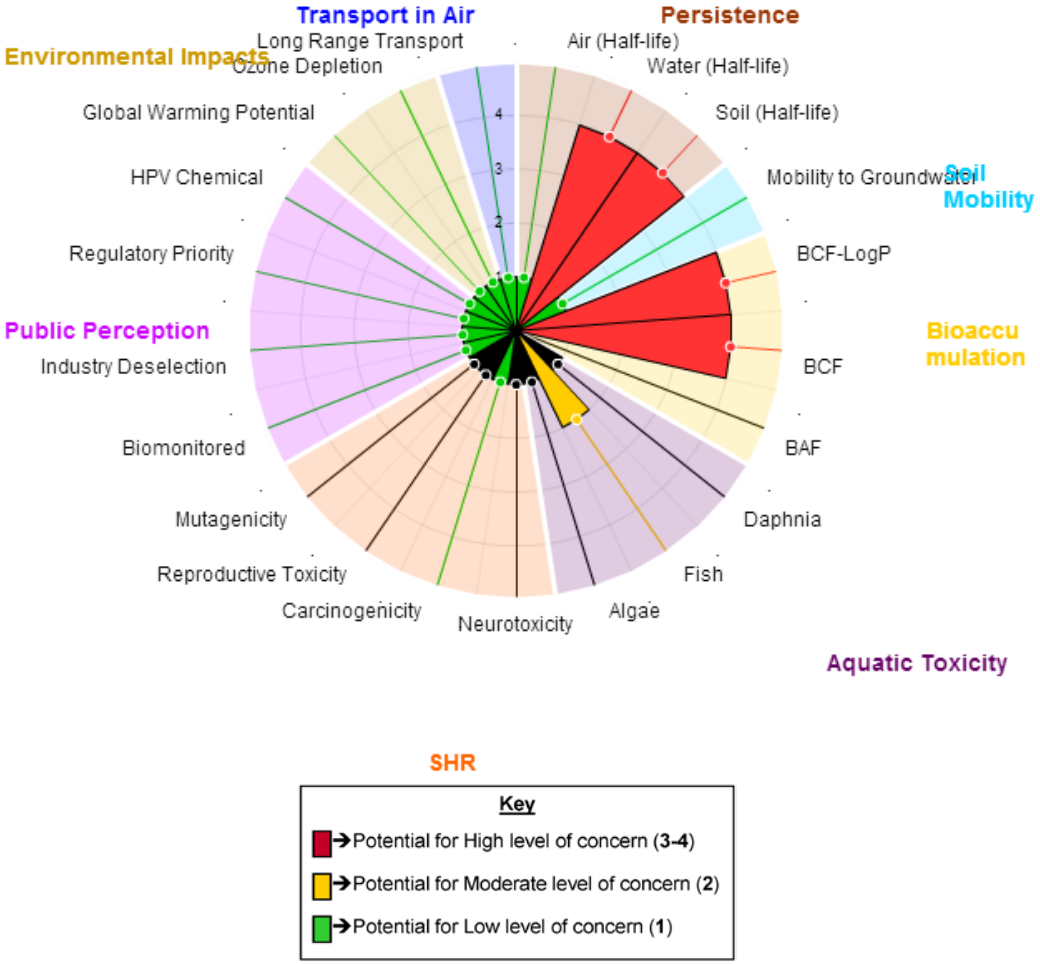
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Methoxychlor

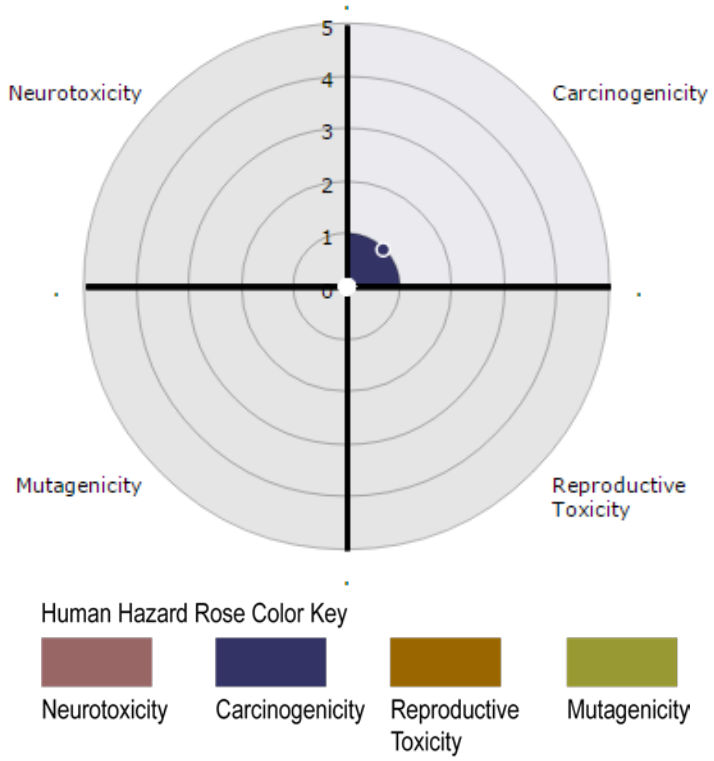
		CAS # 72-43-5
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.1997 days)
	Water (Half-life)	Very High persistence in Water (Estimated Half-life = 180 days)
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Low mobility to groundwater based on LogKoc = 4.629
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=5.08
	BCF	Very High bioconcentration potential based on Experimental LogBCF = 3.91
	BAF	
Aquatic Toxicity	Daphnia	No toxicity estimate.
	Fish	An estimated LC50(96-hr) = 0.156 mg/L indicates a Moderate toxicity to Fish [CLOGP].
	Algae	No toxicity estimate.
SHR	Neurotoxicity	
	Carcinogenicity	CLASS A4 - Not Classifiable as a Human Carcinogen [ACGIH]; Not classifiable [IARC_OE]; D (Not classifiable as to human carcinogenicity) [1986 Guidelines] [IRIS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	0 out of 6 lists
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 85.555 km - A_TRNSPRT)



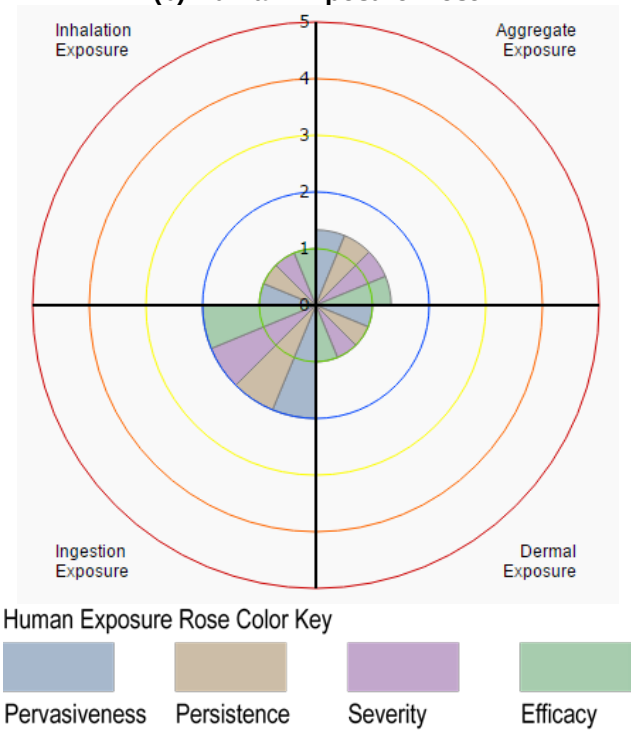
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Methoxychlor

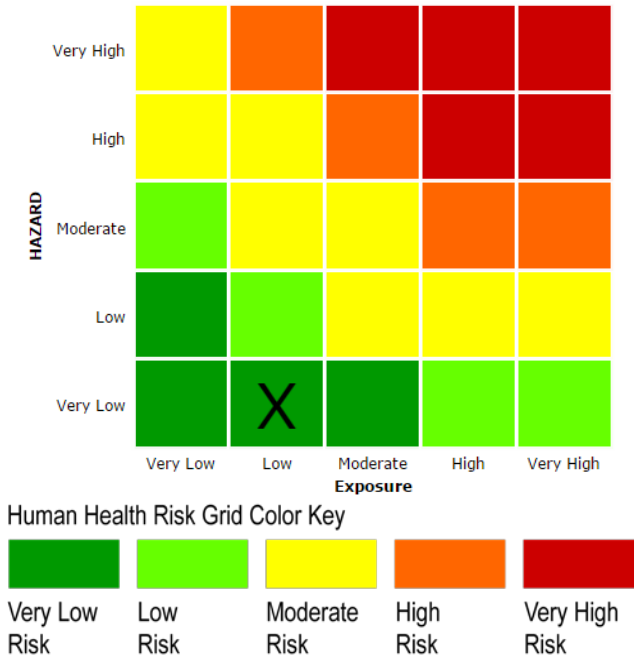
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



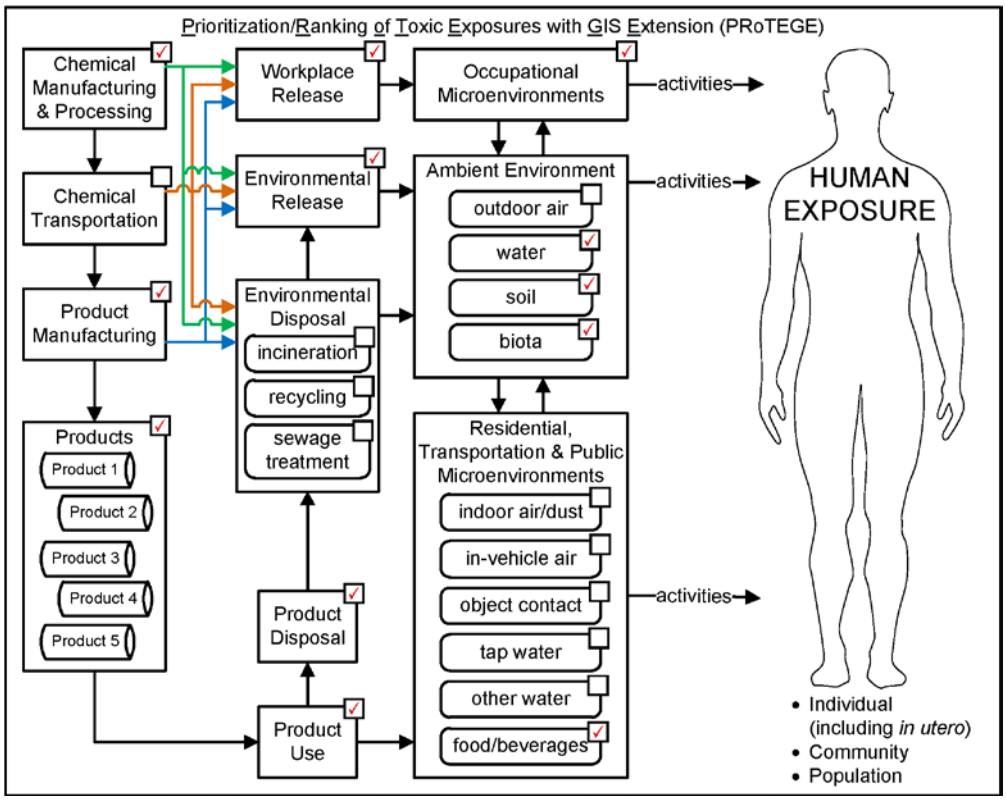
(a) Human Hazard
Estimated ranking of human hazard risk from Methoxychlor, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Methoxychlor (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Methoxychlor, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Methyl Mercury



Summary Physico-Chemical Information	
Name	Methyl Mercury
Other Names	
Chemical Formula	CH_3Hg
Chemical Class	OMt
Identifier	CAS 22967-92-6
Chemical Forms	compound, mixture
Physical Properties	
MW: 215.63 React with free S-H groups of biologically important molecules	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: fetotoxic in mice (single dose of 2.5-7.5 mg/kg)
Toxicological Effects: Carcinogenicity
Exposure Limits: 0.0107 mg/m³
Chemical Use: No industrial uses; formed from methylation of Hg in environment
Exposure Routes: General population may be exposed to methylmercury via ingestion of food, especially fish, and contaminated drinking water
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)				Data sources: Food – TDS 91-03 (5, 50, 95%tile); Surface water and biota (Canada, trees) - HSDB.	Air	0.001	0.03% (NEI)
Ground water (ppb)							
Food (µg/kg)	<LOD	<LOD	3.13		Surface Water		
Indoor Air (units)					Ground Water		
Surface water (ng/L)	0.05-0.3	1-3	10		Soil		
Tap water (units)							
Soil (units)					Chemical Production and Use		
Dust (units)					Production		
Surfaces (units)							
Biota (µg/kg)	0.13	6.13	38.65				
Human Biomarkers							
Urine (µg/L)							
Blood							
Other							

Concentrations of mercury in food were all assumed to be methyl mercury.

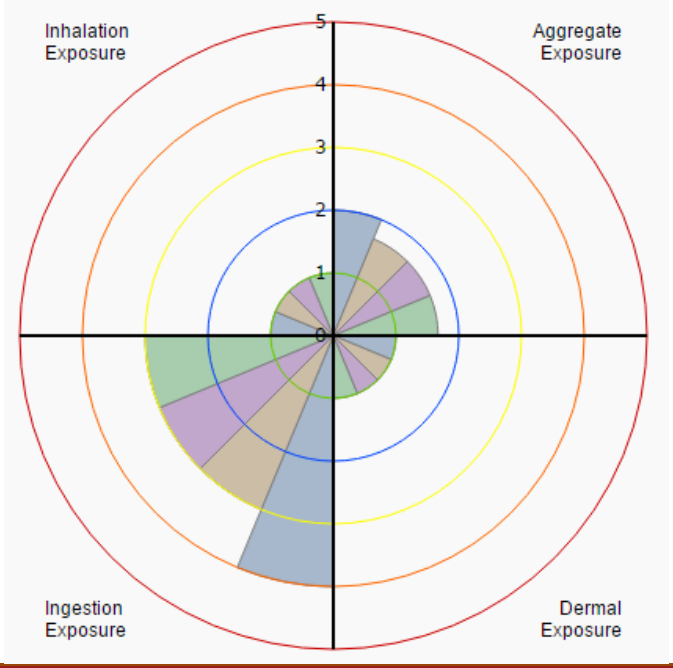
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		
	ICSC		
	Tox Profs		□
	IRIS		●
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		●
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		
	IUR		
	ECD		
	SRD		
Releases	TRI		
	NEI		●
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		●
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	(b)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [53]
	BME		
	ERDEM		

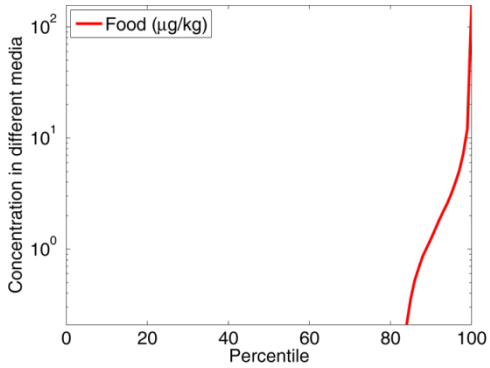
"Tier 1" Exposure Ranking for Methyl Mercury

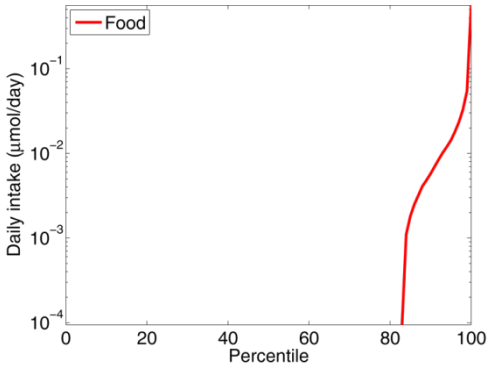
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	4	3	3	2
Dermal	1	1	1	1
Aggregate	2	1.66	1.66	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Methyl Mercury





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0	0.00569	NA	0.00615
% over 0.1 µmol/day	0	0.915	NA	1.79
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

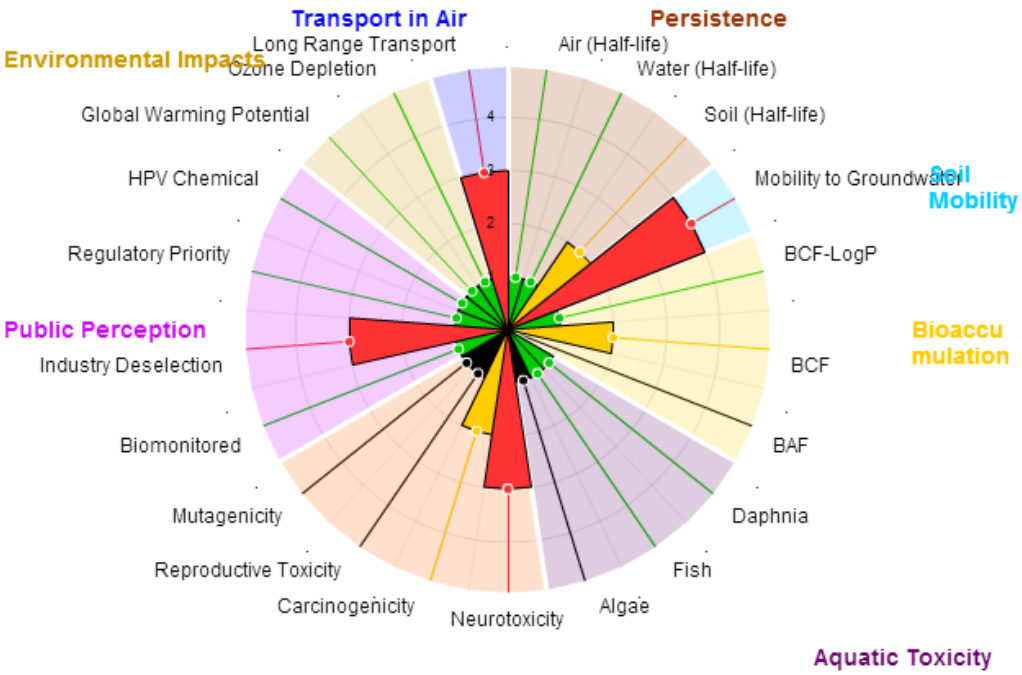
Resources for "Tier 3" Exposure Characterization

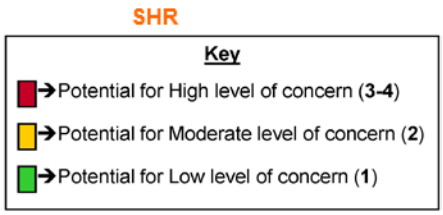
"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Methyl Mercury

		CAS # 22967-92-6
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 1.311 days)
	Water (Half-life)	Low persistence in Water (Estimated Half-life = 37.5 days)
	Soil (Half-life)	Moderate persistence in Soil (Estimated Half-life = 75 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 1.121
Bioaccumulation	BCF-LogP	Low bioconcentration potential based on an Estimated LogP=0.08
	BCF	Moderate bioconcentration potential based on Estimated LogBCF = 2
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 9569.723 mg/L indicates a Low toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 10197.632 mg/L indicates a Low toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	C (Possible human carcinogen) [1986 Guidelines] [IRIS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (GADSL)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 447.483 km - A_TRNSPRT)

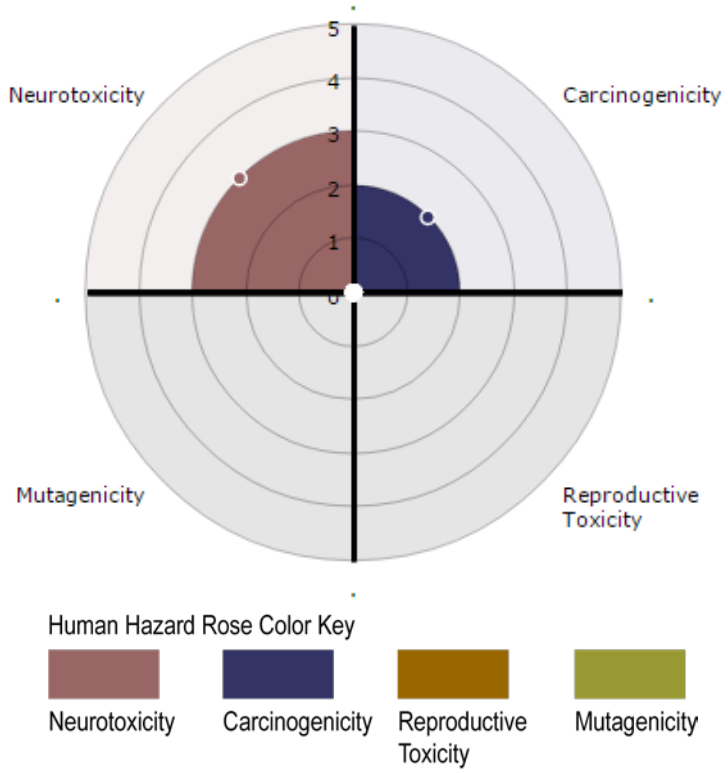




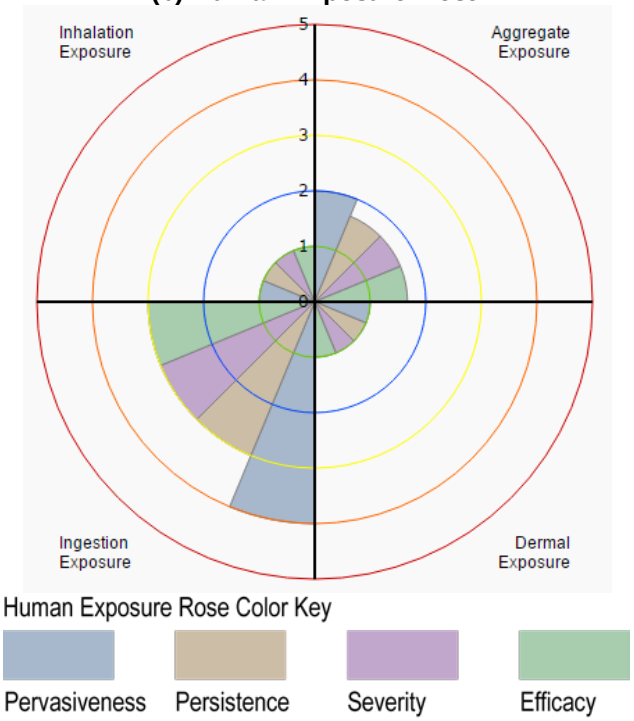
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Methyl Mercury

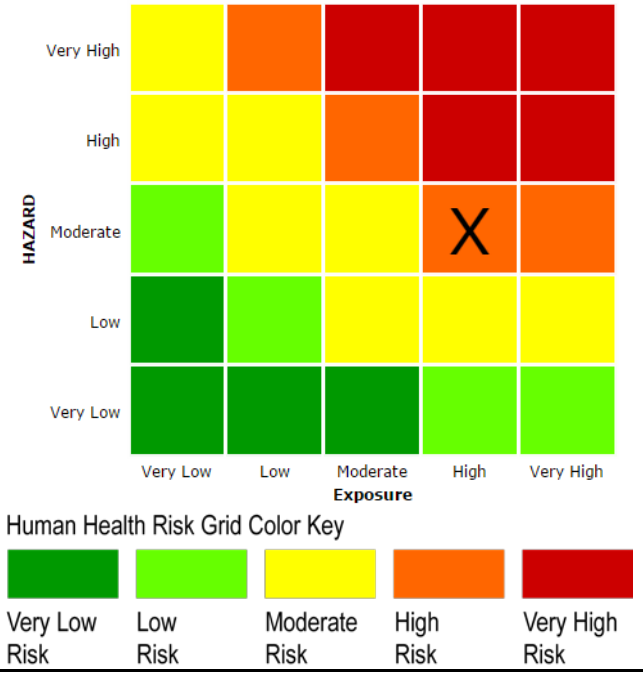
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



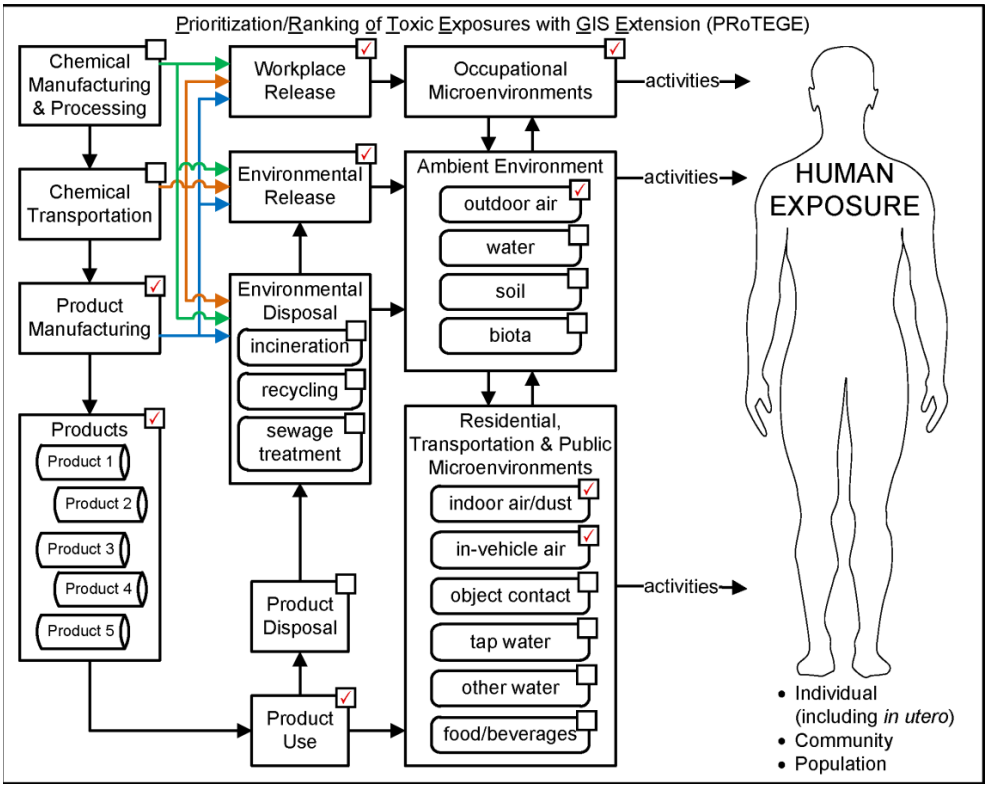
(a) Human Hazard
Estimated ranking of human hazard risk from Methyl Mercury, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Methyl Mercury (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Methyl Mercury, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Ranking for n-Hexane



Summary Physico-Chemical Information	
Name	n-Hexane
Other Names	Hexane, Hexyl hydride, normal-Hexane
Chemical Formula	$CH_3[CH_2]_4CH_3$
Chemical Class	VOC
Identifier	CAS 110-54-3
Chemical Forms	
Physical Properties	
MW: 86.2 BP: 156°F MLT: -219°F Sol: 0.002% VP: 124 mmHg Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F. Colorless liquid with a gasoline-like odor.	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD: NA (IRIS); RfC: 0.7 mg/kg/day (IRIS)
Toxicological Effects: Carcinogenic classification: NA (IRIS)
Exposure Limits: NIOSH REL: TWA 50 ppm (180 mg/m^3); OSHA PEL: TWA 500 ppm (1800 mg/m^3)
Chemical Use: Pure or commercial grade solvent; raw material in the synthesis of polyolefins, elastomers and pharmaceuticals; formulation of glues, stains, varnishes and other industrial chemicals
Exposure Routes: Inhalation, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, respiratory system, central nervous system, peripheral nervous system

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ppb)	0.040	0.185	0.901	Data sources: Outdoor air (5th, 50th, and 95th %iles) - '08 annual means @ AQS monitors; Surface water – HSDB; Indoor air - [87] (5, 50, 95%tiles)	Air	161376.58	99.94%
Ground water							
Food					Surface Water	4.12	2.64%
Indoor Air (µg/m^3)	0.78	2.18	6.06		Ground Water	0.76	0.16%
Surface water (ng/L)	1.5		7.8		Soil	14.43	1.24%
Tap water							
Soil					Chemical Production and Use		
Dust					Production	500 million to < 1 billion Lbs/yr	Data Source: IUR 2006
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

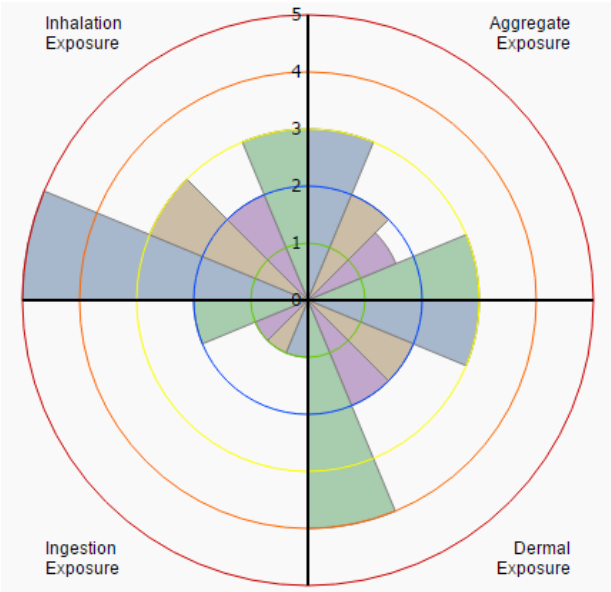
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		●
	ECD		□
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		
	AQS		●
	CERCLIS		
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	(▯)
		09-10	(b)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [88]
	BME		● [48]
	ERDEM		

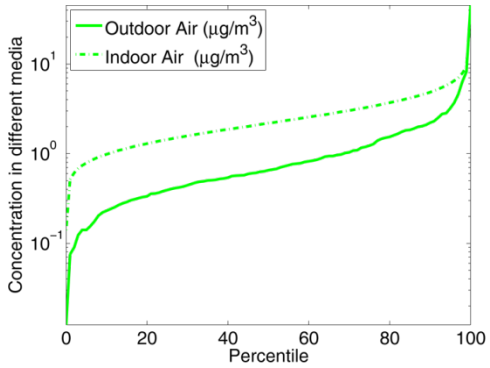
"Tier 1" Exposure Ranking for n-Hexane

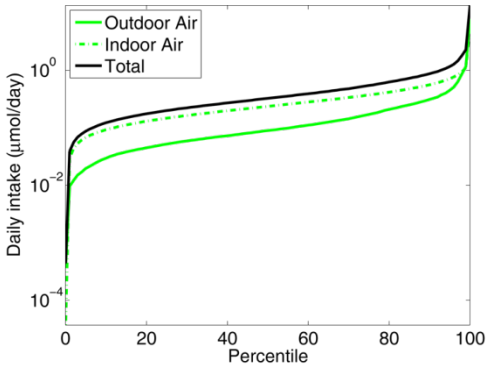
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	5	3	2	3
Ingestion	1	1	1	2
Dermal	3	2	2	4
Aggregate	3	2	1.66	3

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for n-Hexane





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0.368	0	NA	0.368
90 % tile	0.799	0	NA	0.811
% over 0.1 µmol/day	98.1	0	NA	97.5
% over 1 µmol/day	5.34	0	NA	5.81

