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SECONDARY VALUES FOR SIMAZINE (CAS No. 122-34-9)

A search was conducted for information on the chemical properties and toxicity of simazine to human health and to fish and aquatic life using the following databases and search engines: ECOTOX (toxicity to fish and aquatic life), IRIS (Integrated Risk Information System; toxicity to human health), CHEMFATE (environmental fate), BIODEG (degradation), HSDB (Hazardous Substances Data Bank), CCRIS (Chemical Carcinogenesis Research Info System), ATSDR ToxFAQs (Agency for Toxic Substances and Disease Registry chemical fact sheets), and EXTOXNET (Extension Toxicology Network's pesticide information project). This search yielded some useful information on simazine's properties and toxicity.

Fish and Aquatic Life Secondary Values

To derive an acute toxicity criterion for fish and aquatic life, acute toxicity test results are required for at least one species in each of eight different families. Specific requirements and the data available to meet these requirements are found in Table 1. Following a search for information on the toxicity of simazine to fish and other aquatic life, it was determined that data are available to meet six out of the eight requirements. Because data are available for a Daphnid species, it was still possible to calculate a secondary acute value for simazine.

Cold Water

To calculate a secondary acute value (SAV), the lowest genus mean acute value (GMAV) in the database is divided by the secondary acute factor (SAF; an adjustment factor corresponding to the number of satisfied requirements).

SAF for six out of eight requirements met = 5.2
Lowest GMAV = 1,567.31 µg/L (*Daphnia magna*)

SAV = GMAV/SAF
= 1,567.31 µg/L / 5.2
= 301.41 µg/L

There are currently no chronic data available for simazine which meet acceptability requirements. Therefore, a secondary chronic value (SCV) may be calculated using default acute-chronic ratios only.

SACR (secondary acute-chronic ratio) = Geometric mean of three species mean acute-chronic ratios (SMACRs).

SMACR 1 = 18 (default)
SMACR 2 = 18 (default)

SMACR 3 = 18 (default)

SACR = geometric mean of 18, 18, and 18 = 18

SCV = SAV/SACR
= 301.41 μg/L / 18
= 16.74 μg/L

So for cold water-designated waters, the secondary acute value is 301 μg/L and the secondary chronic value is 17 μg/L for simazine.

<u>Warm Water Sportfish, Warm Water Forage Fish, Limited Forage Fish, and Limited Aquatic Life</u>

Because the lowest GMAV in the cold water database is for *Daphnia magna*, an invertebrate species that will not drop out of the database for any of the remaining water body use designations, secondary values calculated for cold water designated waters will apply for warm water sportfish, warm water forage fish, limited forage fish and limited aquatic life-designated waters as well.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for simazine, and corresponding acute toxicity data.

Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference #[a]	Source
1. At least one salmonid fish in the family Salmonidae, in the class Osteichthyes.					
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>100,000**	**9**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**56,000**	**10**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>100,000**	**6**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**25,000**	**13**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>10,000**	**2**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**40,500**	**2**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**70,500**	**2**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>82,000**	**2**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**60,000**	**2**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**44,600**	**2**	**AQUIRE**
SMAV = 49,466.05					
Salmo trutta	**brown trout**	**96-h/LC50**	**83,000**	**14**	**AQUIRE**
SMAV = 83,000					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
Ameiurus melas	**black bullhead**	**96-h/LC50**	**65,000**	**1**	**AQUIRE**
SMAV = 65,000					
Ameiurus natalis	**yellow bullhead**	**96-h/LC50**	**110,000**	**2**	**AQUIRE**
SMAV = 110,000					
Genus Mean Acute Value (GMAV; *Ameirus* sp.) = 84,557.67					

***Ictalurus* sp.** **catfish** **96-h/LC50** **65,000** **9** **AQUIRE**
SMAV = 65,000

Ictalurus punctatus **catfish** **96-h/LC50** **85,000** **2** **AQUIRE**
SMAV = 85,000

GMAV (*Ictalurus* sp.) = 74,330.34

Micropterus salmoides **largemouth bass** **96-h/LC50** **46,000** **2** **AQUIRE**
SMAV = 46,000

Morone saxatilis **striped bass** **96-h/LC50** **>180,000** **11** **AQUIRE**
Morone saxatilis **striped bass** **96-h/LC50** **822,000** **12** **AQUIRE**
Morone saxatilis **striped bass** **96-h/LC50** **>3,000** **2** **AQUIRE**
None of the LC50s were excluded (despite ranging over 10X) since it's unclear whether the high or low values are representative of the range.
SMAV = 76,281.96

Pimephales notatus **bluntnose minnow** **96-h/LC50** **66,000** **2** **AQUIRE**
SMAV = 66,000

Pimephales promelas **fathead minnow** **96-h/LC50** **>100,000** **6** **AQUIRE**
Pimephales promelas **fathead minnow** **96-h/LC50** **6,400** **2** **AQUIRE**
Pimephales promelas **fathead minnow** **96-h/LC50** **>10,000** **7** **AQUIRE**
Pimephales promelas **fathead minnow** **96-h/LC50** **510,000** **7** **AQUIRE**
Pimephales promelas **fathead minnow** **96-h/LC50** **5,000** **7** **AQUIRE**
None of the LC50s were excluded (despite ranging over 10X) since it's unclear whether the high or low values are representative of the range.
SMAV = 43,908.04