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

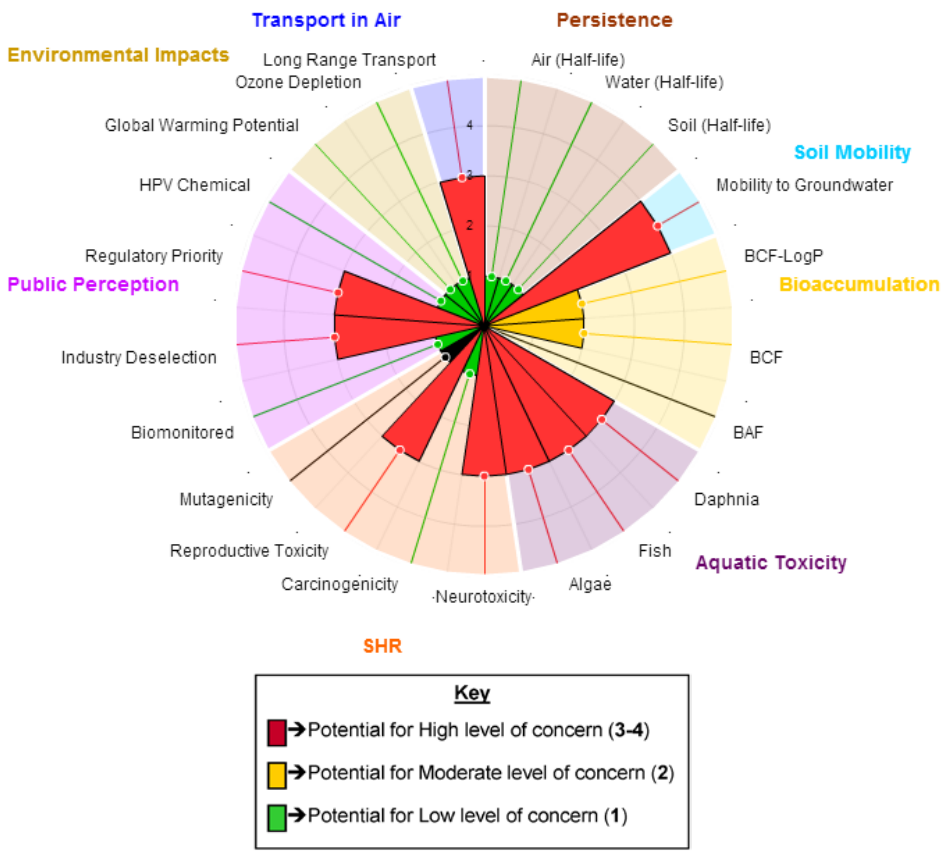
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for n-Hexane

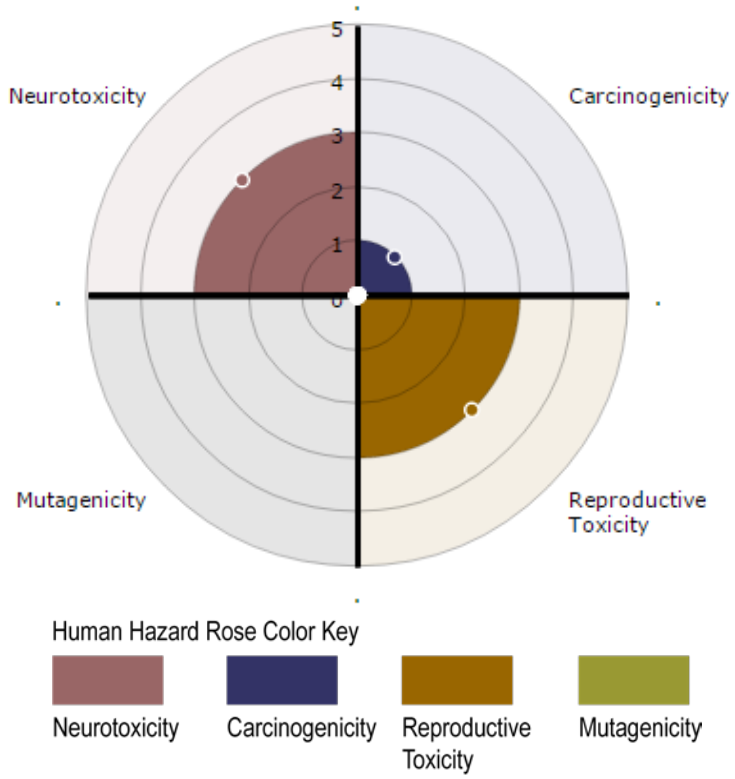
		CAS # 110-54-3
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 1.96 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 100% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is not persistent in water (Min. BOD = 99%, Max. BOD = 103%).
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 17.34 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 2.173
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=3.9
	BCF	Moderate bioconcentration potential based on Estimated LogBCF = 2.303
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 4.587 mg/L indicates a Moderate toxicity to Daphnid. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 3.916 mg/L indicates a Moderate toxicity to Fish. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin [Grandjean et al]
	Carcinogenicity	Inadequate information to assess carcinogenic potential [2005 Guidelines] [IRIS]; [ACGIH]; [EU_GHS]
	Reproductive Toxicity	TOXIC TO REPRODUCTION - Hazard category 2 [EU_GHS]
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	2 out of 6 lists (EUC2; SINLIST)
	Regulatory Priority	2 out of 10 lists (EU_RRAP; JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 587.52 km - A_TRNSPRT)



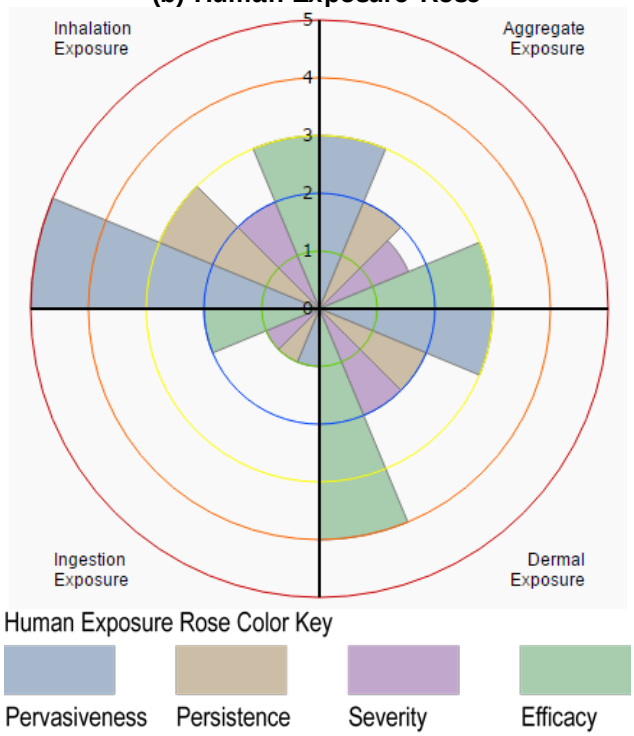
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for n-Hexane

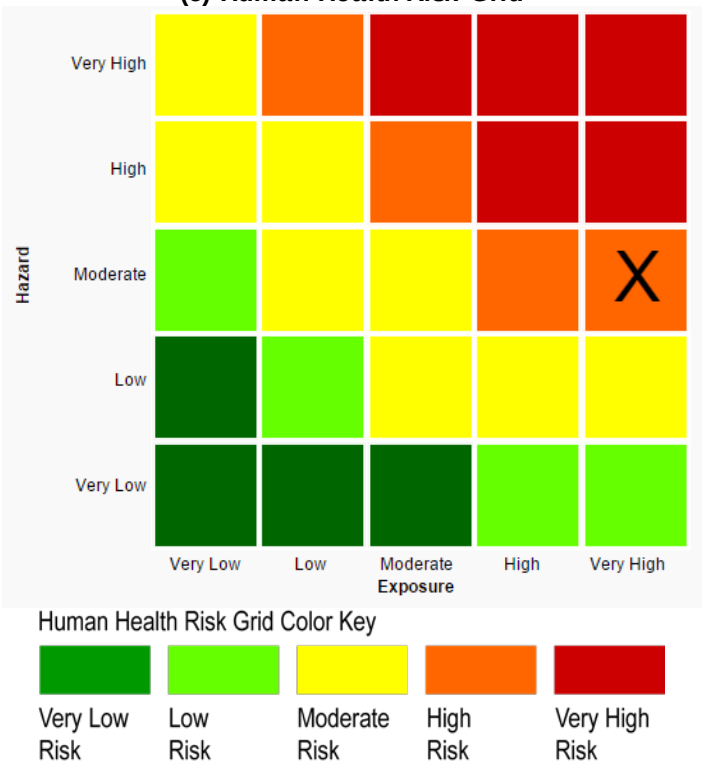
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



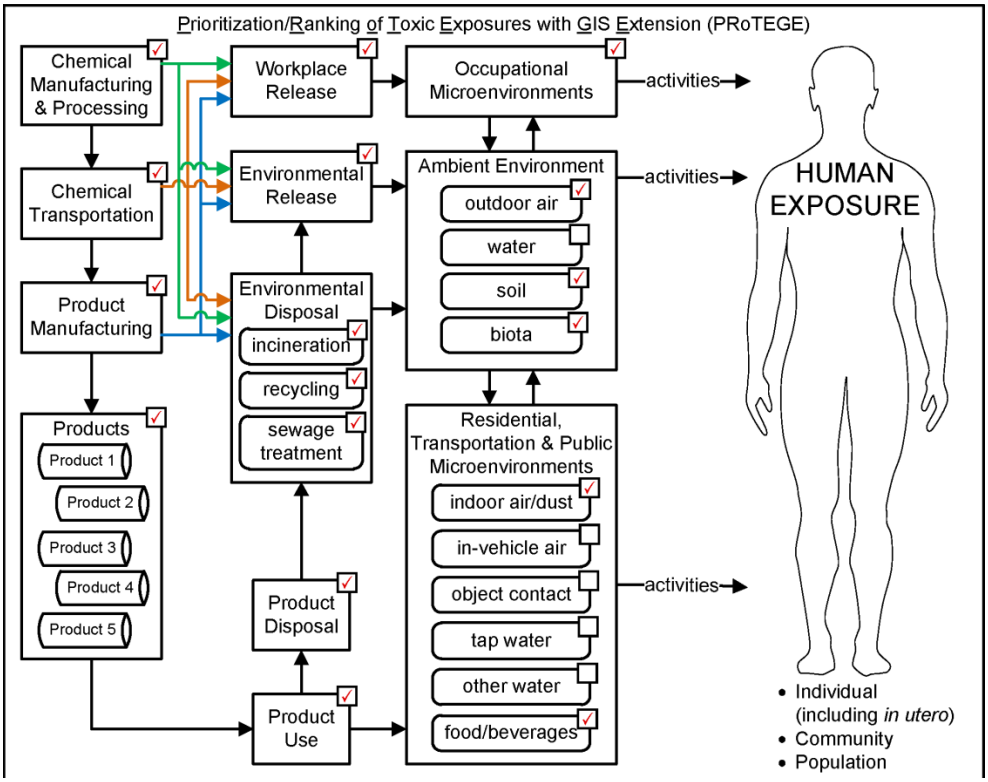
(a) Human Hazard
Estimated ranking of human hazard risk from n-Hexane, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of n-Hexane (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from n-Hexane, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for octaBDE



Summary Physico-Chemical Information	
Name	octaBDE
Other Names	Octabromodiphenyl ether
Chemical Formula	$C_{12}H_2Br_8O$
Chemical Class	PBDEs
Identifier	CAS 32536-52-0
Chemical Forms	mixture of BDE 183, 197, and 207
Physical Properties	
MW: 801.31 SpGr: 2.76	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD 0.003 mg/kg/day
Toxicological Effects: not classifiable as to its carcinogenicity to humans (IRIS)
Exposure Limits:
Chemical Use: flame retardant
Exposure Routes: ingestion (primarily seafood)
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (pg/m³)	<LOD	0.438	2.28	Data source: Surface water and soil (sediment) – HSDB; Food - [39] (5, 50, 95%tiles); Outdoor air - [37] (5, 50, 95%tiles)	Air		
Ground water							
Food (ng/kg)	<LOD	<LOD	0.29		Surface Water		
Indoor Air					Ground Water		
Surface water (µg/L)			<LOD		Soil		
Tap water							
Soil (µg/kg)	8		21		Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

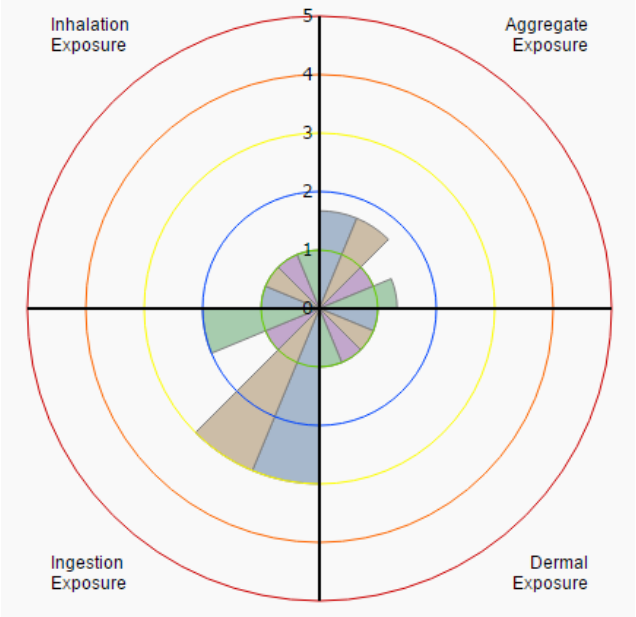
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		●
	PFD		
	MSDS		
	DSSTox		●
	TMI		
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		
	ECD		●
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		
	BME		
	ERDEM		

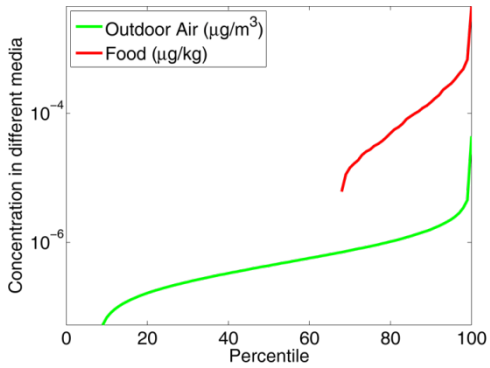
"Tier 1" Exposure Ranking for octaBDE

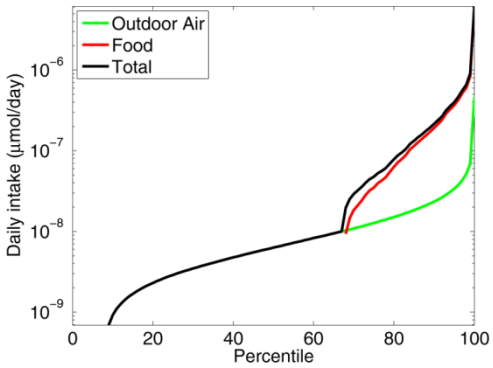
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	3	3	1	2
Dermal	1	1	1	1
Aggregate	1.66	1.66	1	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for octaBDE





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	6.27E-09	0	NA	6.27E-09
90 % tile	2.36E-08	1.87E-07	NA	2.21E-07
% over 0.1 μmol/day	0	0	NA	0
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

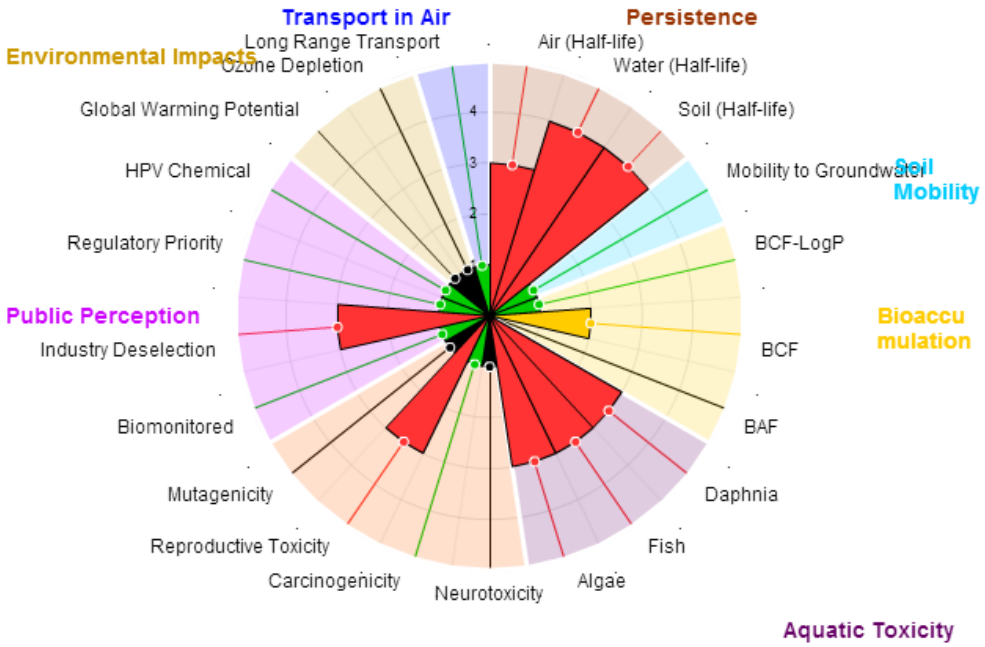
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for octaBDE

		CAS # 32536-52-0
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 140.4 days)
	Water (Half-life)	Very High persistence in Water (Estimated Half-life = 180 days)
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Low mobility to groundwater based on LogKoc = 4.996
Bioaccumulation	BCF-LogP	Low bioconcentration potential based on an Estimated LogP=10.33
	BCF	Moderate bioconcentration potential based on Estimated LogBCF = 2.492
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) >0.011 mg/L indicates a High toxicity to Daphnia.
	Fish	A measured LC50 (96-hr) >0.012 mg/L indicates a High toxicity to Fish.
	Algae	A measured EC50 (72-hr) >0.012 mg/L indicates a High toxicity to Algae.
SHR	Neurotoxicity	
	Carcinogenicity	D (Not classifiable as to human carcinogenicity) [1986 Guidelines] [IRIS]; [EU_GHS]
	Reproductive Toxicity	Toxic to reproduction - Category 1B/2A [EU_RA17_5]; TOXIC TO REPRODUCTION - Hazard category 1B [EU_GHS]
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	3 out of 6 lists (GADSL; EUC2; SINLIST)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 358.565 km - A_TRNSPRT)



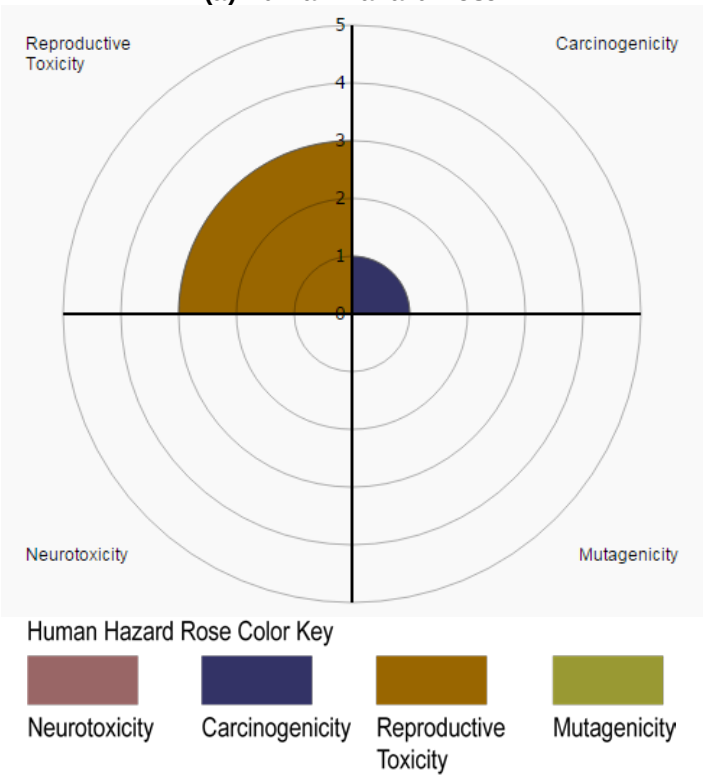
Key

- → Potential for High level of concern (**3-4**)
- → Potential for Moderate level of concern (**2**)
- → Potential for Low level of concern (**1**)

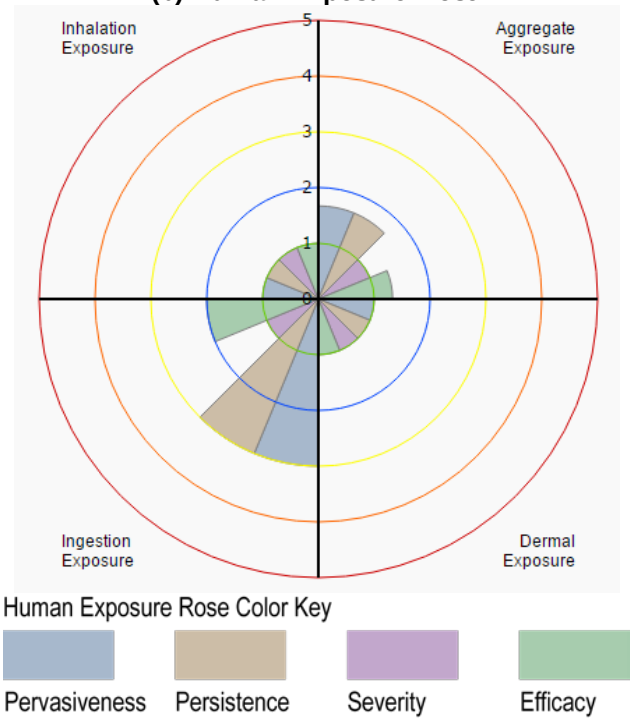
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for octaBDE

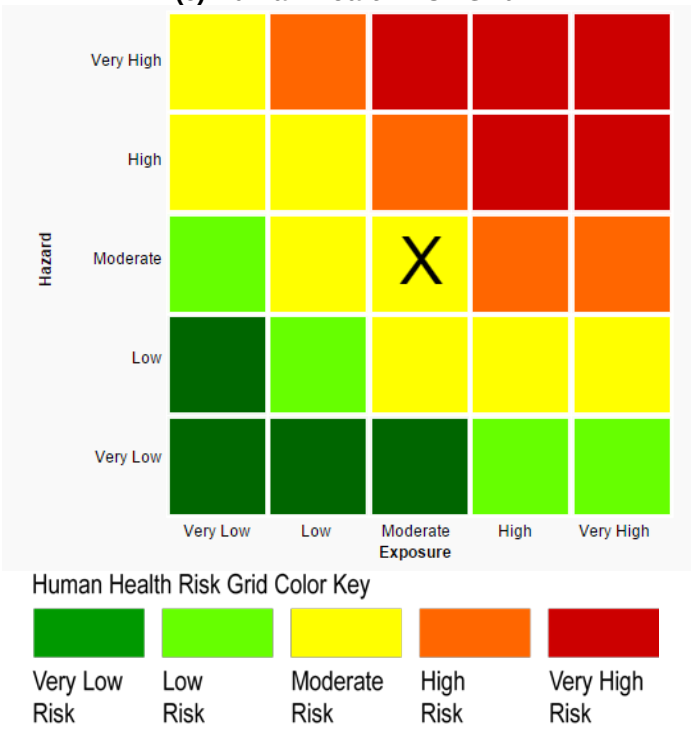
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



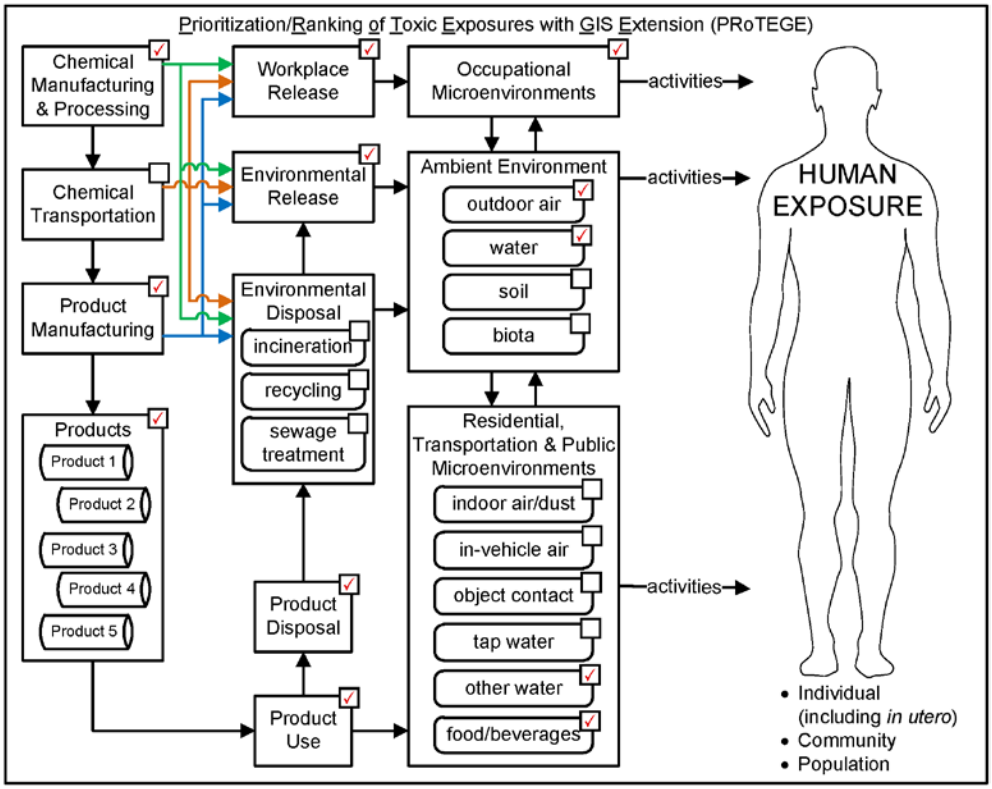
(a) Human Hazard
Estimated ranking of human hazard risk from octaBDE, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of octaBDE (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from octaBDE, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Parathion



Summary Physico-Chemical Information	
Name	Parathion
Other Names	O,O-Diethyl-O(p-nitrophenyl) phosphorothioate; Diethyl parathion; Ethyl parathion; Parathion-ethyl
Chemical Formula	$(C_2H_5O)_2P(S)OC_6H_4NO_2$
Chemical Class	OPP
Identifier	CAS 56-38-2
Chemical Forms	
Physical Properties	
MW:291.3 Sol: 0.001% VP: 0.00004 mmHg	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits:
Toxicological Effects: Carcinogenicity
Exposure Limits: NIOSH REL, TWA 0.05 mg/m³ [skin] ; OSHA PEL, TWA 0.1 mg/m³ [skin]
Chemical Use: Pesticide, insecticide
Exposure Routes: Inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, respiratory system, central nervous system, cardiovascular system, blood cholinesterase

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (pg/m³)	26		13000	Data sources: Outdoor air (rural and remote area) from HSDB, the values are reported minimum and maximum; Food (5th, 50th, and 95th %iles) - TDS 94-02; Tap water, Surface water (Spain) and Ground water - HSDB.	Air		
Ground water (µg/L)	4		6				
Food (ppb)	1	1.5	2		Surface Water		
Indoor Air					Ground Water		
Surface water (mg/L)	0.012		0.176		Soil		
Tap water			<LOD				
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine (µg/L)							
Blood							
Other							

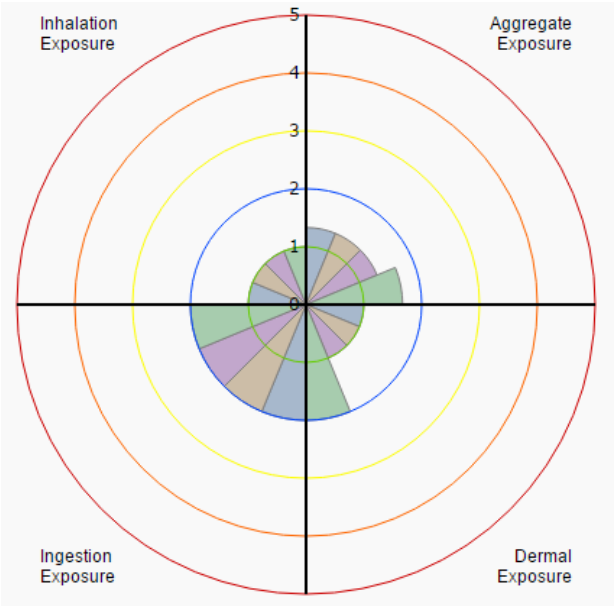
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		
	IARC		
	PSAP		
	NTP		●
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		
	IUR		
	ECD		□
	SRD		
Releases	TRI		●
	NEI		
Environmental Quality	NGA		
	NAWQA		●
	AQS		○
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	(p)
		09-10	(▯)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (H) [54]
	BME		
	ERDEM		●

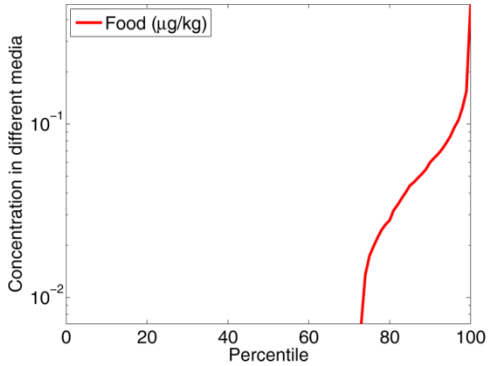
"Tier 1" Exposure Ranking for Parathion

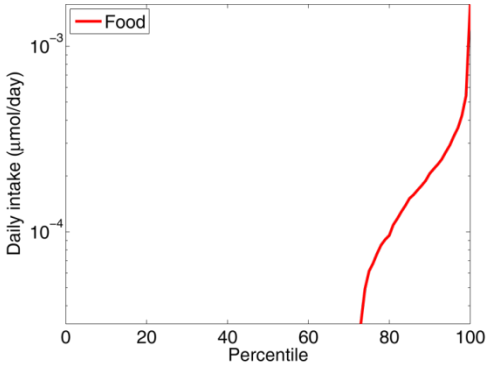
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Parathion





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0	0.000204	NA	0.00021
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

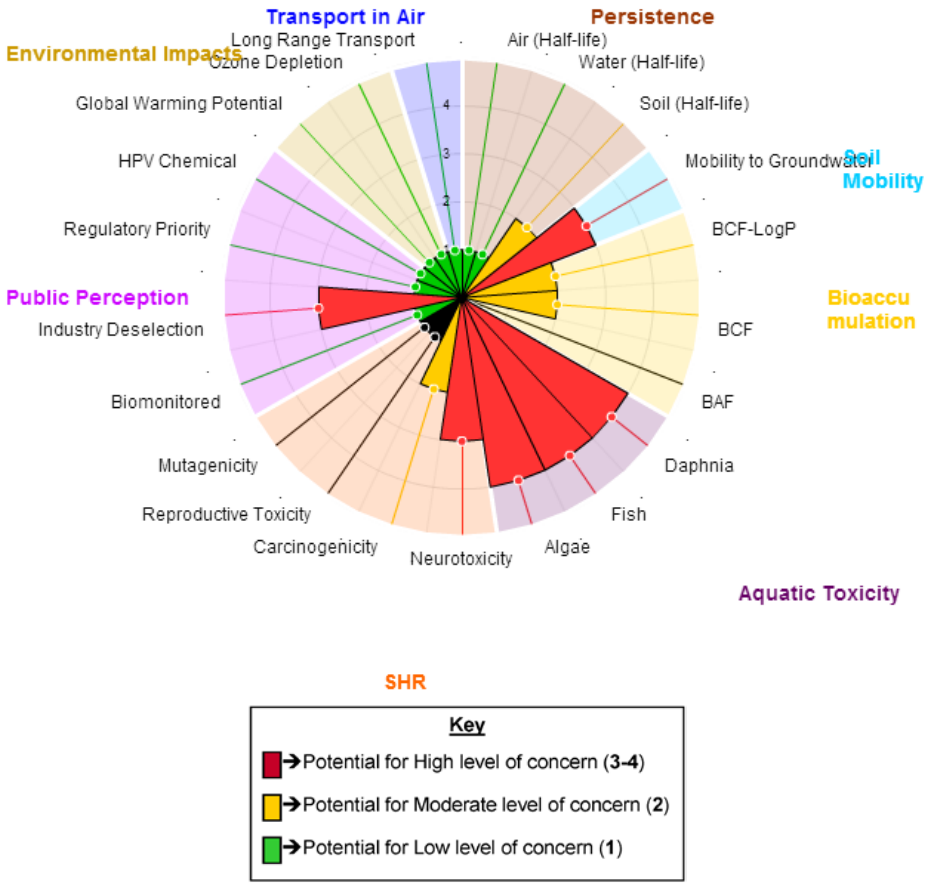
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Parathion

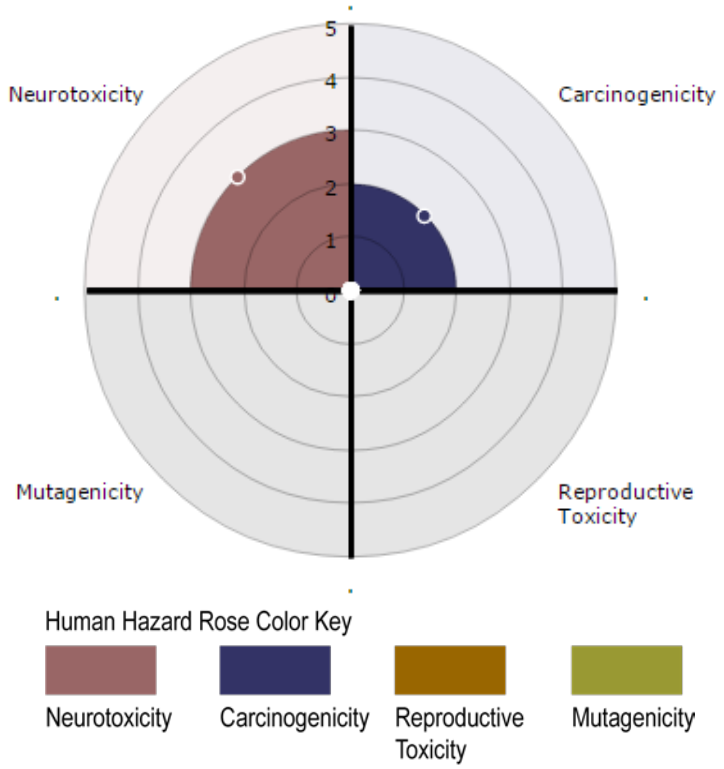
		CAS # 56-38-2
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.1162 days)
	Water (Half-life)	Low persistence in Water (Estimated Half-life = 37.5 days)
	Soil (Half-life)	Moderate persistence in Soil (Estimated Half-life = 75 days)
Soil Mobility	Mobility to Groundwater	High mobility to groundwater based on LogKoc = 3.25
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=3.83
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 2.2
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 6.166 mg/L indicates a Moderate toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 5.233 mg/L indicates a Moderate toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	C (Possible human carcinogen) [1986 Guidelines] [IRIS]; CLASS A4 - Not Classifiable as a Human Carcinogen [ACGIH]; Not classifiable [IARC_OE]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	2 out of 6 lists (RC_PIC; EUC2)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 52.9805 km - A_TRNSPRT)



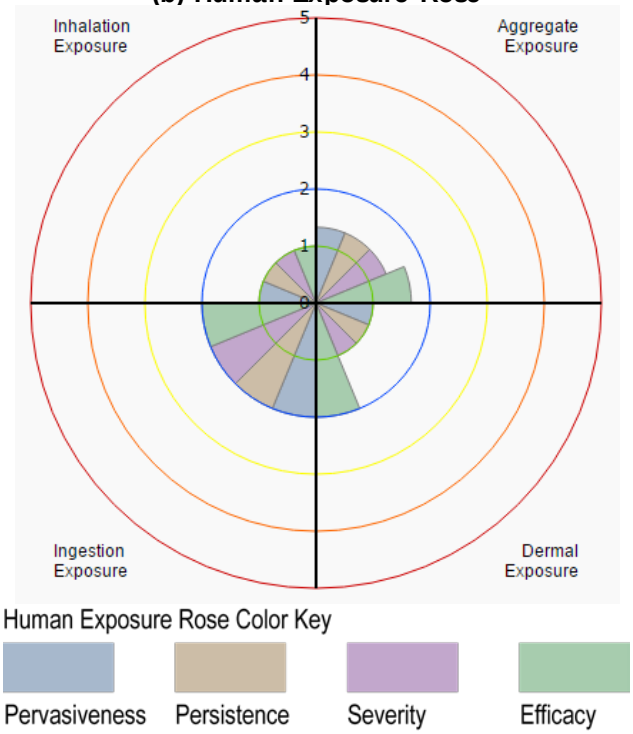
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Parathion

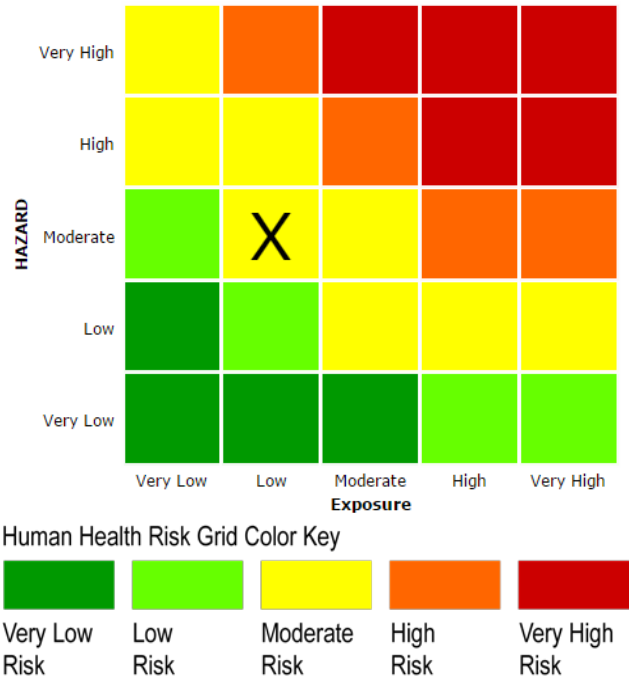
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



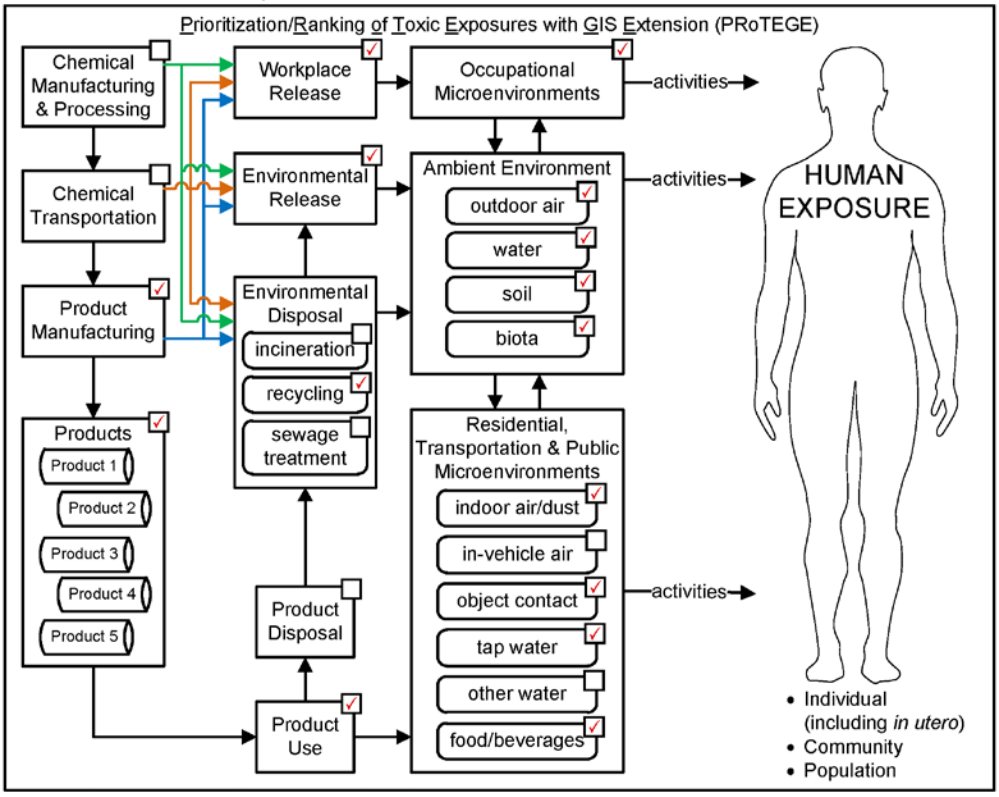
(a) Human Hazard
Estimated ranking of human hazard risk from Parathion, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Parathion (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Parathion, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Pentachlorophenol



Summary Physico-Chemical Information	
Name	Pentachlorophenol
Other Names	PCP; Penta; 2,3,4,5,6-Pentachlorophenol
Chemical Formula	C6Cl5OH
Chemical Class	OCP
Identifier	CAS: 87-86-5
Chemical Forms	
Physical Properties	
MW: 266.4 BP: 588°F (Decomposes) MLT: 374°F Sol: 0.001% VP(77°F): 0.0001 mmHg Noncombustible Solid Colorless to white, crystalline solid with a benzene-like odor. [fungicide]	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.005 mg/kg-day (IRIS); RfC: NA (IRIS)
Toxicological Effects: Carcinogenic Classification: L (IRIS)
Exposure Limits: NIOSH REL: TWA 0.5 mg/m³ [skin]; OSHA PEL: TWA 0.5 mg/m³ [skin]
Chemical Use: Wood preservative and surface disinfectant
Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact
Target Organs: Eyes, skin, respiratory system, cardiovascular system, liver, kidneys, central nervous system

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ng/m³)	14.65	22.81	31.18	Data sources: Outdoor air (5th, 50th, and 95th %iles) - '06 annual means @ AQS monitors; Food (1 measurement of 250 >LOD) - TDS 94-02; Ground water - HSDB; Indoor air - [36] (58% >LOD, 5, 50, 95%tiles); Tap water - [23] (>99% of measurements <RL); Soil - IARC	Air	3.32	81.61%
Ground water (mg/L)	0		3.53				
Food (ppb)		10			Surface Water	0.56	0.37%
Indoor Air (ng/m³)	<LOD	1.2	2.8		Ground Water	NA	
Surface water					Soil	1.19	0.03%
Tap water (µg/L)	<RL	<RL	0.14 (99.9% tile)				
Soil (µg/kg)	25		184		Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

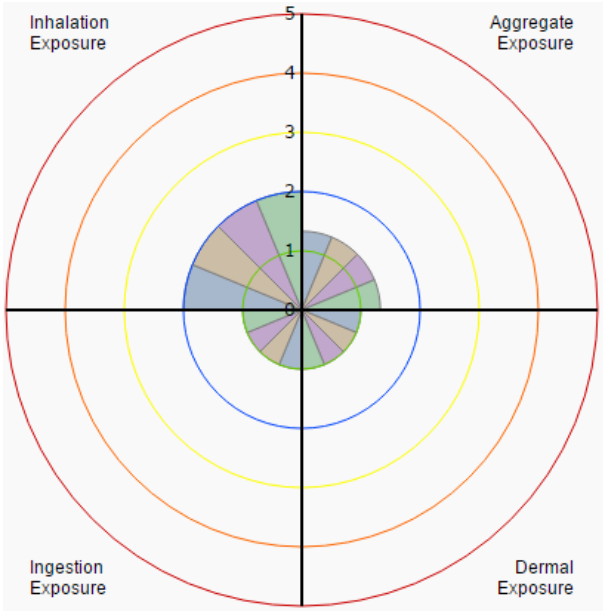
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		
	PSAP		
	NTP		●
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	●
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		
	IUR		
	ECD		
	SRD		
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		●
	NHANES	03-04	u
		05-06	(s,u)
		07-08	(s,u)
		09-10	(,u)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		
	BME		
	ERDEM		

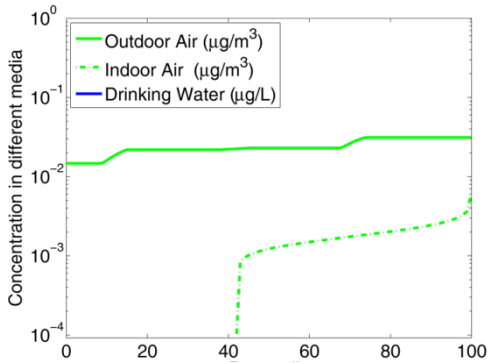
"Tier 1" Exposure Ranking for Pentachlorophenol

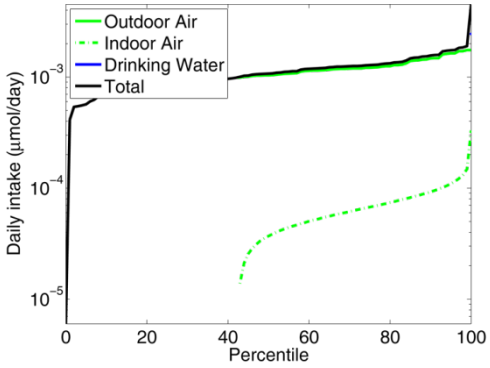
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	2	2	2	2
Ingestion	1	1	1	1
Dermal	1	1	1	1
Aggregate	1.33	1.33	1.33	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Pentachlorophenol





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0.00108	0	NA	0.00108
90 % tile	0.00151	0	NA	0.00152
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

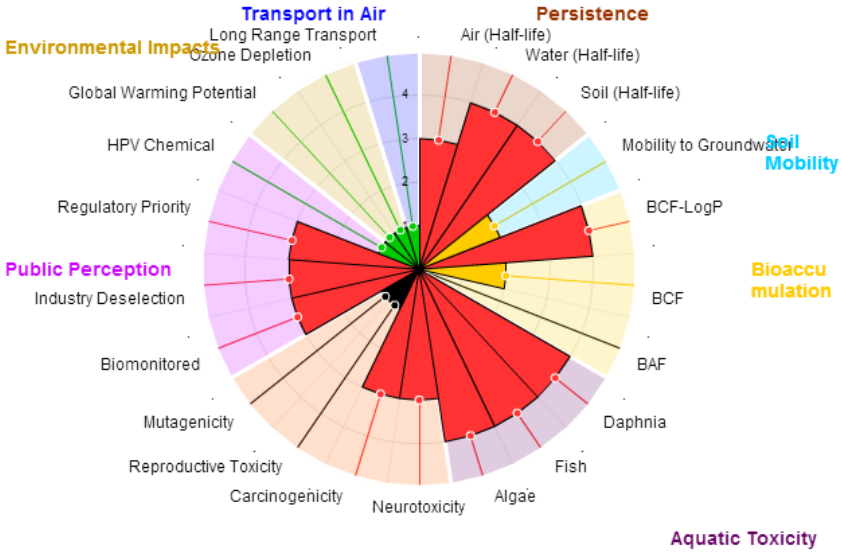
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Pentachlorophenol

		CAS # 87-86-5
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 29.15 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 1% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 1%, Max. BOD = 1%).
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Moderate mobility to groundwater based on LogKoc = 3.695
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=5.12
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 2.89
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) = 0.11 mg/L indicates a Moderate toxicity to Daphnia. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	A measured LC50 (96-hr) = 0.19 mg/L indicates a Moderate toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	A measured EC50 (72-hr) = 0.86 mg/L indicates a Moderate toxicity to Algae. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	Carc. 2: [EU_GHS]; Likely to be carcinogenic to humans [2005 Guidelines] [IRIS]; CLASS A3 - Confirmed Animal Carcinogen with unkown relevance to humans [ACGIH]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	1 out of 2 lists (NHANES IV)
	Industry Deselection	4 out of 6 lists (GADSL; RC_PIC; EUC2; SINLIST)
	Regulatory Priority	2 out of 10 lists (JDES_LST; JMON3)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 127.306 km - A TRNSPRT)



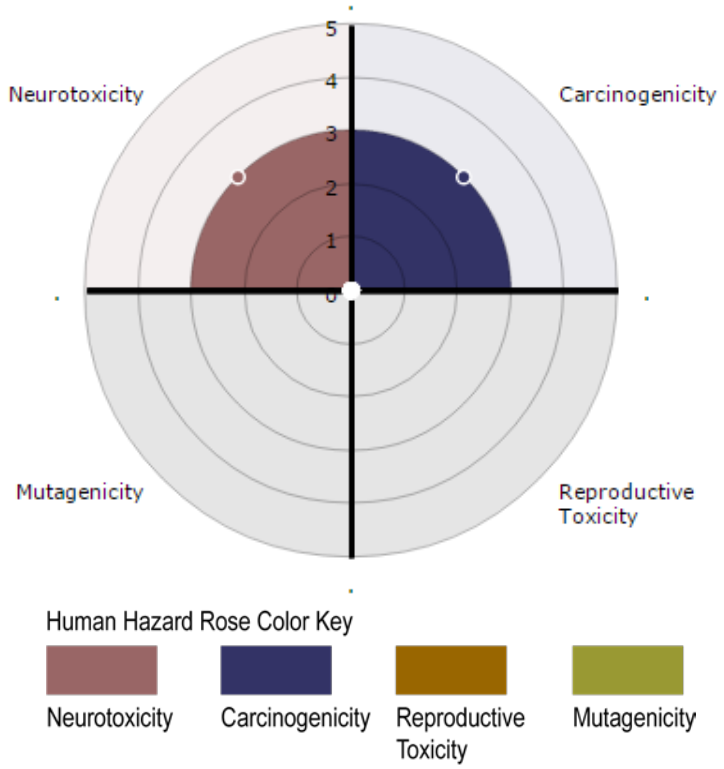
Key

- → Potential for High level of concern (**3-4**)
- → Potential for Moderate level of concern (**2**)
- → Potential for Low level of concern (**1**)

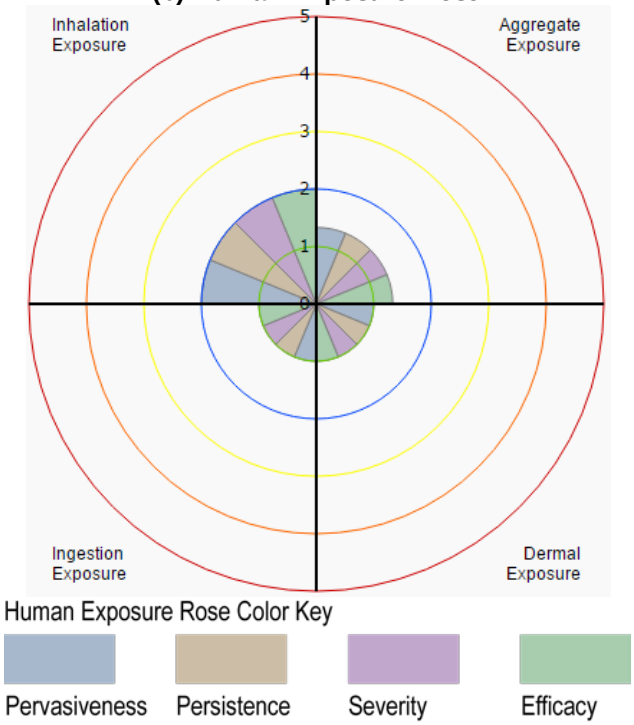
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Pentachlorophenol

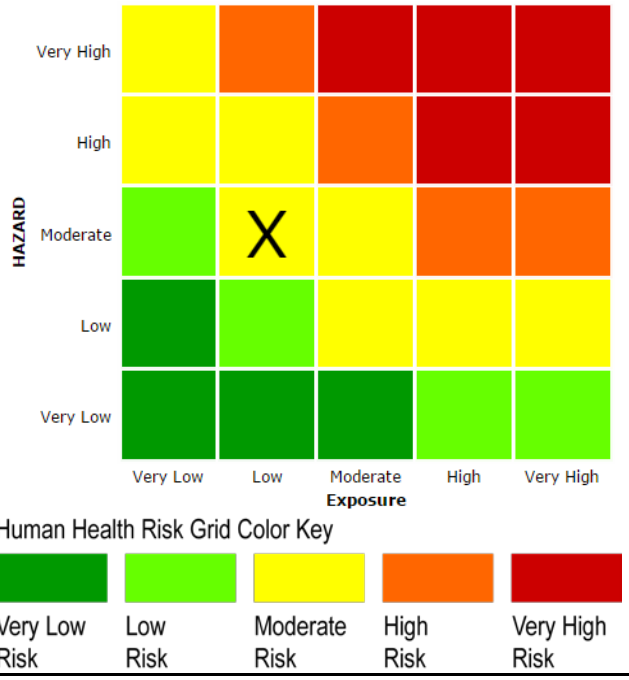
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



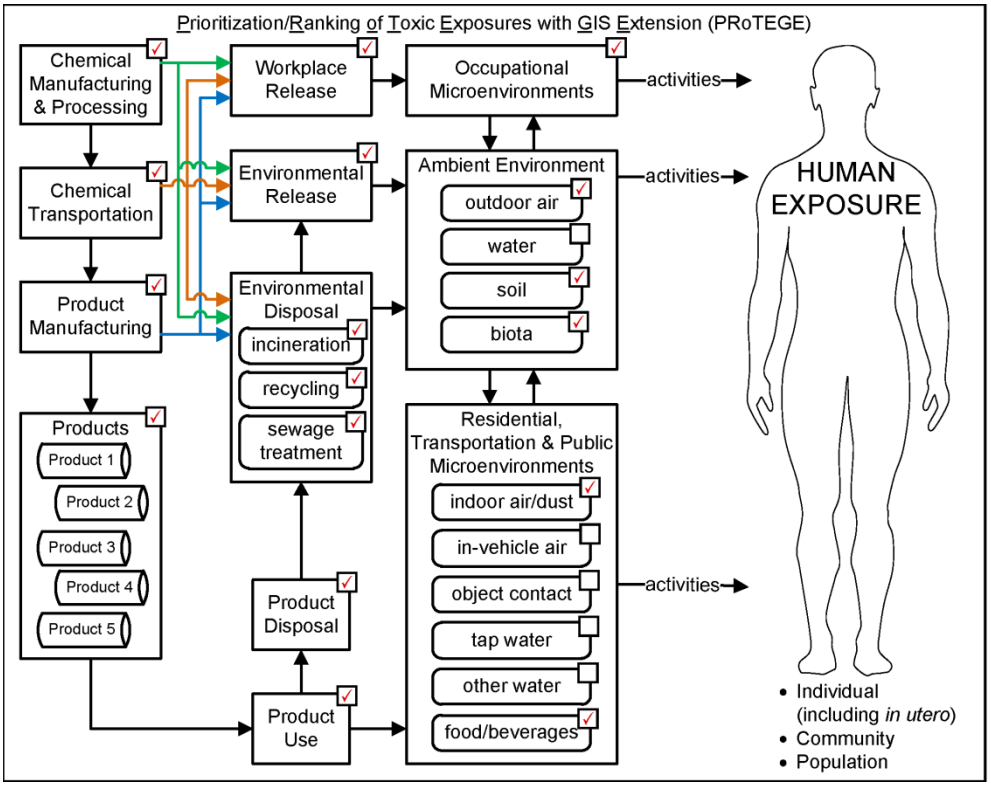
(a) Human Hazard
Estimated ranking of human hazard risk from Pentachlorophenol, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Pentachlorophenol (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Pentachlorophenol, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for pentaBDE



Summary Physico-Chemical Information	
Name	pentaBDE
Other Names	Pentabromodiphenyl ether, 1,2,4-tribromo-5-(2,4-dibromophenoxy)benzene, BDE-99, BDE-100
Chemical Formula	$C_{12}H_5Br_5O$
Chemical Class	PBDEs
Identifier	CAS 32534-81-9
Chemical Forms	mixture of BDE 47, 99, and 100
Physical Properties	
MW: 564.69 MP: -7 to -3°C BP: >300°C Decomp >200°C Sol: 13.3 µg/L	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits:
Toxicological Effects:
Exposure Limits:
Chemical Use: flame retardant
Exposure Routes: ingestion of food
Target Organs:

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (pg/m³)	4.26	13.4	42.3	Data sources: Tap water from NCOD UCMR2, 59402 measurements are less than the minimum reporting requirement; Food - [39] (5, 50, 95%tiles); Outdoor air - [37] (5, 50, 95%tiles)	Air		
Ground water							
Food (ng/kg)	<LOD	1.1	6.6		Surface Water		
Indoor Air					Ground Water		
Surface water					Soil		
Tap water							
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers				Data source: Blood from HSDB			
Urine							
Blood (pmol/g)	0.3		5				
Other							

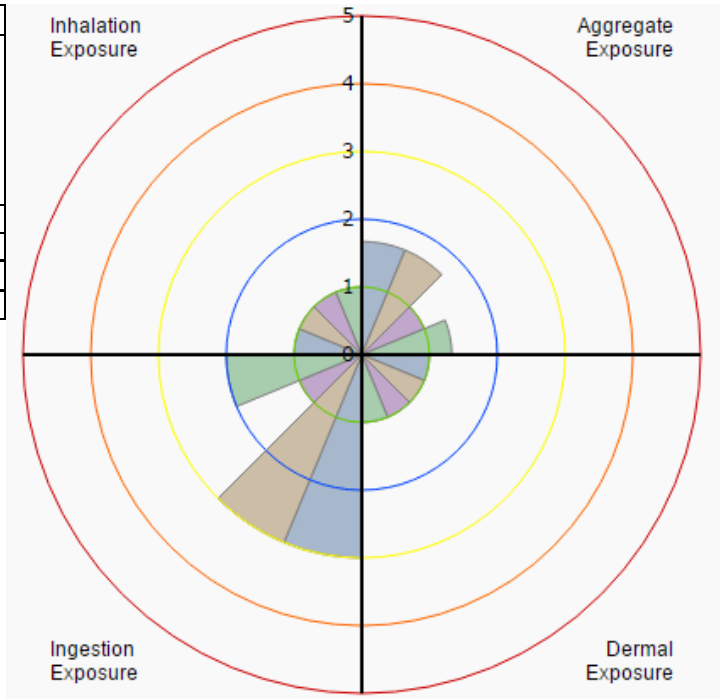
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		
	Tox Profs		□
	IRIS		●
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		●
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		
	ECD		●
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		
	BME		
	ERDEM		

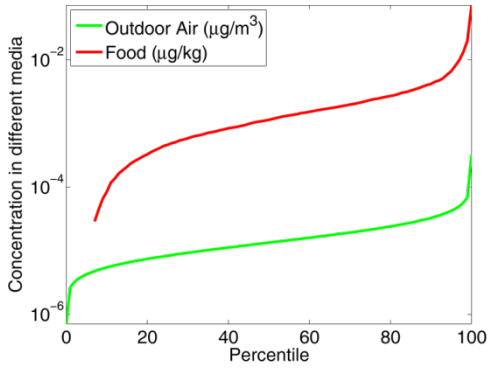
"Tier 1" Exposure Ranking for pentaBDE

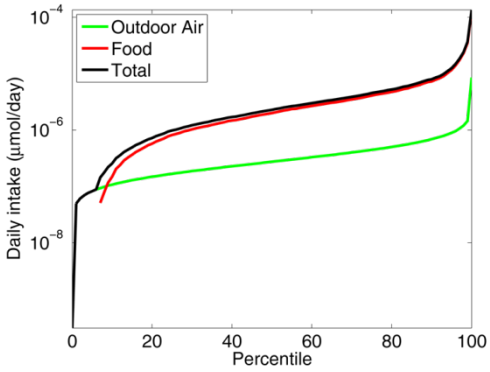
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	3	3	1	2
Dermal	1	1	1	1
Aggregate	1.66	1.66	1	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for pentaBDE





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	2.74E-07	2.04E-06	NA	2.32E-06
90 % tile	6.91E-07	7.52E-06	NA	8.43E-06
% over 0.1 μmol/day	0	0	NA	0
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

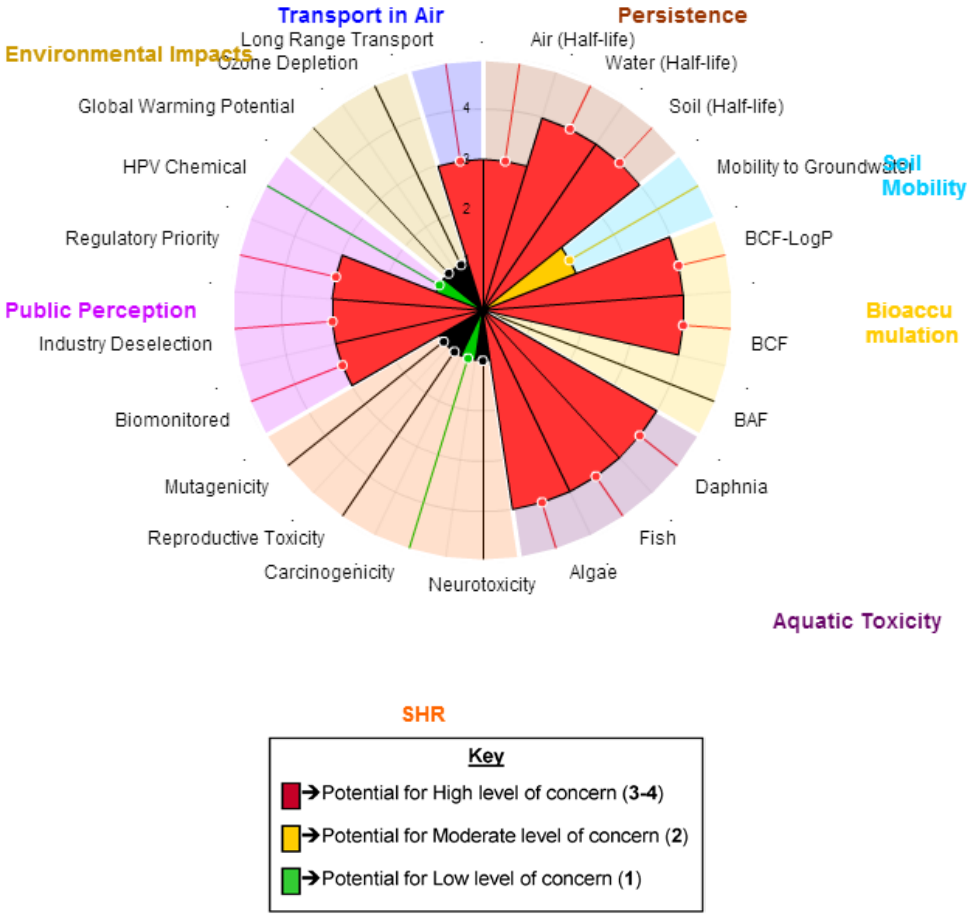
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for pentaBDE

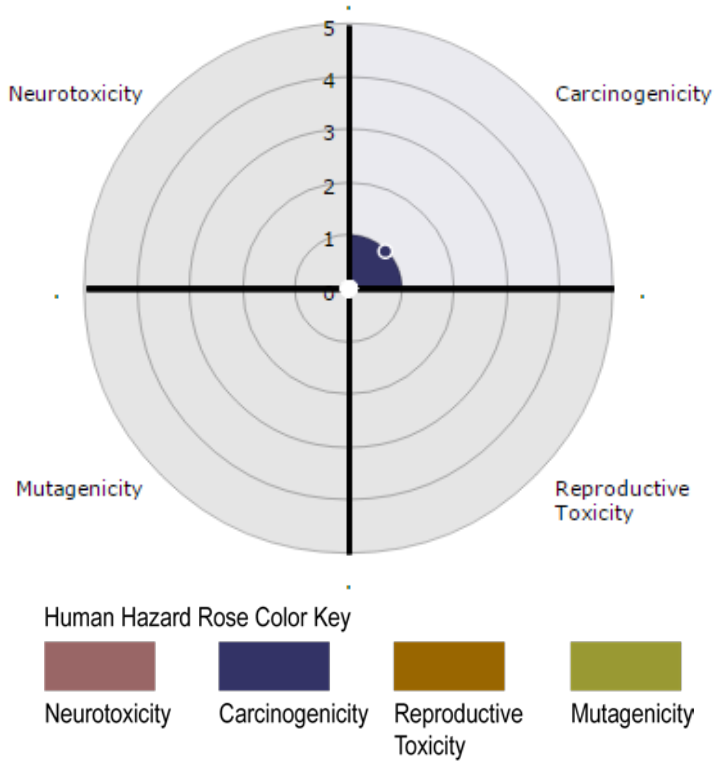
		CAS # 32534-81-9
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 29.16 days)
	Water (Half-life)	Very High persistence in Water (Estimated Half-life = 180 days)
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Moderate mobility to groundwater based on LogKoc = 4.336
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=6.84
	BCF	Very High bioconcentration potential based on Estimated LogBCF = 4.18
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 0.003 mg/L indicates a High toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 0.002 mg/L indicates a High toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	D (Not classifiable as to human carcinogenicity) [1986 Guidelines] [IRIS]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	1 out of 2 lists (NHANES IV)
	Industry Deselection	2 out of 6 lists (GADSL; RC_PIC)
	Regulatory Priority	1 out of 10 lists (JCL1_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 1120.52 km - A TRNSPRT)



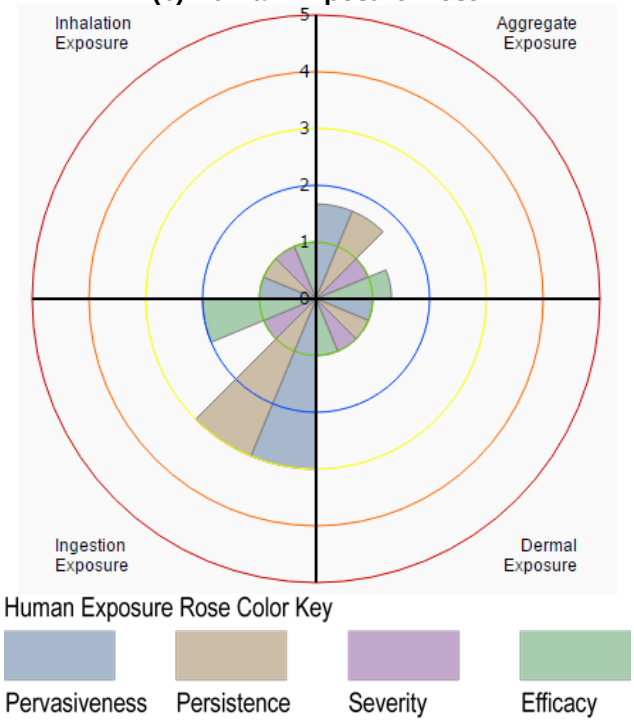
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for pentaBDE

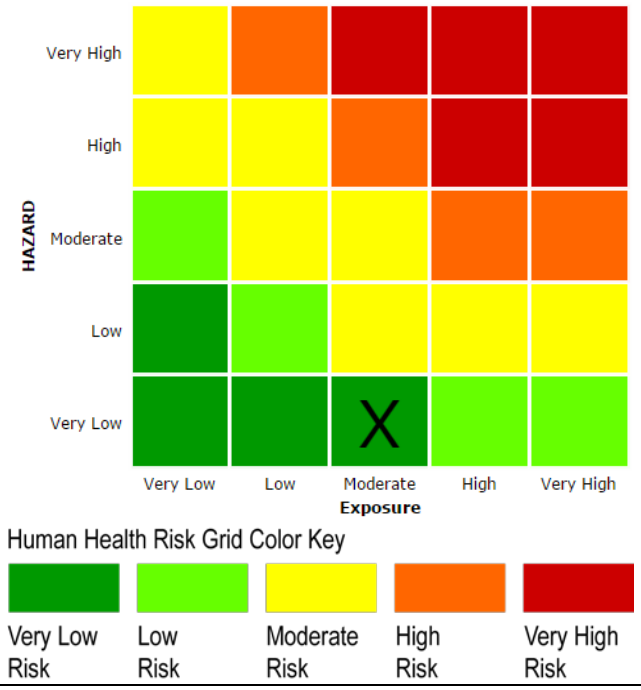
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



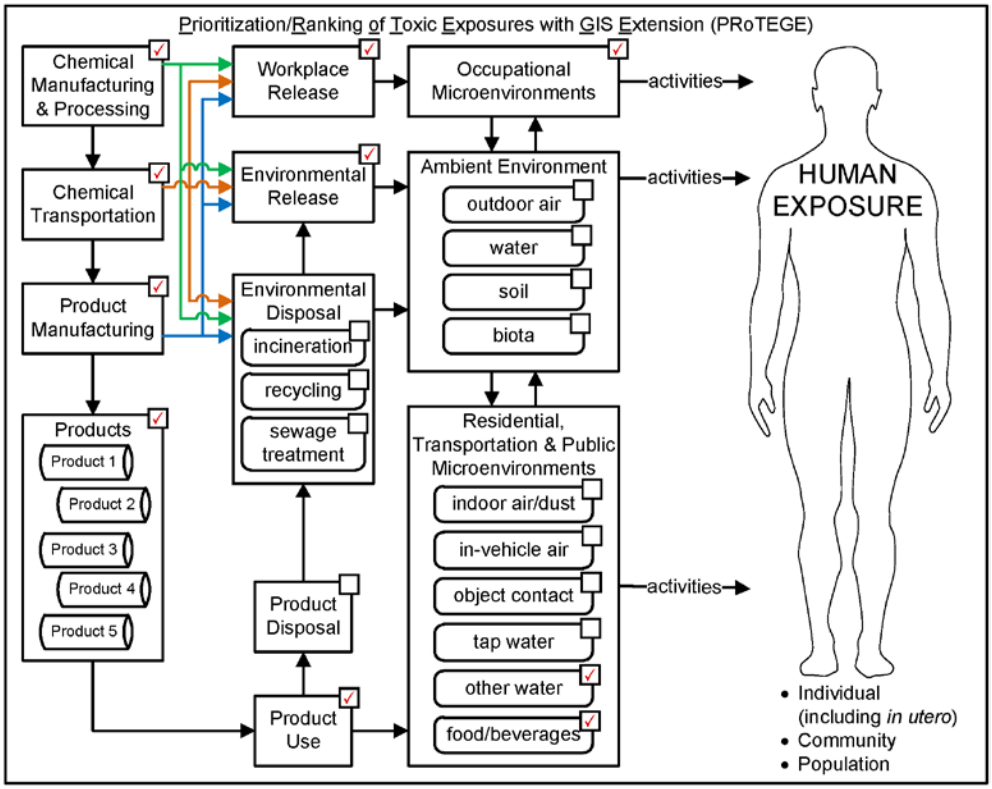
(a) Human Hazard
Estimated ranking of human hazard risk from pentaBDE, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of pentaBDE (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from pentaBDE, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Permethrin



Summary Physico-Chemical Information	
Name	Permethrin
Other Names	IUPAC Name: 3-Phenoxybenzyl (1RS)-cis,trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate; Trade names: Ambush, Dragnet, Eksmin, Qamlin, Torpedo
Chemical Formula	$C_{21}H_{20}Cl_2O_3$
Chemical Class	Pyrethroids
Identifier	CAS: 52645-53-1, 40326 (PubChem)
Chemical Forms	
Physical Properties	
Molecular Weight: 391.3 Boiling point: 200°C Melting point: 34°C Solubility: Insoluble in water (5.5 x 10^{-3} ppm) log Kow = 6.50 Density: 1.19 g/cm^3, solid Specific Gravity: 1.190-1.272 at 20°C Vapor Pressure: 2.18 x 10^{-8} mm Hg at 25°C	
Additional Notes	
Most frequently used pyrethroid in the United States (ATSDR); Have four stereoisomers.	

Exposure and Toxicity Information
Toxicity Limits: RfD0.05 mg/kg/day (IRIS)
Toxicological Effects: Increased liver weight in rats (IRIS); Not classifiable as to its carcinogenicity to humans (IARC)
Exposure Limits: OSHA PEL not established
Chemical Use: pesticide, insecticide
Exposure Routes: Ingestion, Inhalation, Dermal (ATSDR Tox Profile)
Target Organs: Skin, eyes, respiratory tract (NIOSH ICSC: 0312), Neurons [55]

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air				Data sources: Food (5th, 50th and 95th percentiles) - TDS 1994-2002; Ground water (detected in 3 out of 5,728 ambient groundwater samples): HSDB; Surface Water (found in 24 out of 12,253 ambient surface water samples other than spring water) - HSDB; Permethrin was also detected in 3 out of 73 ambient spring water samples (Min, mean and max are 0.01, 0.0133 and 0.02 µg/L respectively) - HSDB; Average daily intake: 3.2 µg/day for an adult 70-kg male (ATSDR Tox. Profile)	Air	1.35 (TRI 2008)	0.16% (TRI 2008)
Ground water (µg/L)	0.006	0.011	0.02				
Food (ppm)	0.0004	0.003	0.5515		Surface Water		
Indoor Air					Ground Water		
Surface water (µg/L)	0.005	0.0137	0.03		Soil		
Tap water							
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota							
Human Biomarkers							
Urine							
Blood							
Other							

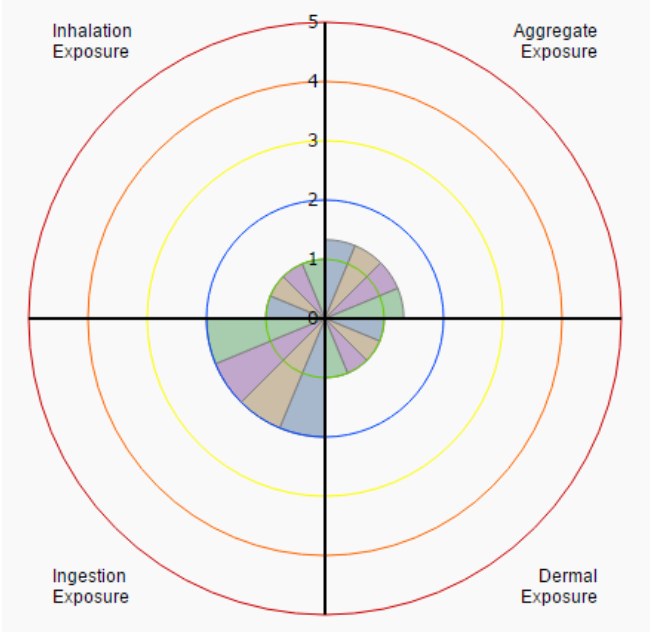
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		●
	Tox Profs		□
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		
	SRD		●
Releases	TRI		●
	NEI		
Environmental Quality	NGA		
	NAWQA		●[1]
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	(p1)
		09-10	(p1)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm (R) [56]
	BME		
	ERDEM		

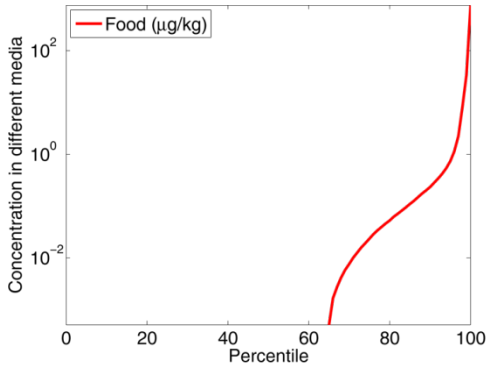
"Tier 1" Exposure Ranking for Permethrin

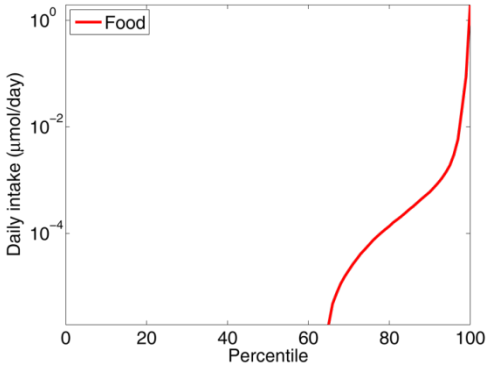
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	1
Aggregate	1.33	1.33	1.33	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Permethrin





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0	0.000615	NA	0.000664
% over 0.1 µmol/day	0	0.997	NA	1.95
% over 1 µmol/day	0	0.508	NA	0.996

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

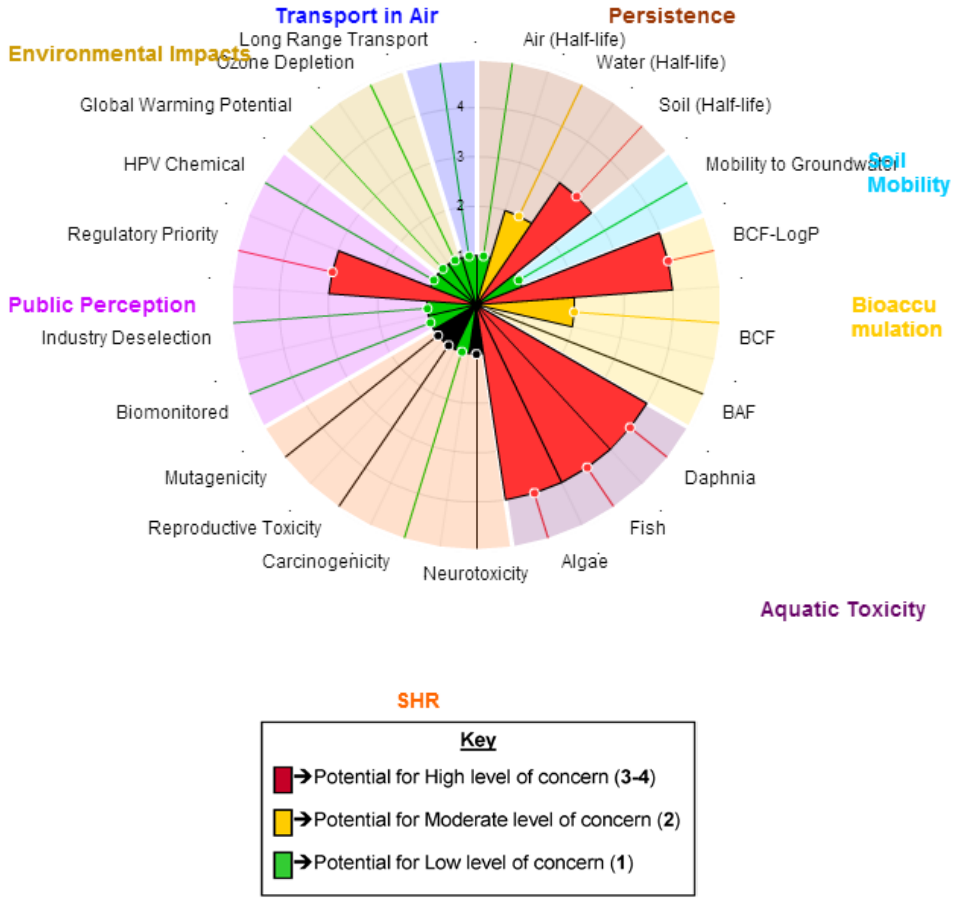
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Permethrin

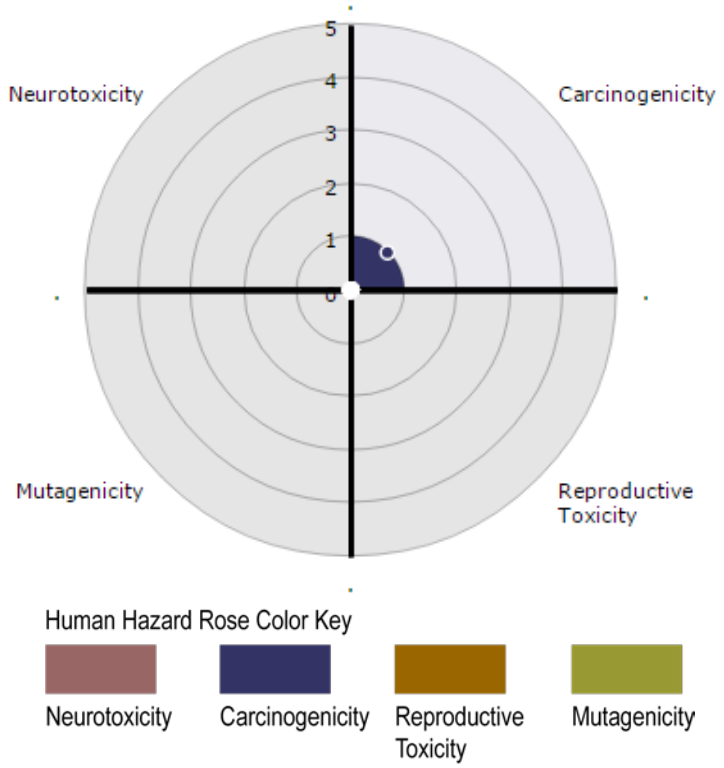
		CAS # 52645-53-1
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.4674 days)
	Water (Half-life)	Moderate persistence in Water (Estimated Half-life = 60 days)
	Soil (Half-life)	High persistence in Soil (Estimated Half-life = 120 days)
Soil Mobility	Mobility to Groundwater	Low mobility to groundwater based on LogKoc = 5.075
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=6.5
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 2.63
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 0.004 mg/L indicates a High toxicity to Daphnid. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 0.074 mg/L indicates a High toxicity to Fish. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	Not classifiable [IARC_OE]; [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	0 out of 6 lists
	Regulatory Priority	1 out of 10 lists (JMON3)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 190.536 km - A_TRNSPRT)



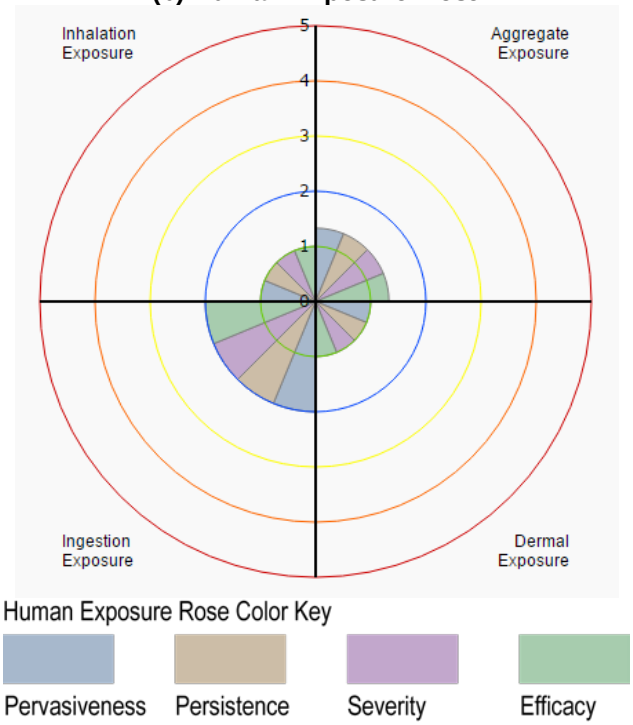
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Permethrin

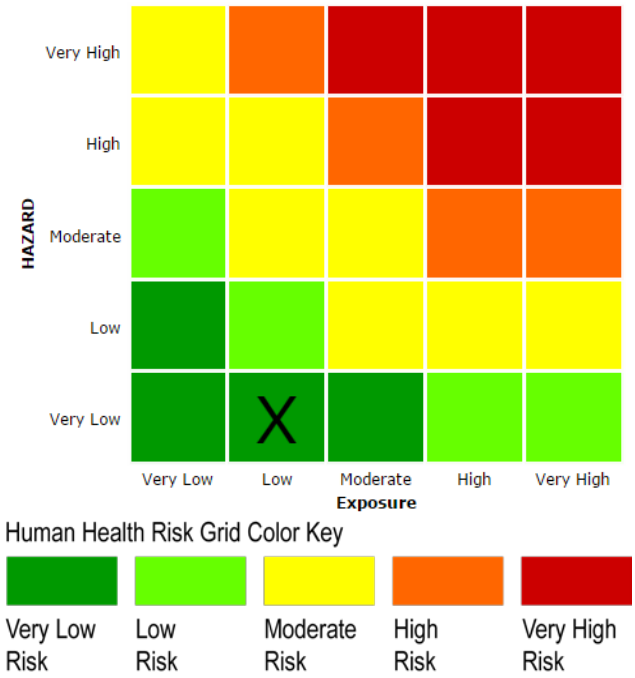
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



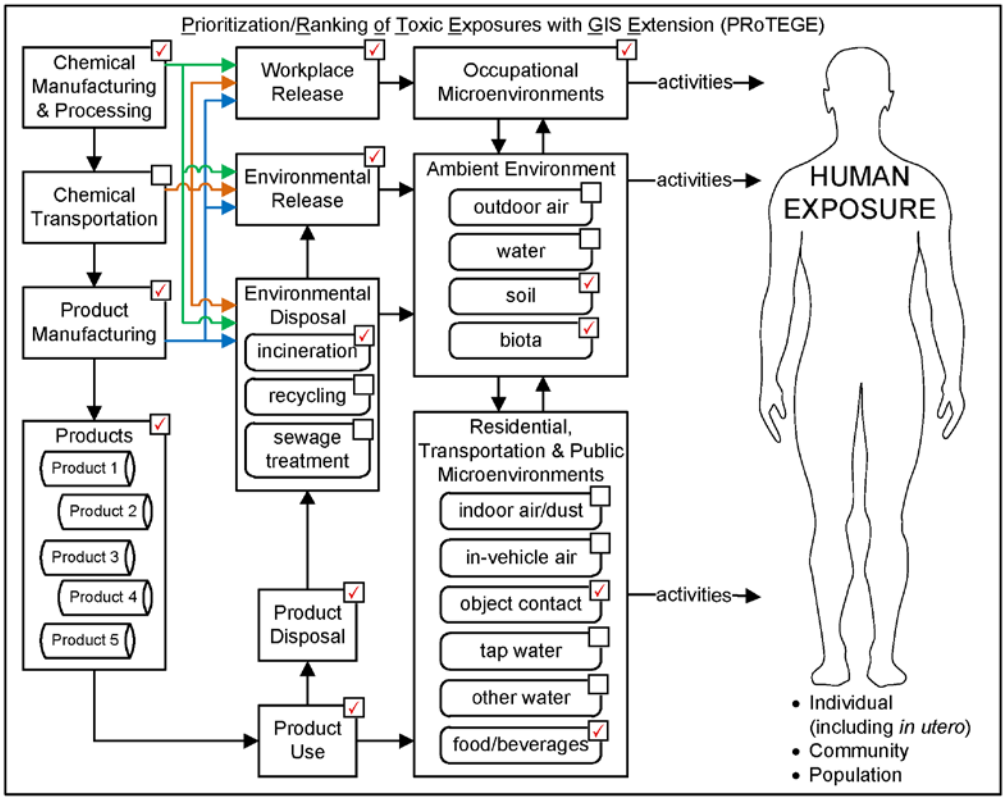
(a) Human Hazard
Estimated ranking of human hazard risk from Permethrin, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Permethrin (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Permethrin, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

PRoTEGE Ranking for PFOS



Summary Physico-Chemical Information	
Name	PFOS
Other Names	Perfluorooctane sulfonic acid
Chemical Formula	$C_8HF_{17}O_3S$
Chemical Class	PFC
Identifier	CAS: 1763-23-1
Chemical Forms	
Physical Properties	
Molecular Weight: 500.13 Color/Form: Liquid Boiling Point: 133 °C @ 0.8 kPa VP: 3.31×10^{-4} Pa @ 20 °C (2.483×10^{-6} mm Hg) /K salt/	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: NA
Toxicological Effects: Subchronic or prechronic exposure/adverse signs of toxicity observed in rat studies included increases in liver enzymes, hepatic vacuolization and hepatocellular hypertrophy, GI effects, hematological abnormalities, weight less, convulsions, and death.
Exposure Limits: NA
Chemical Use: a precursor for fluorinated surfactants. key ingredient in Scotchgard™, a fabric protector made by 3M, and numerous stain repellents. Production of metal plating and fire-fighting foams.
Exposure Routes: inhalation, ingestion and dermal contact
Target Organs: plasma and liver

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	NA			Data sources: Food – not detected in food [79]; Surface water - [93]; Biota – [94,95]	Air	NA	
Ground water (ppb)	NA						
Food (µg/g)	<LOD				Surface Water	NA	
Indoor Air (ng/m³)	NA				Ground Water	NA	
Surface water (µg/L)	0.0168	0.032	0.14		Soil	NA	
Tap water							
Soil					Chemical Production and Use		
Dust					Production		G (Current), 91 tons (ECD)
Surfaces							
Biota (ng/mL)	3	50	475				
Human Biomarkers							
Urine (µg/L)							
Blood							
Other							

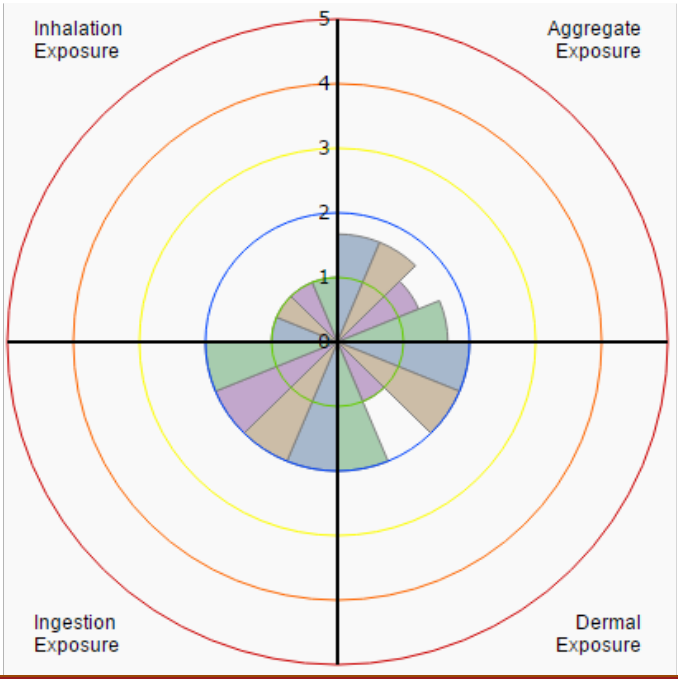
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		
	Tox Profs		□
	IRIS		
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		
	SCP		
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	●
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		
	ECD		●
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	s
		05-06	s
		07-08	s
		09-10	(s)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PK m (H) [52]
	BME		
	ERDEM		

"Tier 1" Exposure Ranking for PFOS

Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	2	2	1	2
Aggregate	1.66	1.66	1.33	1.33

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for PFOS

insufficient data for analysis

insufficient data for analysis

	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0	0	NA	0
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

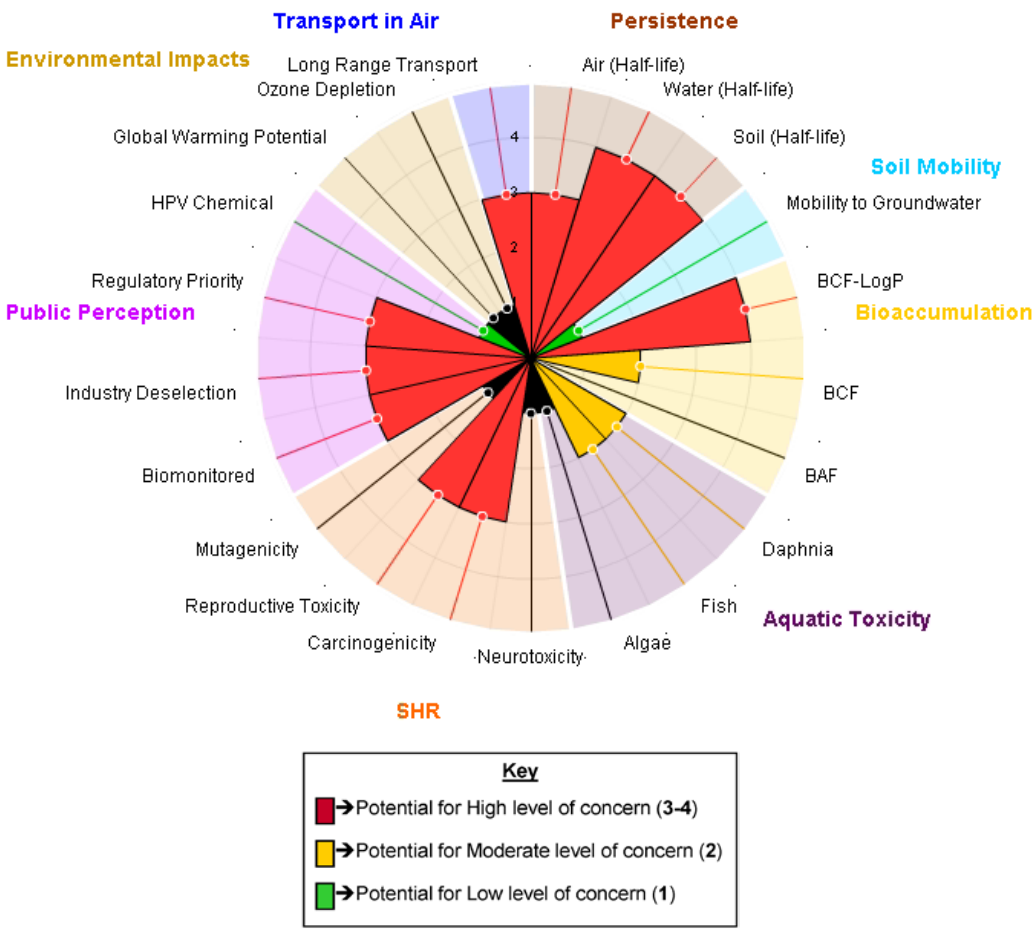
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for PFOS

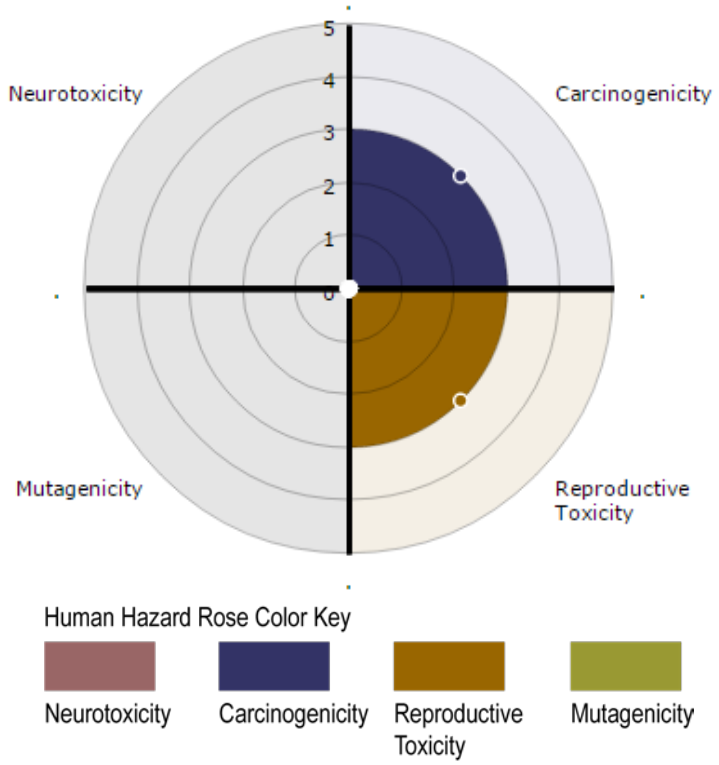
		CAS # 1763-23-1
Persistence	Air (Half-life)	High persistence in Air (Estimated Half-life = 76.4 days)
	Water (Half-life)	Very High persistence in Water (Estimated Half-life = 180 days)
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Low mobility to groundwater based on LogKoc = 5.004
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Estimated LogP=6.28
	BCF	Moderate bioconcentration potential based on Estimated LogBCF = 1.75
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 0.506 mg/L indicates a Moderate toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 0.351 mg/L indicates a Moderate toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	
	Carcinogenicity	Carc. 2: [EU_GHS]
	Reproductive Toxicity	Toxic to reproduction - Category 1B/2A [EU_RA17_5]
	Mutagenicity	
Public Perception	Biomonitored	2 out of 2 lists (NHANES; NHANES IV)
	Industry Deselection	3 out of 6 lists (GADSL; RC_PIC; SINLIST)
	Regulatory Priority	1 out of 10 lists (JCL1_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 1383.78 km - A_TRNSPRT)



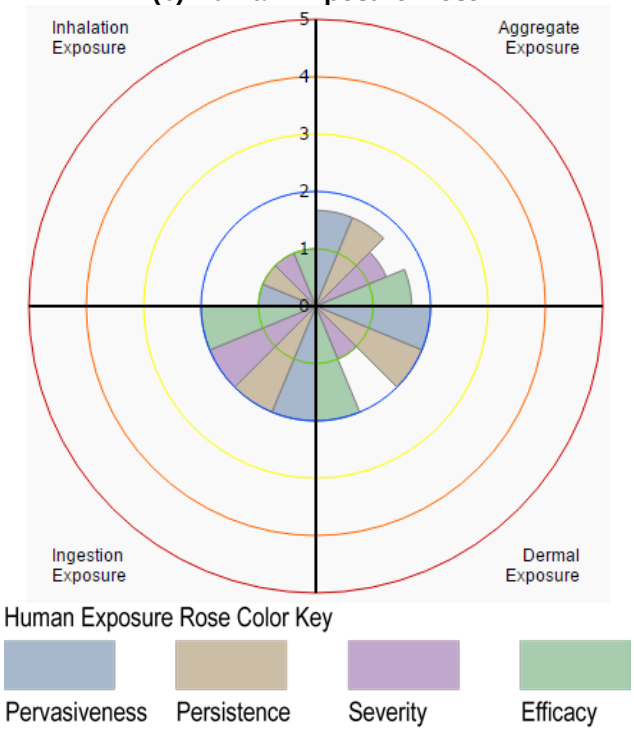
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for PFOS

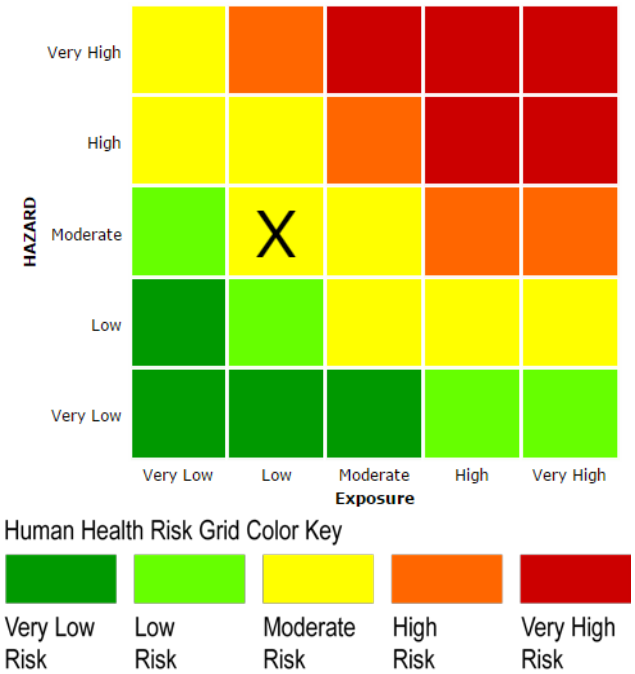
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



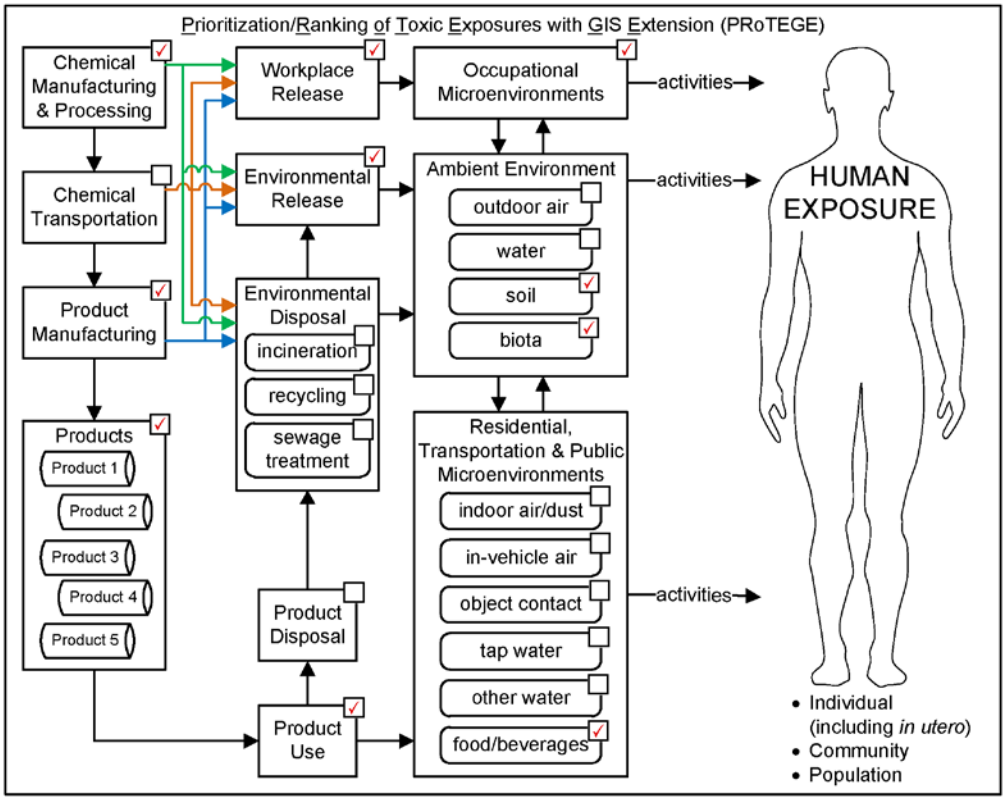
(a) Human Hazard
Estimated ranking of human hazard risk from PFOS, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of PFOS (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from PFOS, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Phenol, (1,1-dimethylethyl)-4-methoxy-



Summary Physico-Chemical Information	
Name	Phenol, (1,1-dimethylethyl)-4-methoxy-
Other Names	Butylated hydroxyanisole, BHA
Chemical Formula	$C_{11}H_{16}O_2$
Chemical Class	FP
Identifier	CAS: 25013-16-5
Chemical Forms	mixture with Butylhydroxyanisole
Physical Properties	
Molecular Weight: 180.24 Melting Point: 48-55 °C Boiling Point: 264-270 °C Sol: Insoluble in water	
Additional Notes	
7 ng/uL detected in industrial wastewater samples	

Exposure and Toxicity Information
Toxicity Limits: LD50 Mouse oral 2000 mg/kg bw, LD50 Rat oral 2200 mg/kg bw, LD50 Rat (male) ip 881 mg/kg bw (IARC)
Toxicological Effects: Reasonably anticipated to be a human carcinogen (NTP RoC 2005) generally recognized as safe (CFR 21)
Exposure Limits: Generally Recognized as Safe (GRAS) for use in food when the total of antioxidants is not greater than 0.02% of fat or oil content (FDA)
Chemical Use: Antioxidant and preservative for fats and oils and in food packaging. Used in cosmetics such as lipstick and eyeshadow. Antioxidant for some rubbers and petroleum products, stabilizer for vitamin A.
Exposure Routes: Ingestion, dermal contact
Target Organs: Blood, liver, respiratory system, eyes, skin

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air	NA				Air		
Ground water	NA					NA	
Food	NA				Surface Water	NA	
Indoor Air	NA				Ground Water	NA	
Surface water	NA				Soil	NA	
Tap water	NA						
Soil	NA				Chemical Production and Use		
Dust	NA				Production	< 500,000 lbs @ US (IUR)	
Surfaces							
Biota							
Human Biomarkers	NA						
Urine	NA						
Blood	NA						
Other	NA						

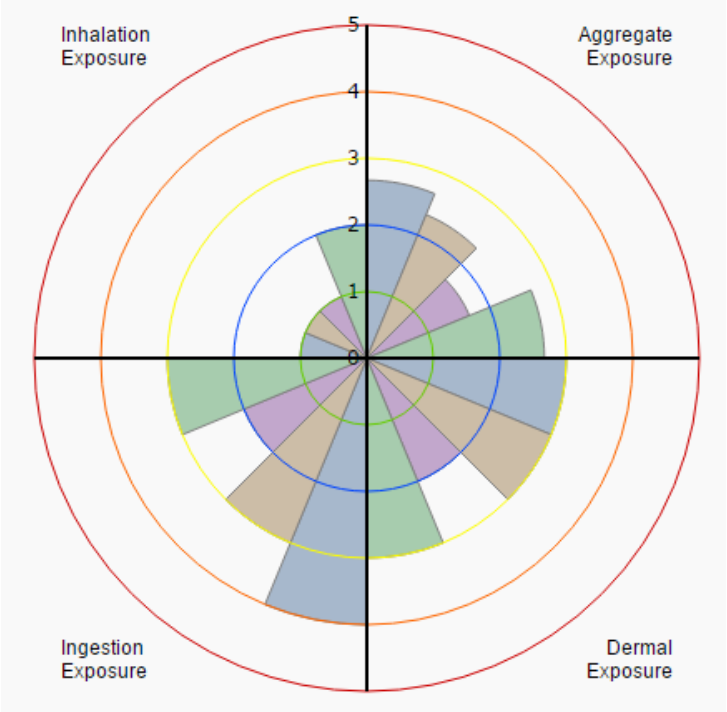
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		
	Tox Profs		
	IRIS		
	HSDB		●
	ITER		
	McKay		
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		●
	ECD		
	SRD		●
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		
	BME		
	ERDEM		

"Tier 1" Exposure Ranking for Phenol, (1,1-dimethylethyl)-4-methoxy-

Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	2
Ingestion	4	3	2	3
Dermal	3	3	2	3
Aggregate	2.66	2.33	1.66	2.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Phenol, (1,1-dimethylethyl)-4-methoxy-

insufficient data for analysis

insufficient data for analysis

	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0	0	NA	0
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

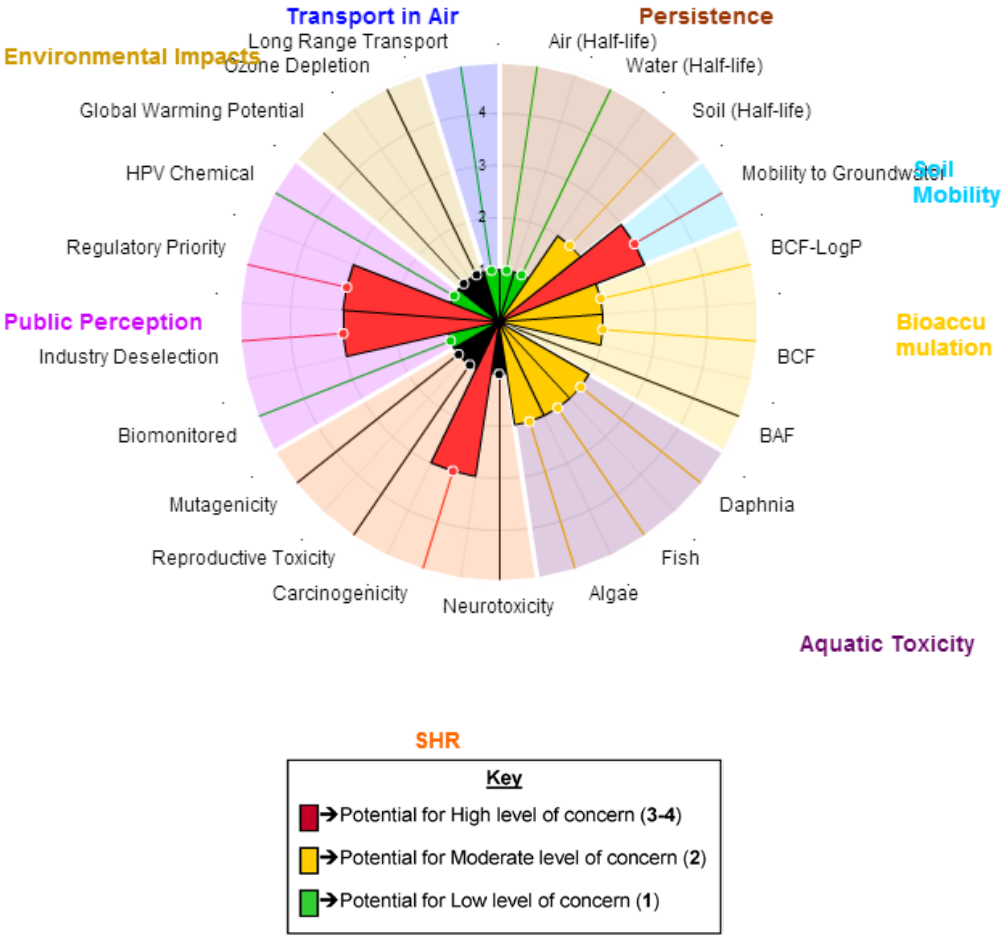
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Phenol, (1,1-dimethylethyl)-4-methoxy-

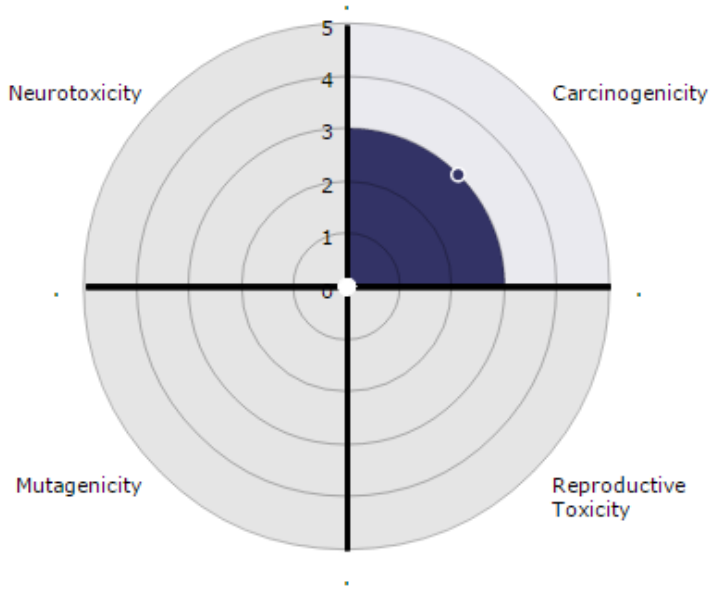
		CAS # 25013-16-5
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.2967 days)
	Water (Half-life)	Low persistence in Water (Estimated Half-life = 37.5 days)
	Soil (Half-life)	Moderate persistence in Soil (Estimated Half-life = 75 days)
Soil Mobility	Mobility to Groundwater	High mobility to groundwater based on LogKoc = 2.925
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Estimated LogP=3.5
	BCF	Moderate bioconcentration potential based on Estimated LogBCF = 1.756
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) = 2.3 mg/L indicates a Moderate toxicity to Daphnia.
	Fish	A measured LC50 (96-hr) = 5.8 mg/L indicates a Moderate toxicity to Fish.
	Algae	A measured EC50 (72-hr) = 5.2 mg/L indicates a Moderate toxicity to Algae.
SHR	Neurotoxicity	
	Carcinogenicity	Anticipated Carcinogen - there is limited evidence of carcinogenicity in humans or sufficient evidence of carcinogenicity in animals [NTP] [NTPLIST]; Possibly carcinogenic to humans [IARC_OE]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (SINLIST)
	Regulatory Priority	1 out of 10 lists (JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 129.6 km - A_TRNSPRT)



IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Phenol, (1,1-dimethylethyl)-4-methoxy-

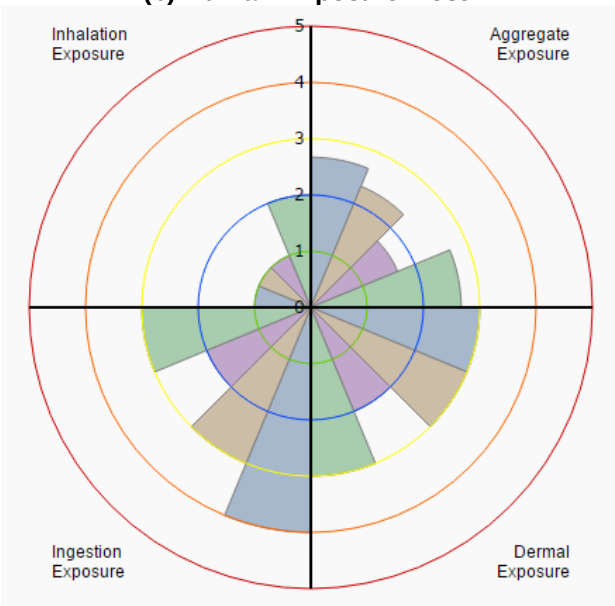
(a) Human Hazard Rose



Human Hazard Rose Color Key

Neurotoxicity | Carcinogenicity | Reproductive Toxicity | Mutagenicity

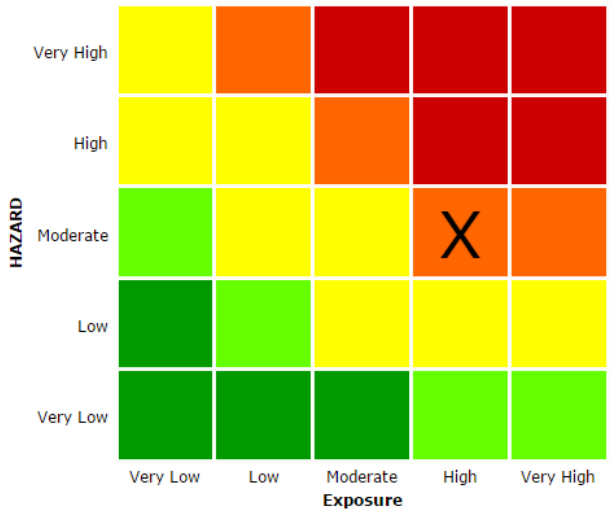
(b) Human Exposure Rose



Human Exposure Rose Color Key

Pervasiveness | Persistence | Severity | Efficacy

(c) Human Health Risk Grid



Human Health Risk Grid Color Key

Very Low Risk | Low Risk | Moderate Risk | High Risk | Very High Risk

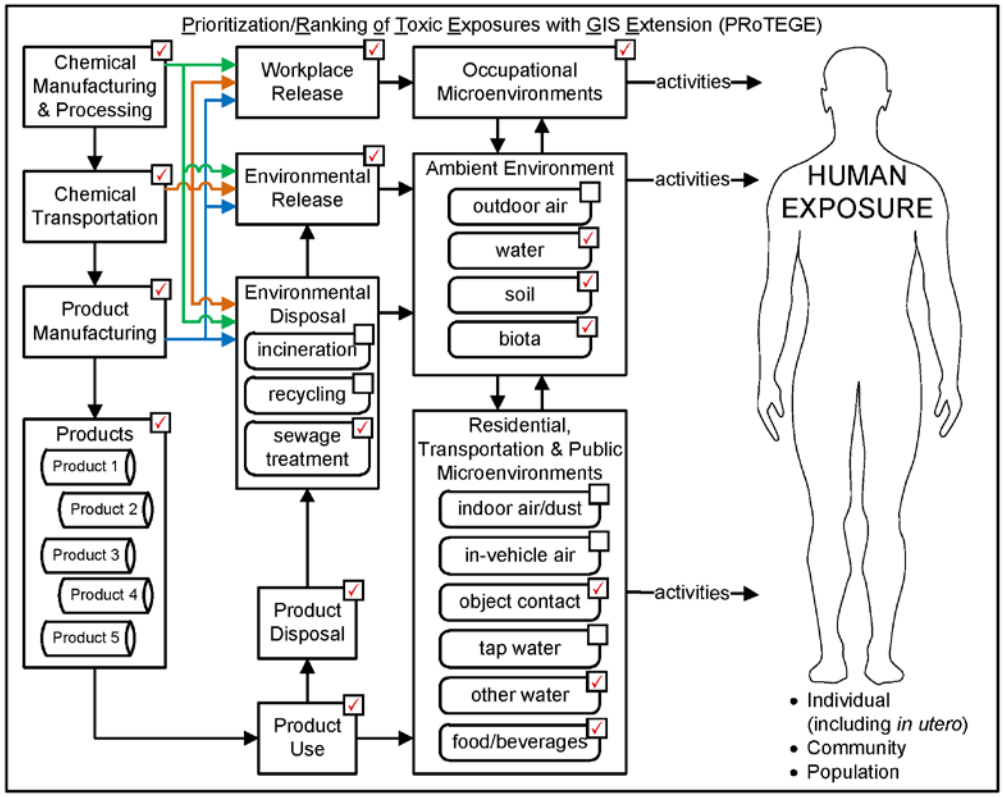
(a) Human Hazard
Estimated ranking of human hazard risk from Phenol, (1,1-dimethylethyl)-4-methoxy-, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Phenol, (1,1-dimethylethyl)-4-methoxy- (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Phenol, (1,1-dimethylethyl)-4-methoxy-, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Ranking for Trifluralin



Summary Physico-Chemical Information	
Name	Trifluralin
Other Names	Agreflan, Elancolan, Treficon, Treflan, Crisalin, Trim
Chemical Formula	$C_{13}H_{16}F_3N_3O_4$
Chemical Class	Herb
Identifier	CAS: 1582-09-8; RTECS: XU9275000; EC: 609-046-00-1
Chemical Forms	
Physical Properties	
Yellow crystalline solid Molecular weight: 335.28 Solubility in water: 18.4 mg/L at 25°C Vapor pressure: negligible at 25°C Density: 1.36 g/cm^3 at 22°C Melting point: 46 – 47 °C Boiling point: 139 – 140 °C at 4.2 mmHg	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD: 7.5 × 10^{-3} mg/kg/day (IRIS); NOEL: 0.75 mg/kg/day (dog), 10 mg/kg/day (rat) (IRIS)
Toxicological Effects: Carcinogenic classification – C (possible human carcinogen)
Exposure Limits:
Chemical Use: Herbicide
Exposure Routes: Dermal absorption, skin and/or eye contact, inhalation
Target Organs: Liver, skin, spleen

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (ng/m^3)	0	0	1094.038	Data sources: Outdoor air (5%,50%,95%) – NATA county-level data; Ground water (mean, max, 1988 in 4 states in US) - HSDB; Food (detected only in animal feed) – FDA pesticide program; Soil (min, max, 1972 in 52 of 1533 soil samples from 37 states) - Natl. Soils Monitoring Program (HSDB); Indoor air - [77] (5, 50, 95%tiles)	Air	0.209 (TRI 2008)	0.47%
Ground water (ppb)		0.4	2.2				
Food	NA				Surface Water	-	
Indoor Air (ng/m^3)	<LOD	<LOD	0.852		Ground Water	-	
Surface water					Soil	3.42 (TRI 2008)	0.06%
Tap water							
Soil (ppm)	0.01		1.29		Chemical Production and Use		
Dust					*Production*	9530 ton/year	
Surfaces							
Biota					*Use*	8.52 million lbs/year	Source: NAWQA
Human Biomarkers							
Urine							
Blood							
Other							

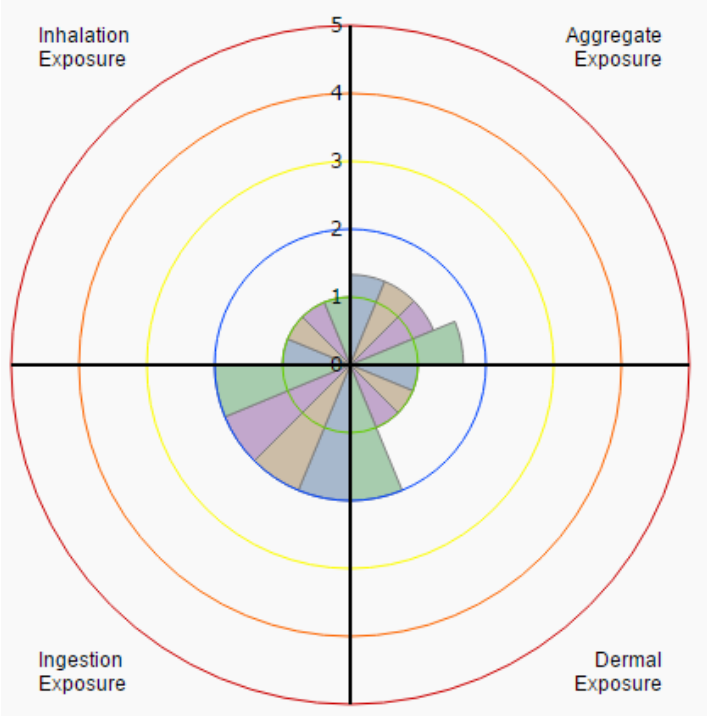
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		
	ICSC		●
	Tox Profs		
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		
	RIVM rprts		
	IARC		●
	PSAP		
	NTP		●
	REACH		
	PFD		●
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		
	SRD		●
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		□
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	(s)
		05-06	(s)
		07-08	(s)
		09-10	(s)
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PKm (F) [55]
	BME		
	ERDEM		

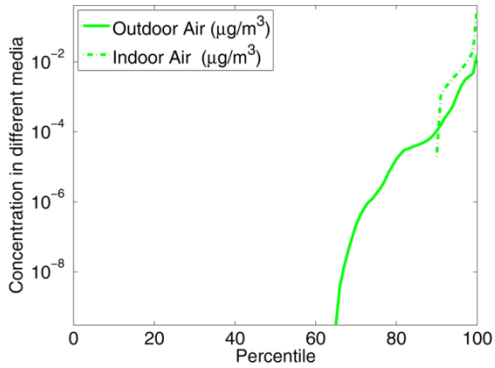
"Tier 1" Exposure Ranking for Trifluralin

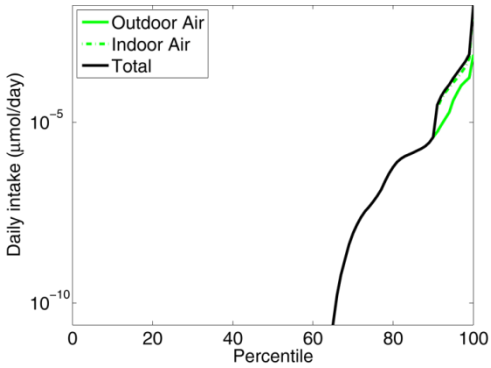
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Trifluralin





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 % tile	0.000026	0	NA	2.73E-05
% over 0.1 µmol/day	0	0	NA	0
% over 1 µmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

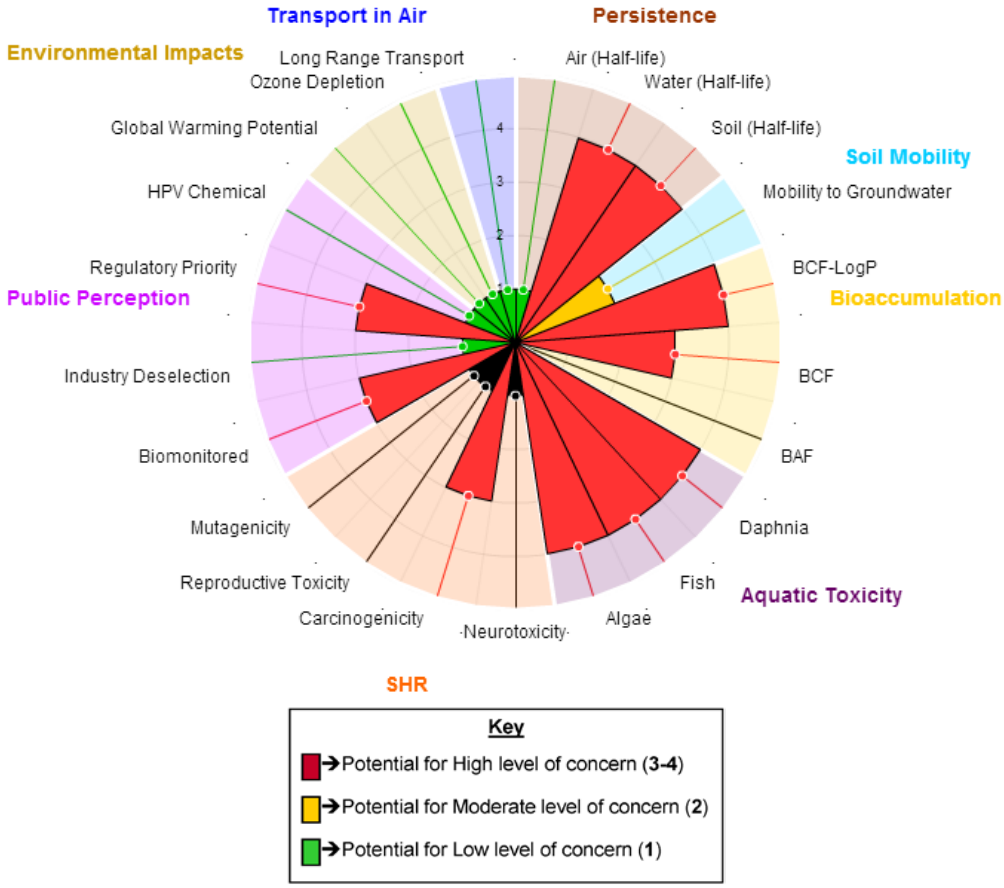
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Trifluralin

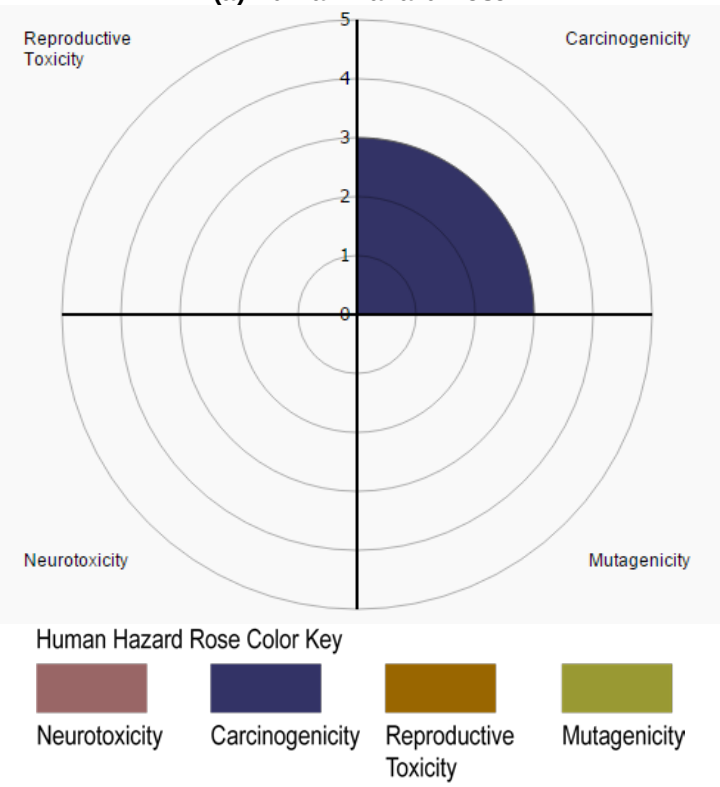
		CAS # 1582-09-8
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.4456 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 4% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 2%, Max. BOD = 5%).
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Moderate mobility to groundwater based on LogKoc = 3.986
Bioaccumulation	BCF-LogP	Very High bioconcentration potential based on an Experimental LogP=5.34
	BCF	High bioconcentration potential based on Experimental LogBCF = 3.62
	BAF	
Aquatic Toxicity	Daphnia	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 1.475 mg/L indicates a Moderate toxicity to Fish [CLOGP]. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R50/53 (Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	Carc. 2: [EU_GHS]; C (Possible human carcinogen) [1986 Guidelines] [IRIS]; Not classifiable [IARC_OE]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	1 out of 2 lists (NHANES)
	Industry Deselection	0 out of 6 lists
	Regulatory Priority	2 out of 10 lists (JDES_LST; JMON3)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 194.504 km - A_TRNSPRT)



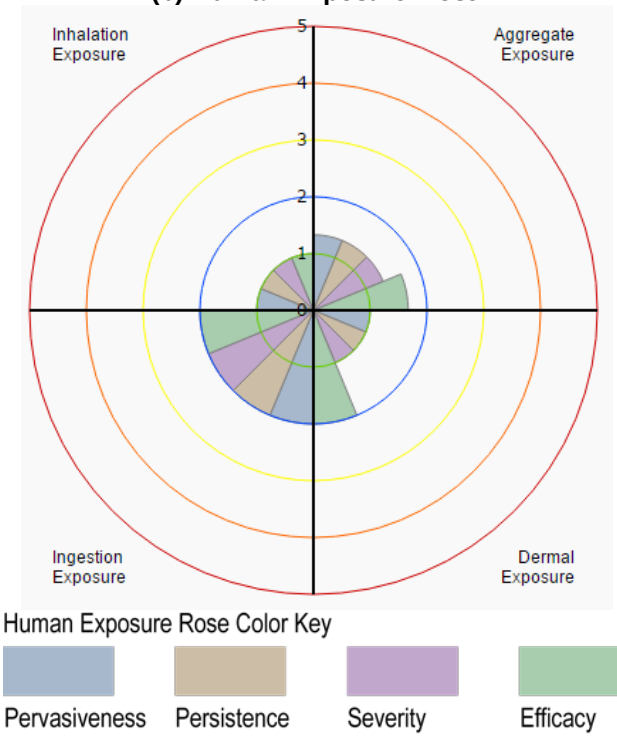
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Trifluralin

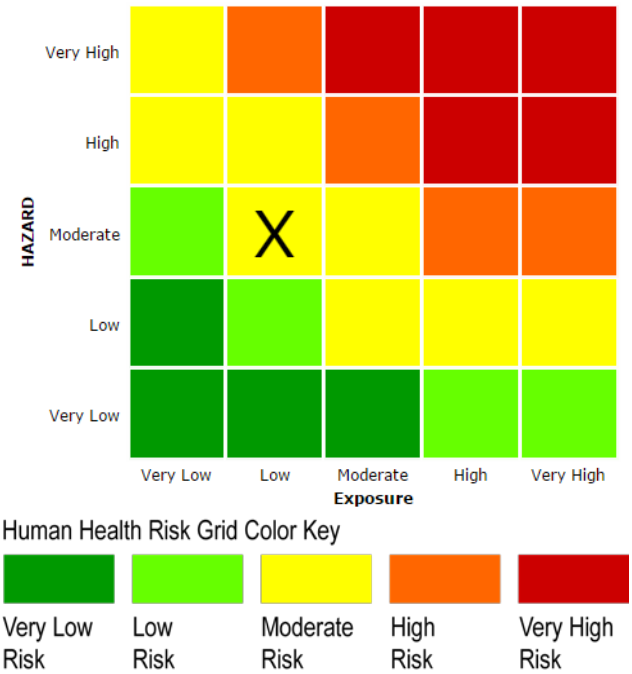
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



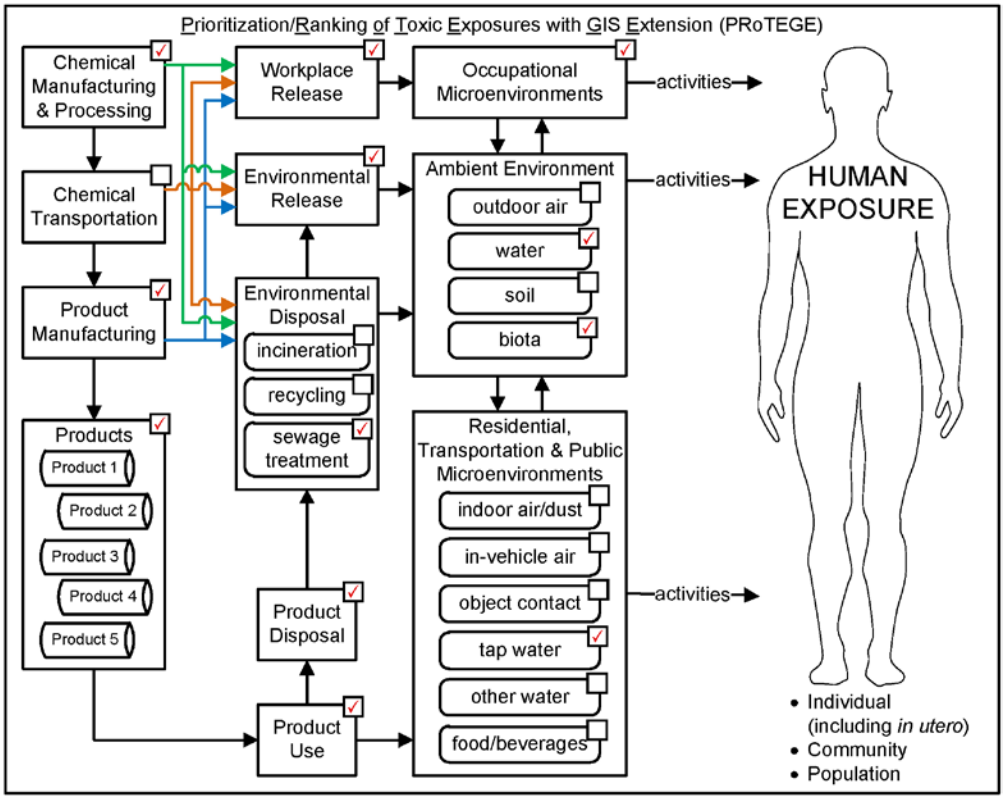
(a) Human Hazard
Estimated ranking of human hazard risk from Trifluralin, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Trifluralin (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Trifluralin, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Ranking for Tris (1,3-dichloro-2-propyl) phosphate



Summary Physico-Chemical Information	
Name	Tris (1,3-dichloro-2-propyl) phosphate
Other Names	phosphoric acid tris(1,3-dichloro-2-propyl)ester; tris(1,3-dichloroisopropyl)phosphate; tris[2-chloro-1-(chloromethyl)ethyl]phosphate
Chemical Formula	$C_9H_{15}Cl_6O_4P$
Chemical Class	PEFR
Identifier	CAS: 13674-87-8
Chemical Forms	
Physical Properties	
Clear, colorless, viscous liquid Molecular weight: 430.90 Solubility in water ≈100 ppm Vapor pressure: 10.3 mmHg at 25°C Boiling point: 236-237°C at 5 mmHg Density: 1.508 g/cm³	
Additional Notes	
Decomposes gradually when heated above 200°C	

Exposure and Toxicity Information
Toxicity Limits: LD50 orally in rat: 1.85 g/kg, LD50 dermal in rat: 2 g/kg, LC50 inhalation in rat: 5.22 g/kg
Toxicological Effects: "Abnormal" EKG
Exposure Limits: NA
Chemical Use: Flame retardant
Exposure Routes: inhalation, skin absorption
Target Organs: Heart

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air				Data sources: Surface water – data from rivers in Canada (HSDB) [101]; Tap water – data from Canada 1980 (HSDB) [102]; Biota – needles of Pinus Ponderosa (HSDB) [103]; Indoor air – [104] (5, 50, 95%tiles); Tap water - [72] (5, 50, 95%tiles)	Air	NA	
Ground water							
Food (µg/g)		<LOD			Surface Water	NA	
Indoor Air (ng/m³)	<LOD	<LOD	150		Ground Water	NA	
Surface water (ng/L)		3.7			Soil	NA	
Tap water (µg/L)	0.207	0.22	0.234				
Soil					Chemical Production and Use		
Dust					Production	10-50 million lbs/yr	USEPA IUR (2006)
Surfaces							
Biota (ng/g)	< 2.5		1260				
Outdoor air (µg/m³)							
Human Biomarkers							
Urine	NA						
Blood	NA						
Other	NA						

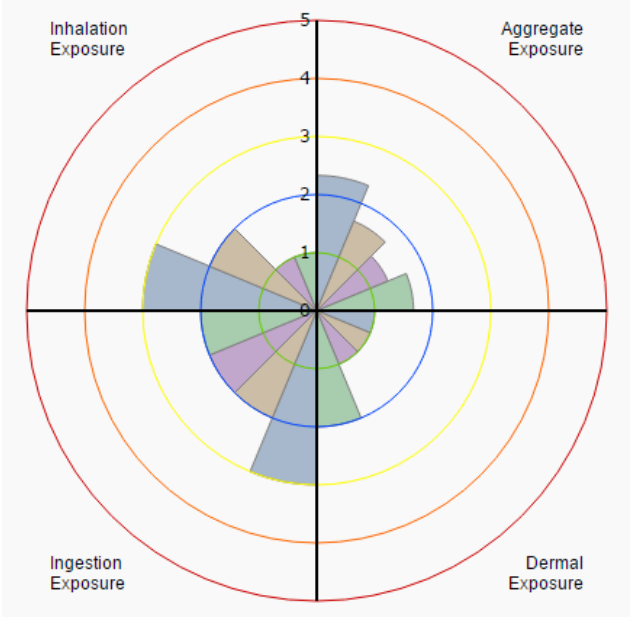
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		
	Tox Profs		□
	IRIS		
	HSDB		●
	ITER		●
	McKay		
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		●
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		●
	Tox Cast	Ph I	
		Ph II	●
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		●
	ECD		●
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		
	BME		
	ERDEM		

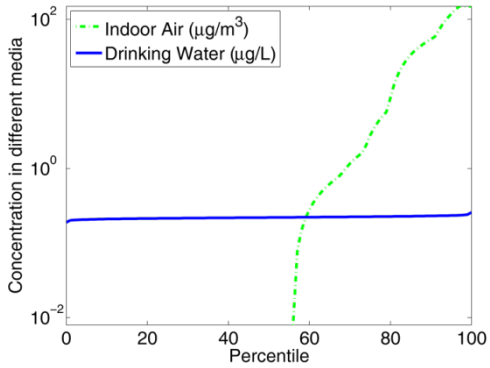
"Tier 1" Exposure Ranking for Tris (1,3-dichloro-2-propyl) phosphate

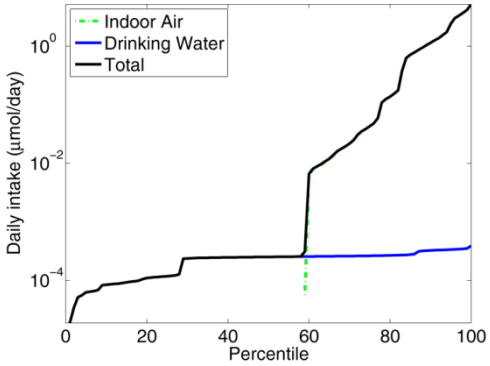
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	3	2	1	1
Ingestion	3	2	2	2
Dermal	1	1	1	2
Aggregate	2.33	1.66	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Tris (1,3-dichloro-2-propyl) phosphate





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0.000252	NA	0.000252
90 % tile	1.17	0.000325	NA	1.21
% over 0.1 µmol/day	22.5	0	NA	22.8
% over 1 µmol/day	11.6	0	NA	12

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

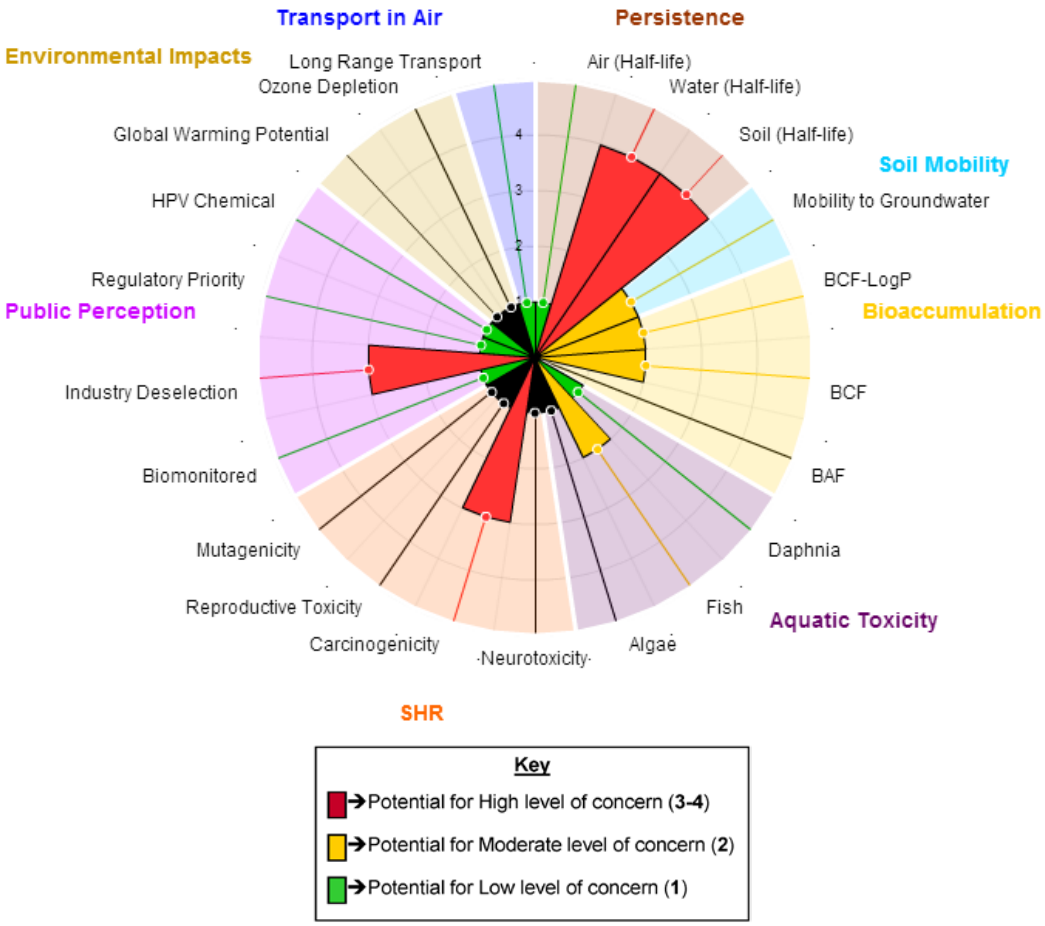
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Tris (1,3-dichloro-2-propyl) phosphate

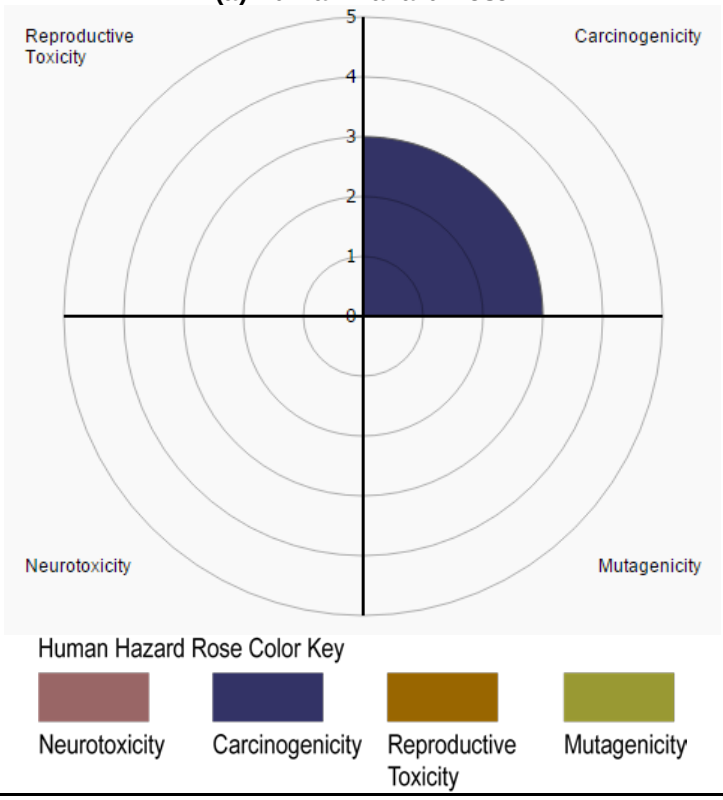
		CAS # 13674-87-8
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.5915 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 1% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 0%, Max. BOD = 4%).
	Soil (Half-life)	Very High persistence in Soil (Estimated Half-life = 360 days)
Soil Mobility	Mobility to Groundwater	Moderate mobility to groundwater based on LogKoc = 4.046
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=3.65
	BCF	Moderate bioconcentration potential based on Experimental LogBCF = 1.86
	BAF	
Aquatic Toxicity	Daphnia	An estimated LC50(48-hr) = 10.787 mg/L indicates a Low toxicity to Daphnid.
	Fish	An estimated LC50(96-hr) = 8.543 mg/L indicates a Moderate toxicity to Fish.
	Algae	No toxicity estimate.
SHR	Neurotoxicity	
	Carcinogenicity	Carc. 2: [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (GADSL)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 23.6477 km - A_TRNSPRT)



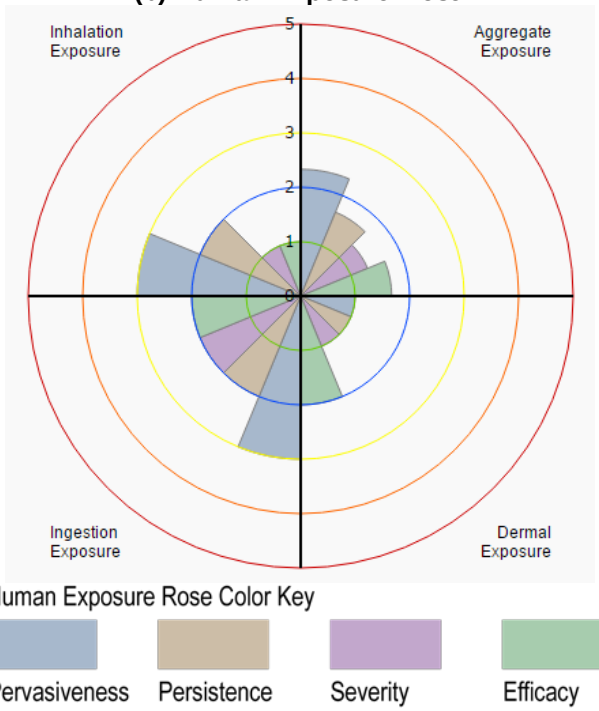
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Tris (1,3-dichloro-2-propyl) phosphate

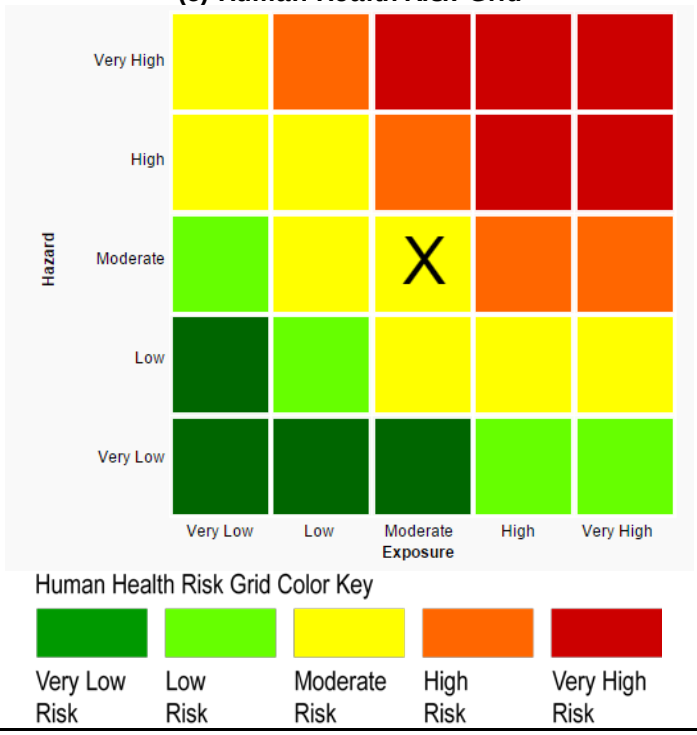
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



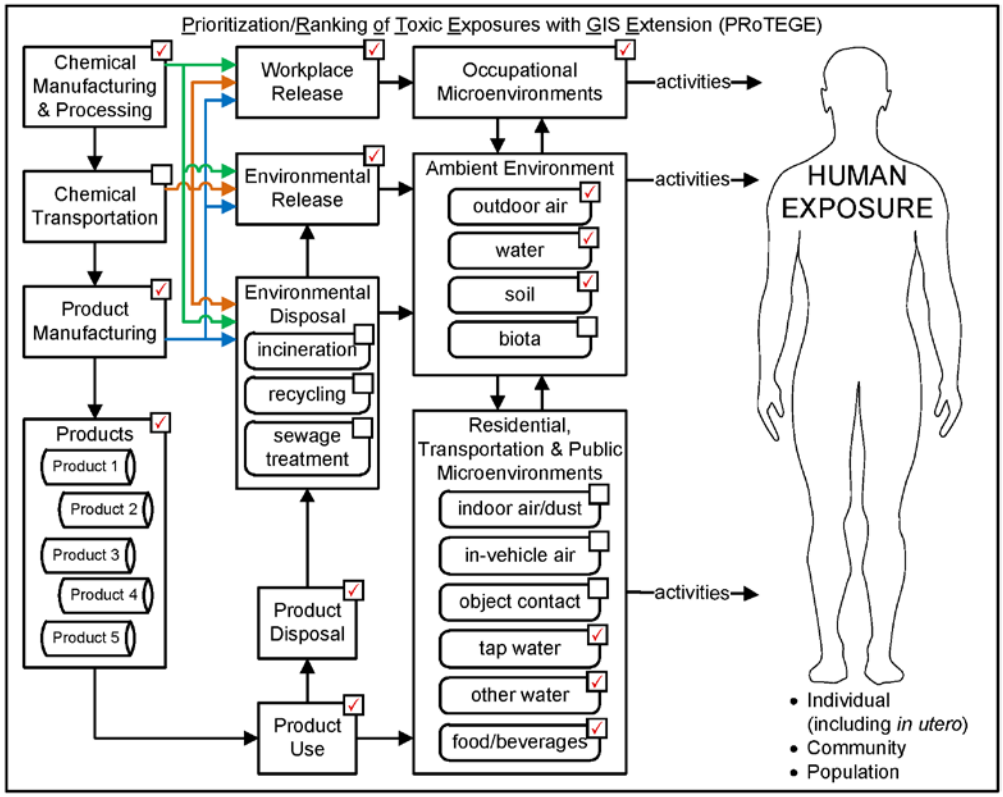
(a) Human Hazard
Estimated ranking of human hazard risk from Tris (1,3-dichloro-2-propyl) phosphate, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Tris (1,3-dichloro-2-propyl) phosphate (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Tris (1,3-dichloro-2-propyl) phosphate, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Ranking for Tris (2-chloroethyl) phosphate



Summary Physico-Chemical Information	
Name	Tris (2-chlorethyl) phosphate
Other Names	Tolgard TCEP, Fyrol CEF
Chemical Formula	$C_6H_{12}Cl_3O_4P$
Chemical Class	PEFR
Identifier	CAS: 115-96-8; RTECS: KK2450000; EC: 015-102-00-0
Chemical Forms	
Physical Properties	
Clear, transparent liquid Molecular weight: 285.5 Soluble in water and most organic solvents Solubility: 7000 mg/L Vapor pressure: 6.125×10^{-2} mmHg at 25°C Boiling point: 330°C Melting point: -55°C Density: 1.39 g/cm^3 at 25°C	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: LD50 rat oral – 1230 mg/kg (HSDB); LD50 rat inhalation > 5 mg/L for 4 hours (HSDB); LD50 rabbit dermal > 5000 mg/kg (HSDB);
Toxicological Effects:
Exposure Limits: 7.5 mg/m^3
Chemical Use: Plasticizer
Exposure Routes: Inhalation, ingestion, dermal contact
Target Organs: Skin, eyes

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m^3)	2		5	Data sources: Outdoor air (min, max)– samples from Kitakyusu, Japan (HSDB) [105]; Ground water – (min, mean, max) samples from Nieschen, Germany (HSDB) [106]; Food -TDS (5, 50, 95%tiles); Indoor air – [104,107] (5, 50, 95%tiles); Tap water - [72] (5, 50, 95%tiles); Soil (min, max) – samples from river and sea sediments near Kitakyushu City, Japan, 1980(HSDB) [108]; Dust (median) – Pilot study in Germany (HSDB) [109];	Air	NA	
Ground water (ppb)	0	71	96				
Food (ppb)	0.74	1	47.6		Surface Water	NA	
Indoor Air (µg/m^3)	0.46	8.55	564		Ground Water	NA	
Surface water					Soil	NA	
Tap water (µg/L)	0.123	0.15	0.18				
Soil (ppm)	13		28		Chemical Production and Use		
Dust (µg/cm^2)		0.1			Production	0.5 – 1 million lbs/year (2006)	Data source: US EPA
Surfaces							
Biota							
Human Biomarkers							
Urine	NA						
Blood	NA						
Other	NA						

Availability of Information in Databases and Reference Documents

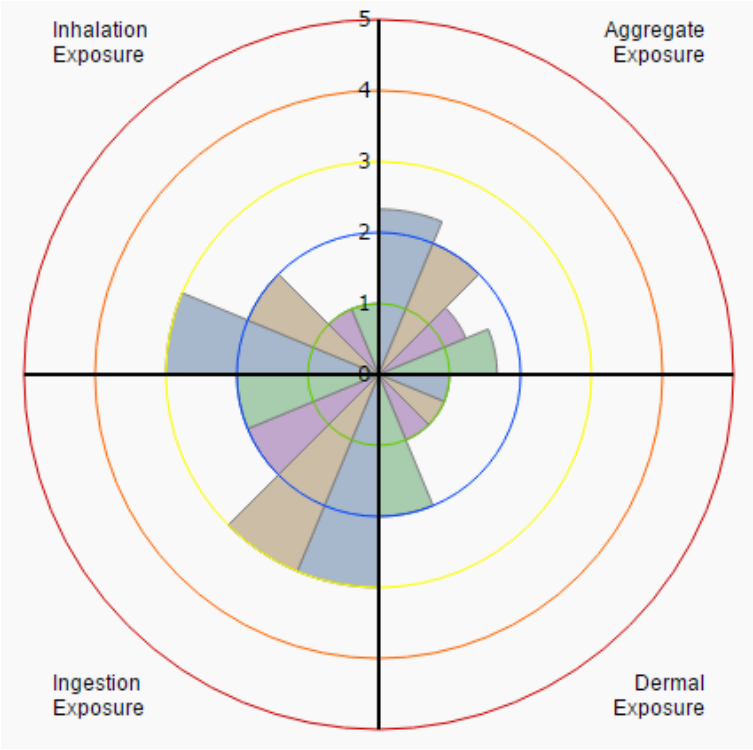
"Tier 1" Exposure Ranking for Tris (2-chloroethyl) phosphate

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

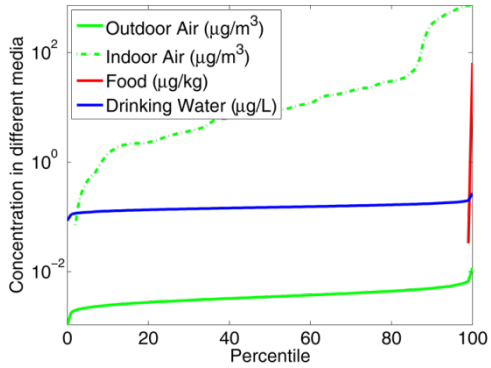
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		
	ICSC		●
	Tox Profs		
	IRIS		
	HSDB		●
	ITER		●
	McKay		●
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		●
	REACH		●
	PFD		
	MSDS		●
	DSSTox		●
	TMI		
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	●
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		●
	ECD		●
	SRD		
Releases	TRI		
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PK m(R/r) [21]
	BME		● [30]
	ERDEM		

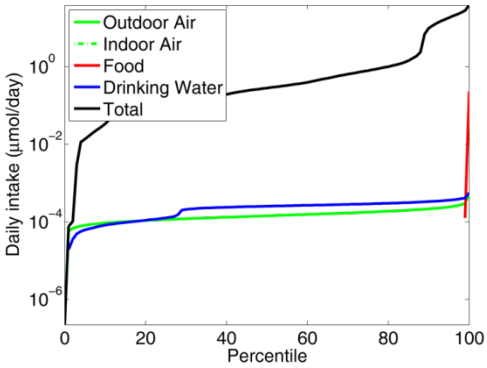
Semi-Quantitative Exposure Ranking				
	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	3	2	1	1
Ingestion	3	3	2	2
Dermal	1	1	1	2
Aggregate	2.33	2	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Tris (2-chloroethyl) phosphate





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.282	0.000253	NA	0.282
90 % tile	10.1	0.000336	NA	10.8
% over 0.1 μmol/day	73.5	0.563	NA	73.4
% over 1 μmol/day	20.3	0	NA	20.6

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

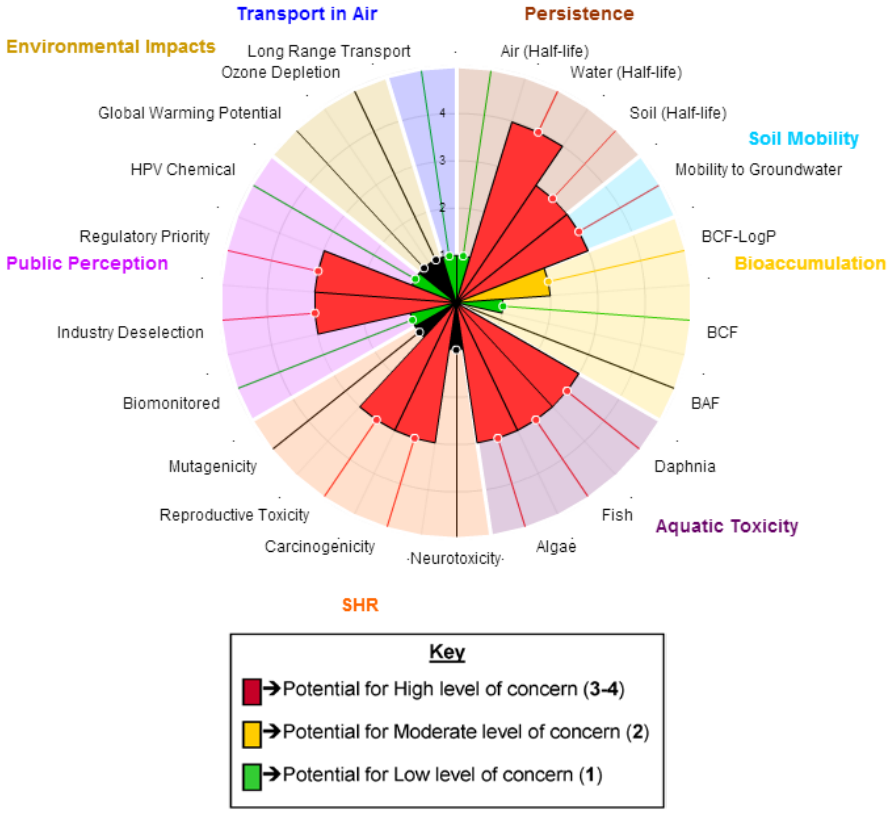
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Tris (2-chloroethyl) phosphate

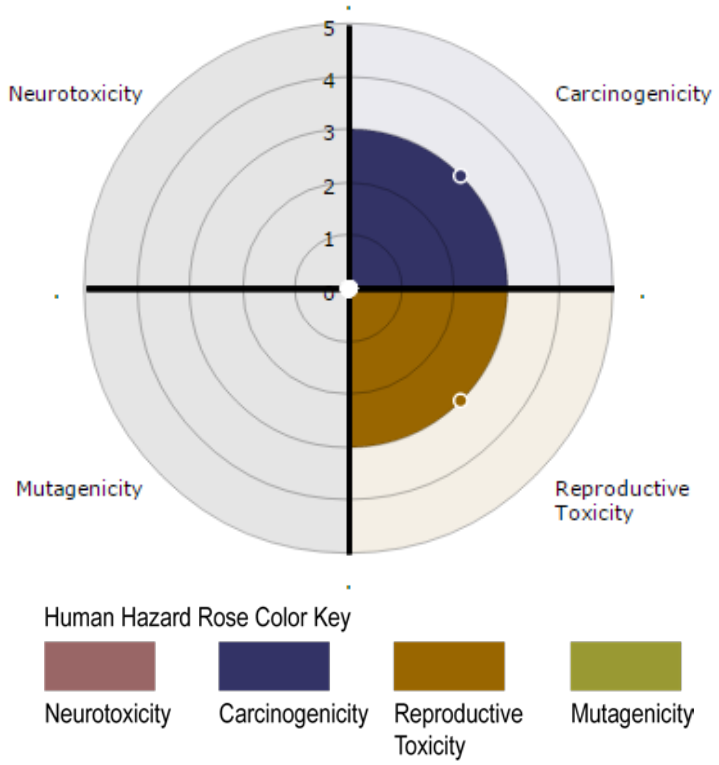
		CAS # 115-96-8
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.4864 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 4% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is very persistent in water (Min. BOD = 1%, Max. BOD = 5%).
	Soil (Half-life)	High persistence in Soil (Estimated Half-life = 120 days)
Soil Mobility	Mobility to Groundwater	High mobility to groundwater based on LogKoc = 2.478
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=1.44
	BCF	Low bioconcentration potential based on Experimental LogBCF = 0.4
	BAF	
Aquatic Toxicity	Daphnia	A measured EC50(48-hr) = 170 mg/L indicates a Low toxicity to Daphnia. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	A measured LC50 (96-hr) >100 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	A measured EC50 (72-hr) = 450 mg/L indicates a Low toxicity to Algae. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	Carc. 2: [EU_GHS]; Not classifiable [IARC_OE]
	Reproductive Toxicity	Toxic to reproduction - Category 1B/2A [EU_RA17_5]; TOXIC TO REPRODUCTION - Hazard category 1B [EU_GHS]
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	3 out of 6 lists (GADSL; EUC2; SINLIST)
	Regulatory Priority	3 out of 10 lists (EU_CAND; EU_RA14; JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 87.5422 km - A_TRNSPRT)



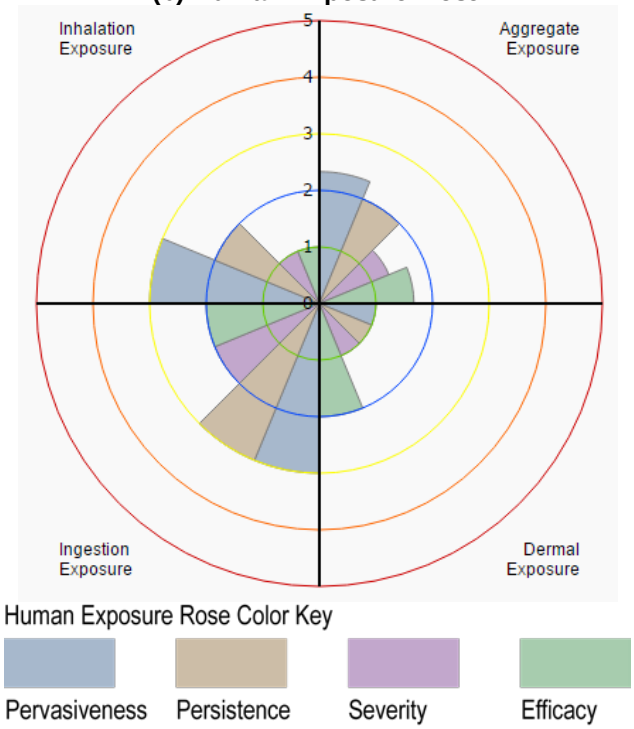
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Tris (2-chloroethyl) phosphate

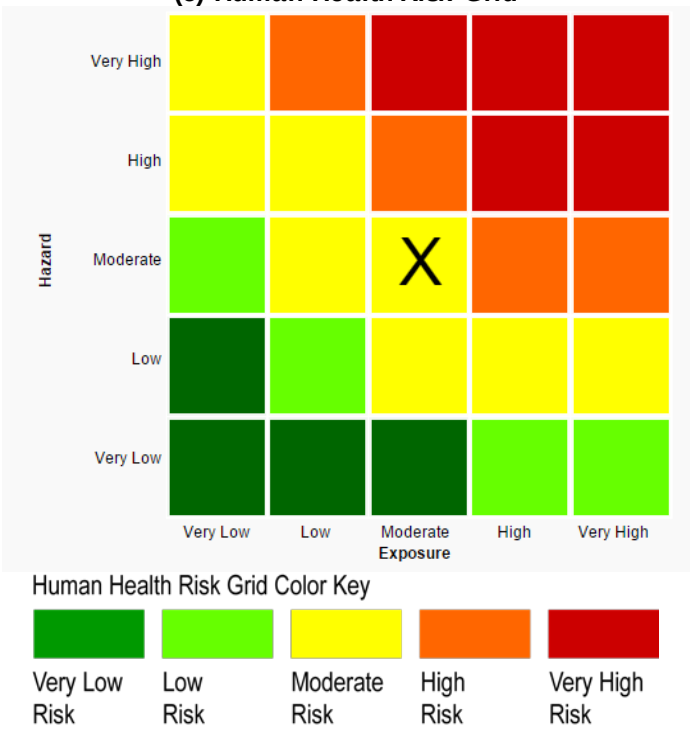
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



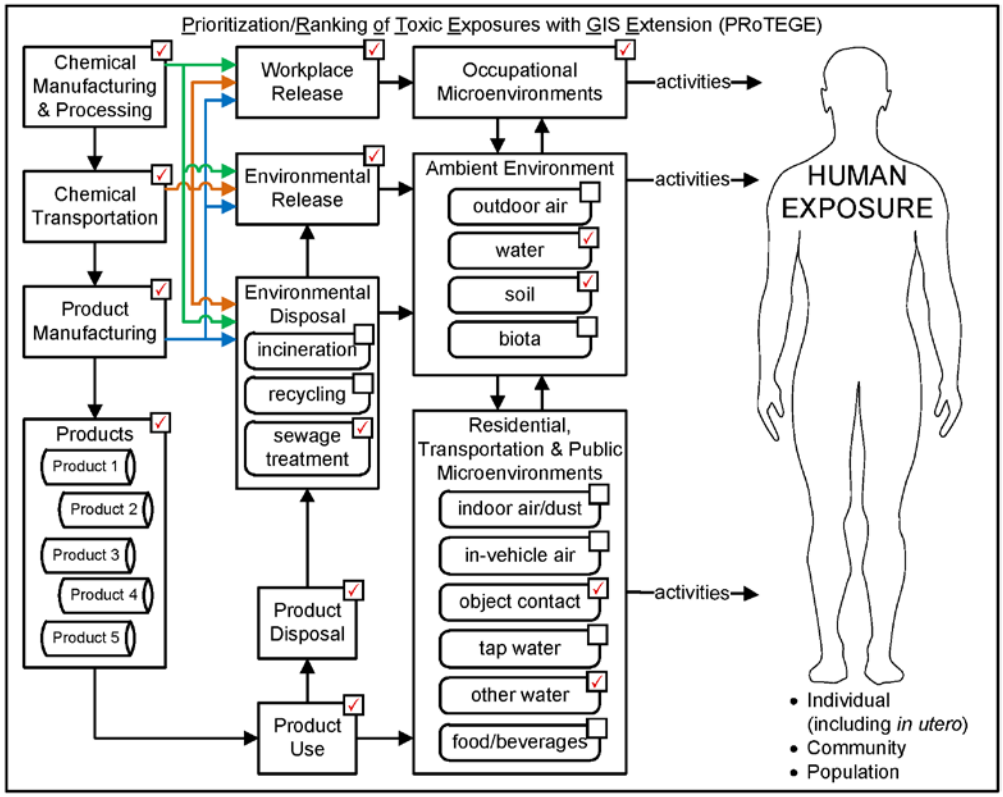
(a) Human Hazard
Estimated ranking of human hazard risk from Tris (2-chloroethyl) phosphate, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Tris (2-chloroethyl) phosphate (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Tris (2-chloroethyl) phosphate, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

PRoTEGE Ranking for Vinclozolin



Summary Physico-Chemical Information	
Name	Vinclozolin
Other Names	Ronilan, Curalan, Vorlan, Touche
Chemical Formula	$C_{12}H_9Cl_2NO_3$
Chemical Class	Fung
Identifier	CAS: 50471-44-8
Chemical Forms	
Physical Properties	
Crystalline solid, with slight aromatic odor Molecular weight: 286.11 Melting point: 108°C Boiling point: 131°C at 0.05 mmHg Density: 1.51 g/cm³ Vapor pressure: 1.2e-7 mmHg at 20°C Solubility in water: 2.6 mg/L at 20°C	
Additional Notes	
Basic manufacturer: BASF Corporation	

Exposure and Toxicity Information
Toxicity Limits: LD50 dermal (rat) > 2.5 g/kg; LD50 oral (rat) 10 g/kg; LC50 inhalation (rat) > 29.1 g/m³ over 4 hr; NOEL: 100 ppm(2.5 mg/kg/day) (IRIS)
Toxicological Effects: Carcinogenic classification – C (Possible Human Carcinogen) (HSDB)
Exposure Limits:
Chemical Use: Fungicide
Exposure Routes: Inhalation of contaminated dust, dermal contact, ingestion of contaminated food
Target Organs: Uterus, placenta

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air				Data sources: Ground water (mean) - estimated environmental conc.(USEPA) [110]; Food (min, median, max) (TDS); Surface water (mean) - estimated environmental conc.(USEPA) [110]; Tap water - [72] (not detected in 15 samples)	Air		
Ground water (ppb)		0.57					
Food (µg/g)	0.6	2	204		Surface Water		
Indoor Air					Ground Water		
Surface water (µg/L)		9.4			Soil		
Tap water	<LOD		<LOD				
Soil					Chemical Production and Use		
Dust					Production		
Surfaces							
Biota					Use	51740 lbs/year	Source: NAWQA
Human Biomarkers							
Urine							
Blood							
Other							

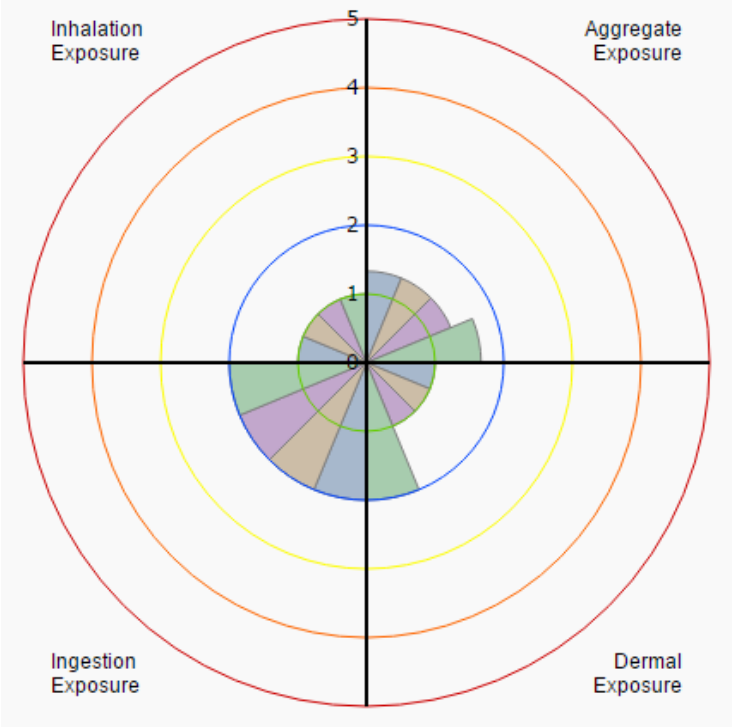
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		
	NIOSH		
	ICSC		
	Tox Profs		
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		
	RIVM rprts		
	IARC		
	PSAP		
	NTP		
	REACH		
	PFD		●
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	●
		Ph II	
	Tox RefDB		●
	CEBS		
Production and Use	SIDS		
	EHPV		
	HPD		●
	IUR		
	ECD		○
	SRD		
Releases	TRI		●
	NEI		
Environmental Quality	NGA		
	NAWQA		
	AQS		
	CERCLIS		
	NATA		
Micro-environments and Biomarkers-Human and Ecological	TDS		●
	SDWIS		
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PKd (R) [57]
	BME		
	ERDEM		

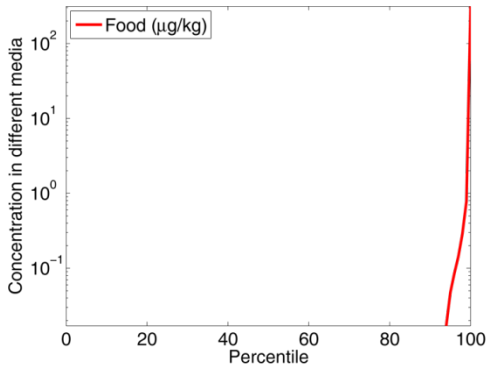
"Tier 1" Exposure Ranking for Vinclozolin

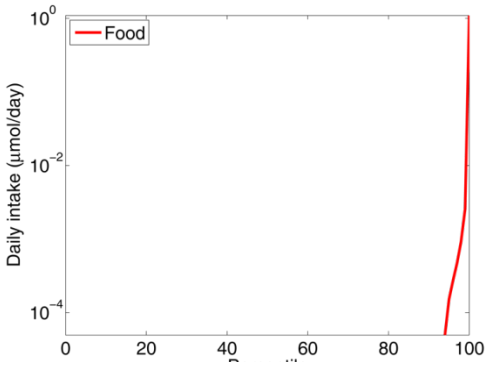
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	1	1	1	1
Ingestion	2	2	2	2
Dermal	1	1	1	2
Aggregate	1.33	1.33	1.33	1.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Vinclozolin





	Inhalation	Ingestion	Dermal	Aggregate
Median (µmol/day)	0	0	NA	0
90 %tile	0	0	NA	0
% over 0.1 µmol/day	0	0.911	NA	1.82
% over 1 µmol/day	0	0.09	NA	0.176

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

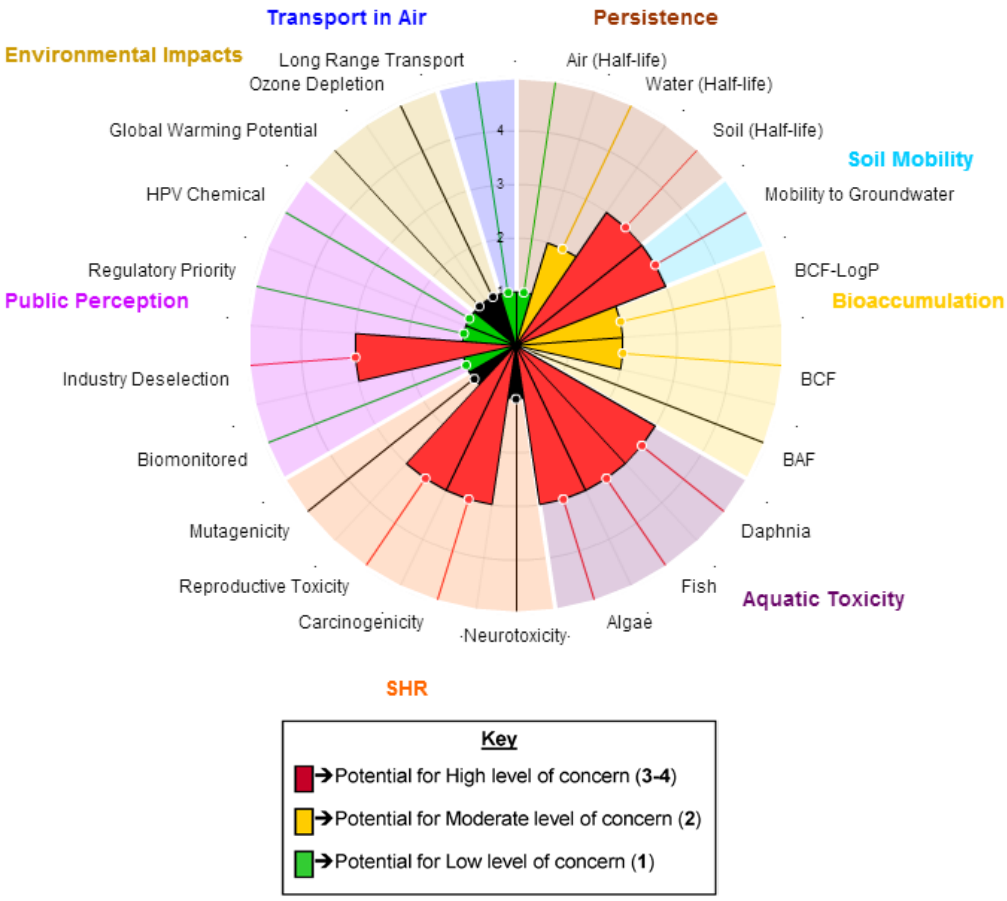
Resources for "Tier 3" Exposure Characterization

"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Vinclozolin

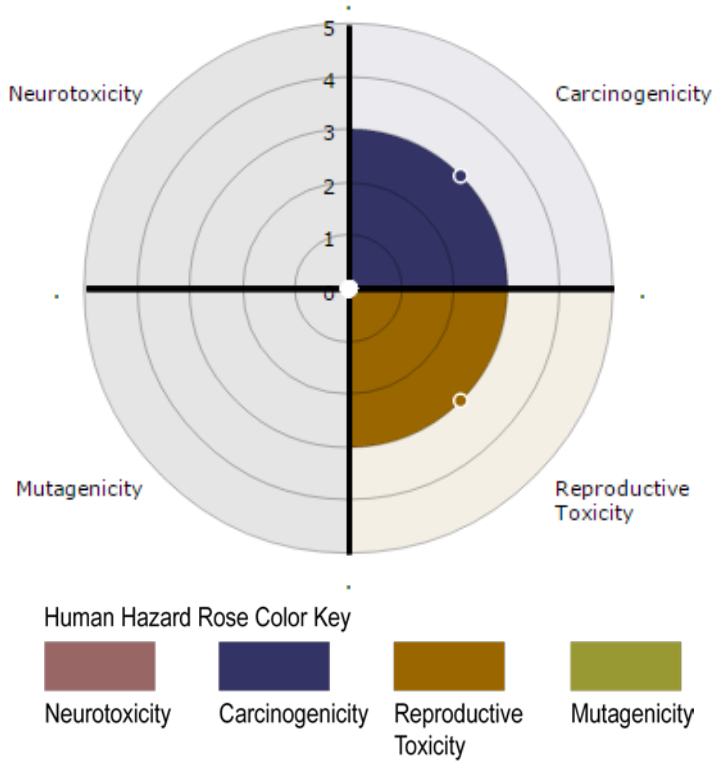
		CAS # 50471-44-8
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 0.3244 days)
	Water (Half-life)	Moderate persistence in Water (Estimated Half-life = 60 days)
	Soil (Half-life)	High persistence in Soil (Estimated Half-life = 120 days)
Soil Mobility	Mobility to Groundwater	High mobility to groundwater based on LogKoc = 2.453
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Experimental LogP=3.1
	BCF	Moderate bioconcentration potential based on Estimated LogBCF = 1.712
	BAF	
Aquatic Toxicity	Daphnia	No toxicity estimate. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Fish	An estimated LC50(96-hr) = 25.689 mg/L indicates a Low toxicity to Fish. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
	Algae	No toxicity estimate. However, this compound is classified as R51/53 (Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.).
SHR	Neurotoxicity	
	Carcinogenicity	Carc. 2: [EU_GHS]
	Reproductive Toxicity	Toxic to reproduction - Category 1B/2A [EU_RA17_5]
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	1 out of 6 lists (EUC2)
	Regulatory Priority	0 out of 10 lists
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	No data on Global Warming potential
	Ozone Depletion	No data on Ozone Depletion
Transport in Air	Long Range Transport	Low potential for Long Range Transport in Air (CTD = 64.1482 km - A_TRNSPRT)



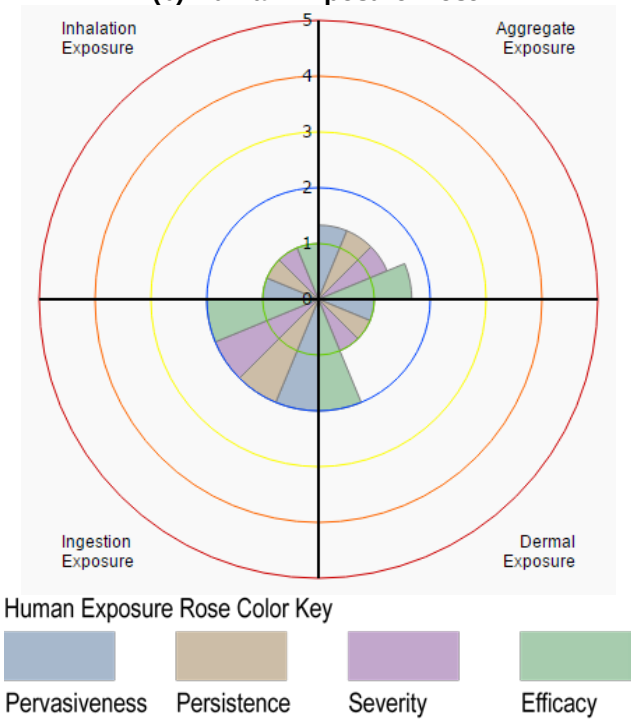
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Vinclozolin

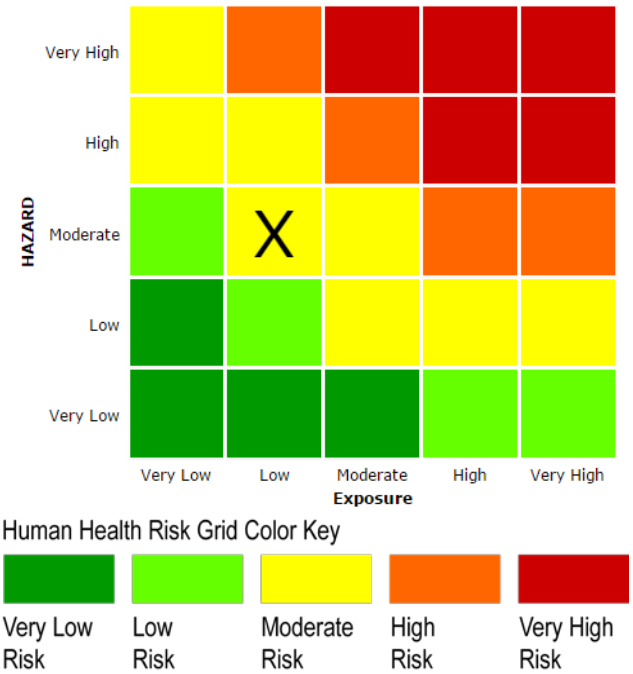
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



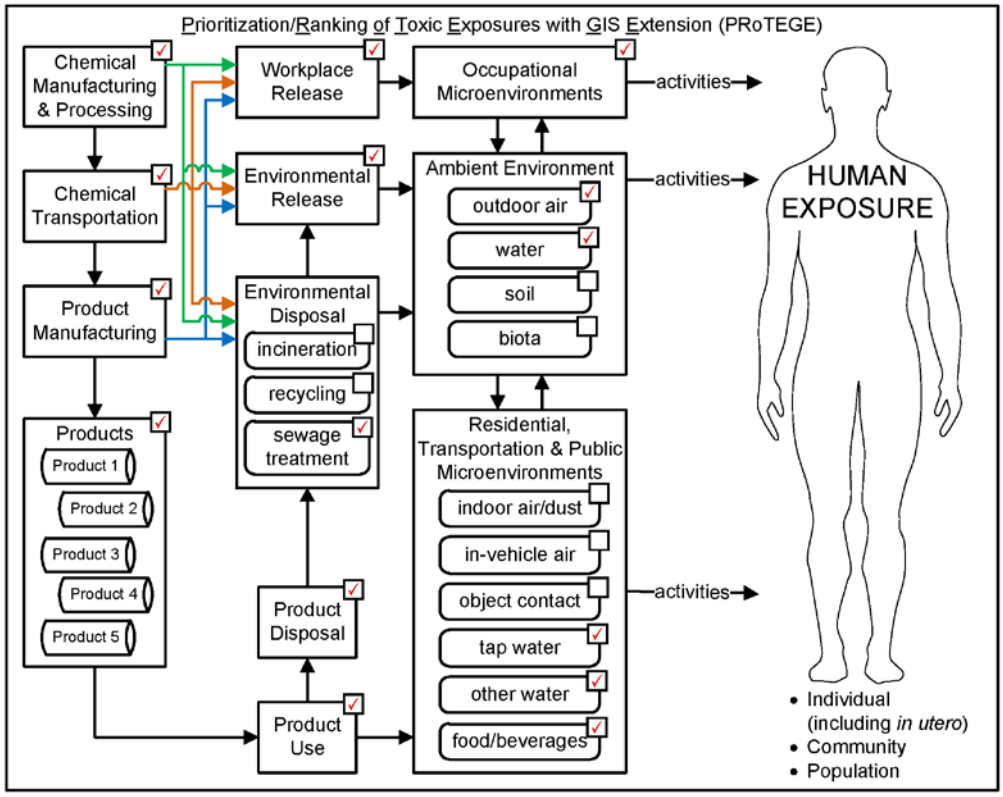
(a) Human Hazard
Estimated ranking of human hazard risk from Vinclozolin, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Vinclozolin (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Vinclozolin, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

PRoTEGE Results for Vinyl Chloride



Summary Physico-Chemical Information	
Name	Vinyl Chloride
Other Names	Chloroethene, Chloroethylene, Ethylene monochloride, Monochloroethene, Monochloroethylene, VC, Vinyl chloride monomer (VCM)
Chemical Formula	CH_2=CHCl
Chemical Class	VOC
Identifier	CAS: 75-01-4; RTECS: KU9625000
Chemical Forms	
Physical Properties	
Molecular weight: 62.5 Solubility in water: 0.1% (77°F) Vapor pressure: 3.3 atm Boiling point: 7°F Freezing point: -256°F Physical characteristics: Colorless gas or liquid (below 7°F) with a pleasant odor at high concentrations. [Note: Shipped as a liquefied compressed gas.]	
Additional Notes	

Exposure and Toxicity Information
Toxicity Limits: RfD: 0.003 mg/kg/day (IRIS); RfC: 0.1 mg/kg/day (IRIS)
Toxicological Effects: Carcinogenic classification: A (IRIS)
Exposure Limits: OSHA PEL: 1910.1017; TWA 1 ppm C 5 ppm [15-minute]; LEL: 36000 ppm (EPA)
Chemical Use: Manufacture of polyvinyl chloride (PVC) and other chlorinated compounds
Exposure Routes: Inhalation, skin and/or eye contact (liquid)
Target Organs: Liver, central nervous system, blood, respiratory system, lymphatic system

Environmental Concentrations					Environmental Releases		
	Low	Medium	High	Notes		Emissions Tons/yr	% Counties Reporting Emissions
Outdoor air (µg/m³)	0	0.05	0.1726	Data sources: Outdoor air (5, 50, 95%tiles) – NATA 2002; Ground water (min, max) – in 2 of 13 US cities groundwater supplies (HSDB) [57]; Food (mean) – in alcoholic beverages packed in vinyl chloride containing packages (IARC); Surface water (min, max) – in US cities (HSDB) [57]; Indoor air - [58]; Tap water - [23] (>99.9% of measurements <RL)	Air	97.46%	97.46%
Ground water (ppb)	2.2		9.4				
Food (mg/kg)		20			Surface Water	0.02 (TRI 2008)	0.19%
Indoor Air (µg/m³)	0.0038	0.025	0.17		Ground Water	NA	
Surface water (ppb)	0.2		5.1		Soil	0.004 (TRI 2008)	0.06%
Tap water	<RL	<RL	0.15 (99.95% tile)				
Soil					Chemical Production and Use		
Dust					Production	18165 million lbs/yr	Data source: CMR 2003
Surfaces							
Biota							
Human Biomarkers				*conc. of metabolite thiodiglycolic acid found in workers exposed to vinyl chloride conc. of 0.14 - 7 ppm in workplace [59].			
Urine (mg/L)*	0.3 - 4						
Blood	NA						
Other	NA						

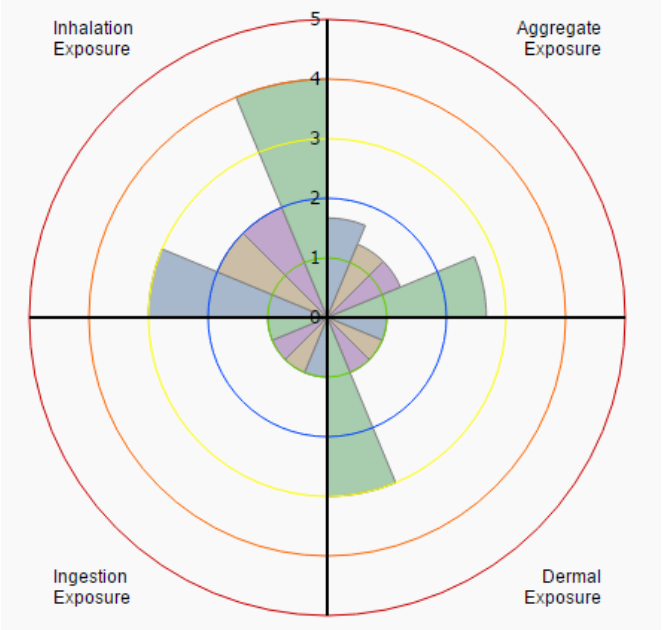
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

Availability of Information in Databases and Reference Documents			
Physicochemical and/or Toxicological Properties	PAC		●
	NIOSH		●
	ICSC		●
	Tox Profs		●
	IRIS		●
	HSDB		●
	ITER		●
	McKay		●
	Howard		●
	RIVM rprts		●
	IARC		●
	PSAP		
	NTP		
	REACH		
	PFD		
	MSDS		●
	DSSTox		●
	TMI		●
	SCP		●
	HPVIS		
	Tox Cast	Ph I	
		Ph II	
	Tox RefDB		
	CEBS		
Production and Use	SIDS		●
	EHPV		
	HPD		
	IUR		●
	ECD		●
	SRD		
Releases	TRI		●
	NEI		●
Environmental Quality	NGA		
	NAWQA		●
	AQS		●
	CERCLIS		●
	NATA		●
Micro-environments and Biomarkers-Human and Ecological	TDS		
	SDWIS		●
	NHANES	03-04	
		05-06	
		07-08	
		09-10	
	NHEXAS		
PK/PBPK Model (or Data)	ScLit		PBPKm(R/M/H) [60]
	BME		
	ERDEM		

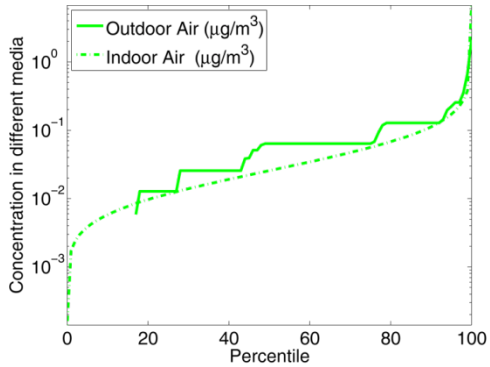
"Tier 1" Exposure Ranking for Vinyl Chloride

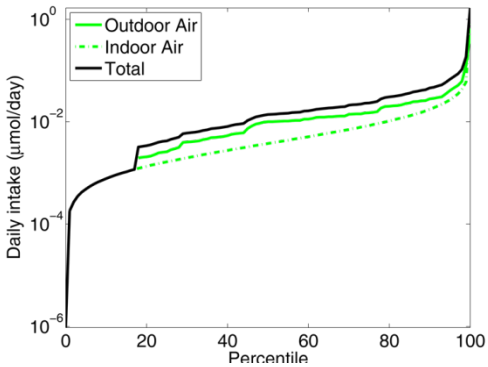
Semi-Quantitative Exposure Ranking	Pervasiveness	Persistence	Severity	Efficacy
Inhalation	3	2	2	4
Ingestion	1	1	1	1
Dermal	1	1	1	3
Aggregate	1.66	1.33	1.33	2.66

The semi-quantitative metrics of "Tier 1" reflect: (i) how widespread the exposures could be within the general US population (*pervasiveness*); (ii) the temporal frequency and/or duration of such exposures (*persistence*); (iii) the potential for high levels of such exposures (*severity*); (iv) the potential of the contact with the chemical to result in intake/uptake (*efficacy*).



"Tier 2" Exposure Ranking for Vinyl Chloride





	Inhalation	Ingestion	Dermal	Aggregate
Median (μmol/day)	0.0147	0	NA	0.0147
90 % tile	0.0414	0	NA	0.0423
% over 0.1 μmol/day	1.81	0.505	NA	2.54
% over 1 μmol/day	0	0	NA	0

"Tier 2" estimates are based on (a) different exposure factors sampled from national distributions for the general US population (inhalation rates, food intake rates, drinking water intake, time spent indoors, etc.); and (b) concentrations of the chemical in multiple media sampled from national measured distributions. (Contributions from Environmental Tobacco Smoke are not considered in "Tier 2" Exposure Characterization.)

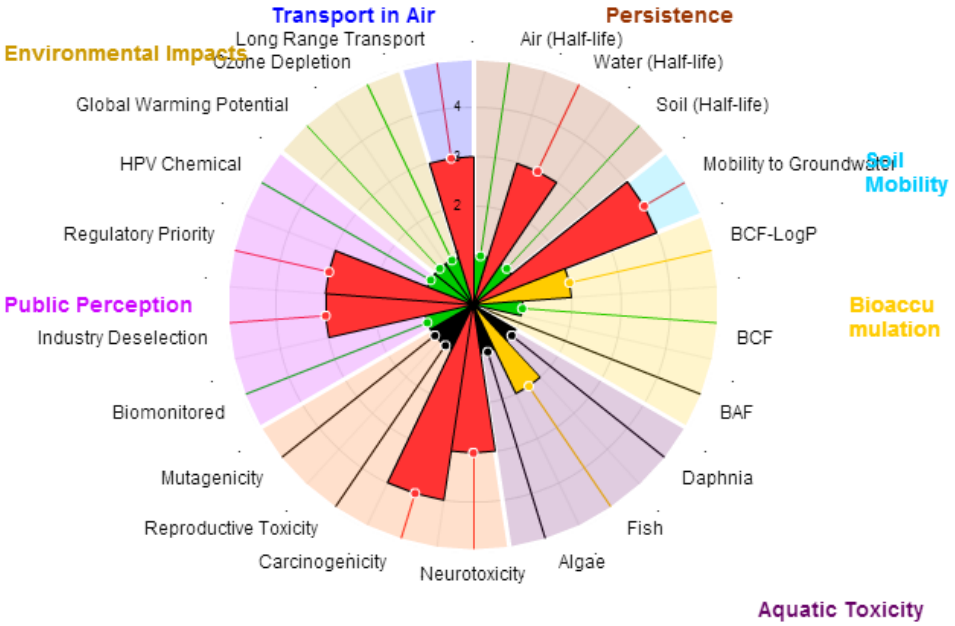
Resources for "Tier 3" Exposure Characterization

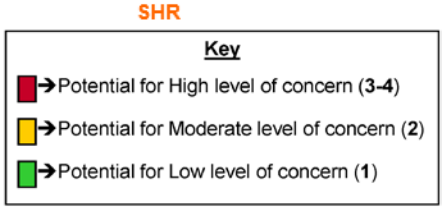
"Tier 3" exposure characterization should consider issues such as: exposures of susceptible subpopulations; occupational exposures; spatial and temporal heterogeneity of exposures, etc.

IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

METIS Results for Vinyl Chloride

		CAS # 75-01-4
Persistence	Air (Half-life)	Low persistence in Air (Estimated Half-life = 1.937 days)
	Water (Half-life)	A measured average Biochemical Oxygen Demand (BOD) = 16% using a Modified MITI Biodegradation Test (OECD 301C) would indicate that this chemical is persistent in water (Min. BOD = 16%, Max. BOD = 16%).
	Soil (Half-life)	Low persistence in Soil (Estimated Half-life = 30 days)
Soil Mobility	Mobility to Groundwater	Very High mobility to groundwater based on LogKoc = 1.375
Bioaccumulation	BCF-LogP	Moderate bioconcentration potential based on an Estimated LogP=1.62
	BCF	Low bioconcentration potential based on Estimated LogBCF = 0.55
	BAF	
Aquatic Toxicity	Daphnia	No toxicity estimate.
	Fish	An estimated LC50(96-hr) = 2.315 mg/L indicates a Moderate toxicity to Fish [CLOGP].
	Algae	No toxicity estimate.
SHR	Neurotoxicity	Known Neurotoxin Grandjean and Landrigan [22]
	Carcinogenicity	CLASS A1 - Confirmed Human Carcinogen [ACGIH]; Known Carcinogen - human studies indicate a causal relationship between exposure and human cancer [NTPLIST]; Carcinogenic to humans [IARC_OE]; Carc. 1A: [EU_GHS]; Known/likely human carcinogen [1996 Guidelines] [IRIS]; CARCINOGENICITY - Hazard category 1A [EU_GHS]
	Reproductive Toxicity	
	Mutagenicity	
Public Perception	Biomonitored	0 out of 2 lists
	Industry Deselection	3 out of 6 lists (GADSL; EUC2; SINLIST)
	Regulatory Priority	1 out of 10 lists (JDES_LST)
	HPV Chemical	out of lists
Environmental Impacts	Global Warming Potential	A GWP= 0 indicates that this compound does not contribute to Global Warming
	Ozone Depletion	This compound does not contribute to Ozone Depletion
Transport in Air	Long Range Transport	High potential for Long Range Transport in Air (CTD = 483.356 km - A_TRNSPRT)

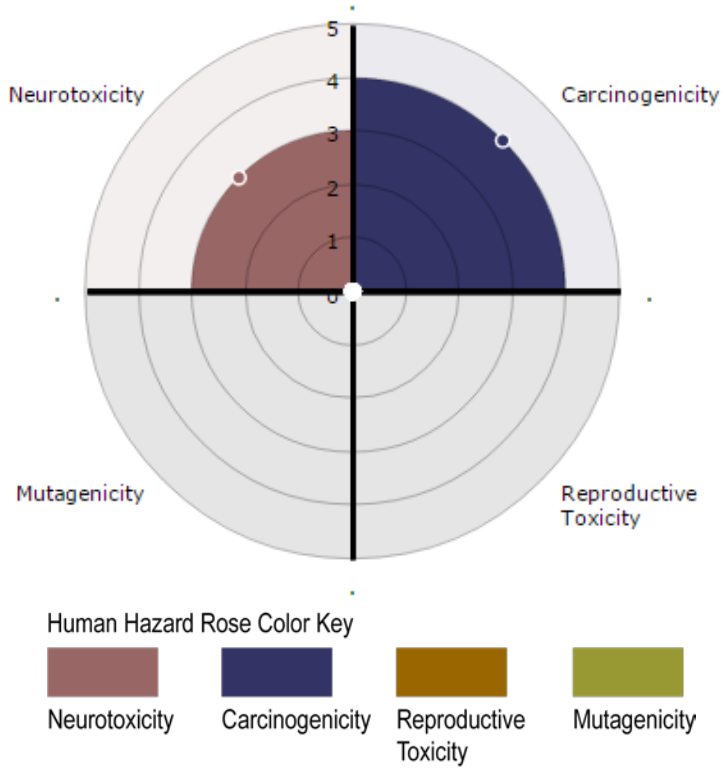




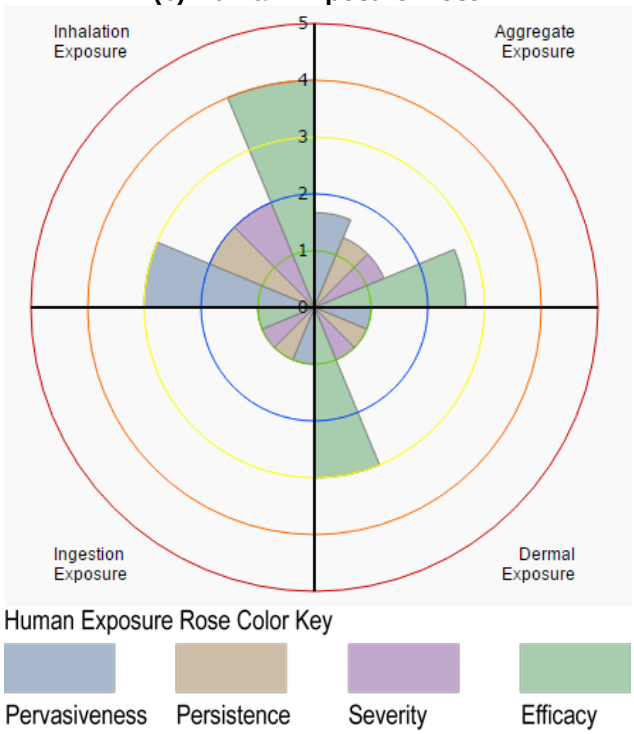
IMPORTANT NOTE: All results are preliminary and are shown for demonstration and testing purposes only

NJrisk Preliminary Results for Vinyl Chloride

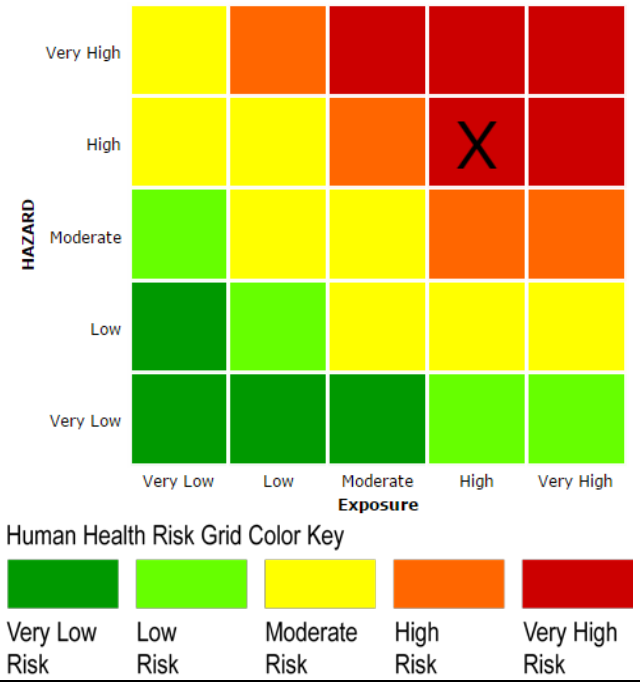
(a) Human Hazard Rose



(b) Human Exposure Rose



(c) Human Health Risk Grid



(a) Human Hazard
Estimated ranking of human hazard risk from Vinyl Chloride, in terms of neurotoxicity, carcinogenicity, reproductive toxicity, and mutagenicity.

(b) Human Exposure
Estimated human exposure ranking based on semi-quantitative metrics of pervasiveness, persistence, severity, and efficacy of Vinyl Chloride (refer to page 10 for a more detailed explanation of these metrics).

(c) Human Health Risk
Estimated human health risk from Vinyl Chloride, based on calculation of exposure values from PRoTEGE combined with hazard values from METIS (refer to page 16 for a more detailed explanation of how this ranking is calcualted).

IMPORTANT NOTE: All results are preliminary and are show n for demonstration and testing purposes only

References

1. Judson, R., Richard, A., Dix, D., Houck, K., Elloumi, F., Martin, M., Cathey, T., Transue, T.R., Spencer, R., and Wolf, M. 2008. ACTOR - Aggregated Computational Toxicology Resource. *Toxicology and Applied Pharmacology* 233 (1):7-13. PMID: WOS:000261477800004
2. Georgopoulos, P. 2008. A multiscale approach for assessing the interactions of environmental and biological systems in a holistic health risk assessment framework. *Water, Air, and Soil Pollution: Focus* 8 (1):3-21.
3. Judson, R.S., Kavlock, R.J., Setzer, R.W., Hubal, E.A., Martin, M.T., Knudsen, T.B., Houck, K.A., Thomas, R.S., Wetmore, B.A., and Dix, D.J. 2011. Estimating toxicity-related biological pathway altering doses for high-throughput chemical risk assessment. *Chemical Research in Toxicology* 24 (4):451-62. PMID: 21384849
4. Chen, M. 2010. Chemical Screening Visualization Tool: Resource for Rapid Chemical Assessment. Research Triangle Park, NC: USEPA Computational Toxicology Communities of Practice
5. NJ DEP SAB CEC Subcommittee. 2012. Proposed CEC Framework. Trenton, NJ: NJ DEP Science Advisory Board CEC Workgroup.
6. Mitchell, J., Arnot, J.A., Jolliet, O., Georgopoulos, P., Isukapalli, S., Dasgupta, S., Pandian, M., Wambaugh, J., Egeghy, P., Cohen-Hubal, E.A., and Vallero, D.A. 2013. Comparison of modeling approaches to prioritize chemicals based on estimates of exposure and exposure potential. *Science of The Total Environment* (in press).
7. Georgopoulos, P.G., Isukapalli, S.S., and Lioy, P.J. 2011. PRoTEGE - A Three-Tier System that Supports Exposure-Based Prioritization of Chemicals. US EPA Exposure-Based Chemical Prioritization Workshop: Exploring Opportunities for Collaboration, September 26-27, 2011, Research Triangle Park, NC.
8. Georgopoulos, P.G., Wang, S.W., Vyas, V.M., Sun, Q., Burke, J., Vedantham, R., McCurdy, T., and Ozkaynak, H. 2005. A source-to-dose assessment of population exposures to fine PM and ozone in Philadelphia, PA, during a summer 1999 episode. *Journal of Exposure Analysis and Environmental Epidemiology* 15 (5):439−457. PMID: 15714222
9. Georgopoulos, P.G., Wang, S.-W., Yang, Y.-C., Xue, J., Zartarian, V.G., McCurdy, T., and Ozkaynak, H. 2008. Biologically based modeling of multimedia, multipathway, multiroute population exposures to arsenic. *Journal of Exposure Science and Environmental Epidemiology* 18 (5):462-476. PMCID: 3068596. PMID: 18073786
10. Georgopoulos, P.G., and Lioy, P.J. 2006. From a theoretical framework of human exposure and dose assessment to computational system implementation: the Modeling ENvironment for TOtal Risk Studies (MENTOR). *J Toxicol Environ Health B Crit Rev* 9 (6):457-83. PMID: 17090483
11. Mackay, D., Shiu, W.Y., Ma, K.-C., and Lee, S.C. 2006. *Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals*. Boca Raton, FL: CRC Press.
12. Rosenbaum, R.K., Huijbregts, M.A.J., Henderson, A.D., Margni, M., McKone, T.E., van de Meent, D., Hauschild, M.Z., Shaked, S., Li, D.S., Gold, L.S., and Jolliet, O. 2011. USEtox human exposure and toxicity factors for comparative assessment of toxic emissions in life cycle analysis: sensitivity to key chemical properties. *International Journal of Life Cycle Assessment* 16 (8):710-727. PMID: WOS:000294060700003
13. Nazaroff, W.W. 2008. Inhalation intake fraction of pollutants from episodic indoor emissions. *Building and Environment* 43 (3):269-277.
14. Bennett, D.H., Margni, M.D., McKone, T.E., and Jolliet, O. 2002. Intake Fraction for Multimedia Pollutants: A Tool for Life Cycle Analysis and Comparative Risk Assessment. *Risk Analysis* 22 (5):905-918.

15. Hays, S.M., and Aylward, L.L. 2009. Using Biomonitoring Equivalents to interpret human biomonitoring data in a public health risk context. *Journal of Applied Toxicology* 29 (4):275-288.
16. USEPA. 2012. TSCA Work Plan Chemicals: Methods Document. Environmental Protection Agency, Office of Pollution Prevention and Toxics. http://www.epa.gov/oppt/existingchemicals/pubs/wpmethods.pdf
17. USEPA. 2011. Design for the Environment Program Alternatives Assessment Criteria for Hazard Evaluation. Version 2. USEPA Office of Pollution Prevention and Toxics. http://www.epa.gov/dfe/alternatives_assessment_criteria_for_hazard_eval.pdf
18. Wiegers, K. 2003. *Software Requirements 2*. Redmond, WA: Microsoft Press.
19. Lowdermilk, T. 2013. *User-Centered Design: A Developer's Guide to Building User-Friendly Applications*. Sebastopol, CA: O'Reilly Media.
20. Sipes, N.S., Martin, M.T., Reif, D.M., Kleinstreuer, N.C., Judson, R.S., Singh, A.V., Chandler, K.J., Dix, D.J., Kavlock, R.J., and Knudsen, T.B. 2011. Predictive models of prenatal developmental toxicity from ToxCast high-throughput screening data. *Toxicological Sciences* 124 (1):109-27. PMID: 21873373
21. Egeghy, P.P., Judson, R., Gangwal, S., Mosher, S., Smith, D., Vail, J., and Hubal, E.A.C. 2012. The exposure data landscape for manufactured chemicals. *Science of the Total Environment* 414:159-166. PMID: ISI:000300459500020
22. Grandjean, P., and Landrigan, P.J. 2006. Developmental neurotoxicity of industrial chemicals. *The Lancet* 368 (9553):2167-2178.
23. USEPA. 2010. Six-Year Review of Drinking Water Standards, edited by USEPA.
24. Kim, C.S., Gargas, M.L., and Andersen, M.E. 1994. Pharmacokinetic modeling of 2,4-dichlorophenoxyacetic acid (2,4-D) in rat and in rabbit brain following single dose administration. *Toxicol Lett* 74 (3):189-201. PMID: 7871543
25. Aylward, L.L., and Hays, S.M. 2008. Biomonitoring Equivalents (BE) dossier for 2,4-dichlorophenoxyacetic acid (2,4-D) (CAS No. 94-75-7). *Regul Toxicol Pharmacol* 51 (3 Suppl):S37-48. PMID: 18579270
26. Knaak, J.B., Dary, C.C., Okino, M.S., Power, F.W., Zhang, X., Thompson, C.B., Tornero-Velez, R., and Blancato, J.N. 2008. Parameters for Carbamate Pesticide QSAR and PBPK/PD Models for Human Risk Assessment. *Rev Environ Contam Toxicol* 193:53-212. PMID: 20614344
27. Bidleman, T.F., Billings, W.N., and Foreman, W.T. 1986. Vapor Particle Partitioning of Semivolatile Organic-Compounds - Estimates from Field Collections. *Environmental Science & Technology* 20 (10):1038-1043. PMID: ISI:A1986E251900014
28. USDA. 2009. Dioxin 08 Survey:Dioxins and Dioxin-Like Compounds in the US Meat and Poultry Supply. Risk Assessment Division, Office of Public Health, Food Safety and Inspection Service, US Department of Agriculture. http://www.fsis.usda.gov/PDF/Dioxin_Report_1009.pdf
29. Parham, F.M., and Portier, C.J. 1998. Using structural information to create physiologically based pharmacokinetic models for all polychlorinated biphenyls. II. Rates of metabolism. *Toxicol Appl Pharmacol* 151 (1):110-6. PMID: 9705893
30. Clayton, C.A., Pellizzari, E.D., Whitmore, R.W., Perritt, R.L., and Quackenboss, J.J. 1999. National Human Exposure Assessment Survey (NHEXAS): distributions and associations of lead, arsenic and volatile organic compounds in EPA region 5. *J Expo Anal Environ Epidemiol* 9 (5):381-92. PMID: 10554141
31. Ling, M.P., and Liao, C.M. 2009. A human PBPK/PD model to assess arsenic exposure risk through farmed tilapia consumption. *Bull Environ Contam Toxicol* 83 (1):108-14. PMID: 19452117
32. Hays, S.M., Aylward, L.L., Gagné, M., Nong, A., and Krishnan, K. 2010. Biomonitoring Equivalents for inorganic arsenic. *Regulatory Toxicology and Pharmacology* 58 (1):1-9.

33. Benotti, M.J., Trenholm, R.A., Vanderford, B.J., Holady, J.C., Stanford, B.D., and Snyder, S.A. 2009. Pharmaceuticals and endocrine disrupting compounds in U.S. drinking water. *Environ Sci Technol* 43 (3):597-603. PMID: 19244989
34. McMullin, T.S., Hanneman, W.H., Cranmer, B.K., Tessari, J.D., and Andersen, M.E. 2007. Oral absorption and oxidative metabolism of atrazine in rats evaluated by physiological modeling approaches. *Toxicology* 240 (1-2):1-14. PMID: 17767989
35. Hays, S.M., Nordberg, M., Yager, J.W., and Aylward, L.L. 2008. Biomonitoring Equivalents (BE) dossier for cadmium (Cd) (CAS No. 7440-43-9). *Regul Toxicol Pharmacol* 51 (3 Suppl):S49-56. PMID: 18579269
36. Rudel, R.A., Camann, D.E., Spengler, J.D., Korn, L.R., and Brody, J.G. 2003. Phthalates, Alkylphenols, Pesticides, Polybrominated Diphenyl Ethers, and Other Endocrine-Disrupting Compounds in Indoor Air and Dust. *Environmental Science & Technology* 37 (20):4543-4553.
37. Strandberg, B., Dodder, N.G., Basu, I., and Hites, R.A. 2001. Concentrations and Spatial Variations of Polybrominated Diphenyl Ethers and Other Organohalogen Compounds in Great Lakes Air. *Environmental Science & Technology* 35 (6):1078-1083.
38. Ritter, R., Scheringer, M., MacLeod, M., Schenker, U., and Hungerbuhler, K. 2009. A multi-individual pharmacokinetic model framework for interpreting time trends of persistent chemicals in human populations: application to a postban situation. *Environ Health Perspect* 117 (8):1280-6. PMCID: 2721873. PMID: 19672409
39. Schecter, A., Haffner, D., Colacino, J., Patel, K., Papke, O., Opel, M., and Birnbaum, L. 2010. Polybrominated Diphenyl Ethers (PBDEs) and Hexabromocyclodecane (HBCD) in Composite U.S. Food Samples. *Environ Health Perspect* 118 (3):357-62. PMCID: 2854763. PMID: 20064778
40. Clark, K., Cousins, I., Mackay, D., and Yamada, K. 2003. Observed Concentrations in the Environment. In *Series Anthropogenic Compounds*: Springer Berlin / Heidelberg. 125-177.
41. Lorber, M., Angerer, J., and Koch, H.M. 2010. A simple pharmacokinetic model to characterize exposure of Americans to Di-2-ethylhexyl phthalate. *J Expo Sci Environ Epidemiol* 20 (1):38-53. PMID: 19127283
42. Wilkes, C.R., Mason, A.D., Niang, L.L., Rector, H.E., Power, F.W., Tsang, A.M., Stephen, P.M., Harrison, L.S., Blancato, J.N., and Hern, S.C. 2002. Developing Individual Human Exposure Estimates for Individual DBPs. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment. Cincinnati OH. NCEA-C-1257.
43. Aylward, L.L., Hays, S.M., Gagne, M., and Krishnan, K. 2009. Derivation of Biomonitoring Equivalents for di-n-butyl phthalate (DBP), benzylbutyl phthalate (BzBP), and diethyl phthalate (DEP). *Regul Toxicol Pharmacol* 55 (3):259-67. PMID: 19751787
44. Kostiainen, R. 1995. Volatile Organic-Compounds in the Indoor Air of Normal and Sick Houses. *Atmospheric Environment* 29 (6):693-702. PMID: ISI:A1995QX17200005
45. Gargas, M.L., and Andersen, M.E. 1989. Determining kinetic constants of chlorinated ethane metabolism in the rat from rates of exhalation. *Toxicol Appl Pharmacol* 99 (2):344-53. PMID: 2734795
46. Aylward, L.L., Kirman, C.R., Blount, B.C., and Hays, S.M. 2010. Chemical-specific screening criteria for interpretation of biomonitoring data for volatile organic compounds (VOCs) - Application of steady-state PBPK model solutions. *Regulatory Toxicology and Pharmacology* 58 (1):33-44.
47. Byczkowski, J.Z., Kinkead, E.R., Leahy, H.F., Randall, G.M., and Fisher, J.W. 1994. Computer simulation of the lactational transfer of tetrachloroethylene in rats using a physiologically based model. *Toxicol Appl Pharmacol* 125 (2):228-36. PMID: 8171430
48. Conolly, R.B., Lilly, P.D., and Kimbell, J.S. 2000. Simulation modeling of the tissue disposition of formaldehyde to predict nasal DNA-protein cross-links in Fischer 344 rats, rhesus monkeys, and humans. *Environ Health Perspect* 108 Suppl 5:919-24. PMID: 11036001

49. Lane, D.A., Johnson, N.D., Hanley, M.J.J., Schroeder, W.H., and Ord, D.T. 1992. Gas- and particle-phase concentrations of .alpha.-hexachlorocyclohexane, .gamma.-hexachlorocyclohexane, and hexachlorobenzene in Ontario air. *Environmental Science & Technology* 26 (1):126-133.
50. DeJongh, J., and Blaauboer, B.J. 1997. Simulation of lindane kinetics in rats. *Toxicology* 122 (1-2):1-9. PMID: 9274797
51. USEPA. 2003. Health Effects Support Document for Manganese. USEPA Office of Water, Health and Ecological Criteria Division. Washington DC. EPA 822-R-03-003. http://www.epa.gov/safewater/ccl/pdfs/reg_determine1/support_cc1_magnese_healtheffects.pdf
52. Nong, A., Teeguarden, J.G., Clewell, H.J., 3rd, Dorman, D.C., and Andersen, M.E. 2008. Pharmacokinetic modeling of manganese in the rat IV: Assessing factors that contribute to brain accumulation during inhalation exposure. *J Toxicol Environ Health A* 71 (7):413-26. PMID: 18306088
53. Young, J.F., Wosilait, W.D., and Luecke, R.H. 2001. Analysis of methylmercury disposition in humans utilizing a PBPK model and animal pharmacokinetic data. *J Toxicol Environ Health A* 63 (1):19-52. PMID: 11346132
54. Knaak, J.B., Dary, C.C., Patterson, G.T., and Blancato, J.N. 2002. Worker Hazard Posed by Reentry into Pesticide-Treated Foliage: Reassessment of Reentry Levels/Intervals Using Foliar Residue Transfer-Percutaneous Absorption PBPK/PD Models, with Emphasis on Isofenphos and Parathion. In *Human and Ecological Risk Assessment: Theory and Practice*, edited by D. J. Paustenbach. NY, NY: John Wiley & Sons
55. Toynton, K., Luukinen, B., Buhl, K., and Stone, D. 2009. Permethrin Technical Fact Sheet. National Pesticide Information Center, Oregon State University Extension Services. http://npic.orst.edu/factsheets/Permtech.pdf
56. Tornero-Velez, R., Nichols, H.P., Evans, M.V., Devito, M.J., Dary, C.C., Dellarco, M., and Blancato, J. 2004. Towards a Generic PBPK Model of Pyrethroid Pesticides: Modeling Deltamethrin and Permethrin in the Rat. In *Society of Toxicology*. Baltimore, MD.
57. Coniglio, W.A., Miller, K., and MacKeever, D. 1980. The occurrence of volatile organics in drinking water. U.S. Environmental Protection Agency, Criteria and Standards Division. Washington, DC.
58. Hodgson, A., and Levin, H. 2003. Volatile organic compounds in indoor air: A review of concentrations measured in North America since 1990. Lawrence Berkeley National Laboratory. Berkeley, CA. LBNL-51715. http://eetd.lbl.gov/ied/pdf/LBNL-51715.pdf
59. Müller, G., Norpoth, K., Kusters, E., Herweg, K., and Versin, E. 1978. Determination of thiodiglycolic acid in urine specimens of vinyl chloride exposed workers. *International Archives of Occupational and Environmental Health* 41 (3):199-205.
60. Reitz, R.H., Gargas, M.L., Andersen, M.E., Provan, W.M., and Green, T.L. 1996. Predicting cancer risk from vinyl chloride exposure with a physiologically based pharmacokinetic model. *Toxicol Appl Pharmacol* 137 (2):253-67. PMID: 8661351