Poecilia reticulata **guppy** **96-h/LC50** **49,000** **9** **AQUIRE**
SMAV = 49,000

3. At least one planktonic crustacean (e.g., cladoceran, copepod).

Daphnia magna	**water flea**	**48-h/EC50**	**1,000**	**3**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**>3,500**	**4**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**1,100**	**2**	**AQUIRE**
SMAV = 1,567.31					
Daphnia pulex	**water flea**	**48-h/LC50**	**92,100**	**5**	**AQUIRE**
Daphnia pulex	**water flea**	**48-h/LC50**	**424,000**	**5**	**AQUIRE**
SMAV = 197,611.74					

Excluded from GMAV calculation since result was more than 10X the SMAV for *D. magna.*

4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).

Gammarus fasciatus	**scud**	**96-h/LC50**	**>100,000**	**6**	**AQUIRE**
Gammarus fasciatus	**scud**	**96-h/LC50**	**130,000**	**7**	**AQUIRE**
Gammarus fasciatus	**scud**	**96-h/LC50**	**13,000**	**8**	**AQUIRE**
SMAV = 55,287.75					

5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).

Pteronarcys californicus	**stonefly**	**96-h/EC50**	**1,900**	**2**	**AQUIRE**
SMAV = 1,900					

6. At least one fish or amphibian from a family in the phylum Chordata not already represented in one of the other subdivisions.

Carassius auratus	**goldfish**	**96-h/LC50**	**>32,000**	**2**	**AQUIRE**
SMAV = 32,000					
Lepomis gibbosus	**pumpkinseed**	**96-h/LC50**	**27,000**	**2**	**AQUIRE**
SMAV = 27,000					
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**90,000**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**118,000**	**10**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**100,000**	**6**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**16,000**	**2**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**35,000**	**2**	**AQUIRE**

Lepomis macrochirus SMAV = 62,476.80	**bluegill**	**96-h/LC50**	**100,000**	**7**	**AQUIRE**
Lepomis microlophus SMAV = 54,000	**redear sunfish**	**96-h/LC50**	**54,000**	**2**	**AQUIRE**
GMAV (*Lepomis* sp.) = 44,994.43					
Notropis atherinoides SMAV = 18,000	**emerald shiner**	**96-h/LC50**	**>18,000**	**2**	**AQUIRE**

7. At least one organism from a family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca).

8. At least one organism from a family in any order of insect or any other phylum not already represented in subdivisions 1 through 7.

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HUMAN HEALTH

To calculate a criteria or secondary value for the protection of human health, it is first necessary to determine if the substance has been shown to be carcinogenic (which will result in the calculation of a human cancer criteria or secondary value) or not (which will result in the calculation of a human threshold criteria or secondary value). The U.S. EPA has not yet classified simazine's carcinogenicity due to insufficient data (U.S. EPA's IRIS database). Because an oral reference dose and a log octanol water partition coefficient are available, however, it is possible to calculate a secondary threshold value for simazine.

There are several steps to calculating a human threshold secondary value: 1) calculation of the fraction of freely dissolved chemical; 2) calculation of the "baseline BAF"; 3) calculation of the "human health BAF"; and 4) calculation of the human threshold secondary value.

1) Calculation of the freely-dissolved fraction = f_{fd}

Given a standard dissolved organic carbon (DOC) concentration of 0.000002 Kg/L and a particulate organic carbon (POC) concentration of 0.00000004 Kg/L in water, the equation

$$f_{fd} = 1/\{1 + [(DOC)(K_{ow})/10] + [(POC)(K_{ow})]\}$$

can be reduced to:

$$= 1/\{1 + [(0.00000024\ Kg/L)(K_{ow})]\}$$

A log K_{ow} of 2.18 (K_{ow} of 151.3561) has been published for simazine (National Institutes of Health, Hazardous Substance Database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(151.3561)]\}$$

$$= 1/1.000036$$

$$\mathbf{= 1.0000}$$

2) Calculation of the baseline BAF

The baseline BAF is calculated according to the equations contained in 40 CFR part 132 (Final Water Quality Guidance for the Great Lakes System), Appendix B, using BAF data that was collected in one of four ways (listed in order of most preferred to least preferred):

a) a measured BAF from a field study
b) a predicted BAF based on field-measured BSAFs
c) a predicted BAF using a laboratory-measured bioconcentration factor (BCF) and a food chain multiplier (FCM)
d) a predicted BAF using a K_{ow} and a FCM

Currently, there are no BAFs, BSAFs, or BCFs available for simazine; therefore, the baseline BAF was calculated using the K_{ow} and a food chain multiplier (method d above).

Given simazine's log K_{ow} of 2.18 (K_{ow} of 151.3561), the FCMs (taken from table B-1 in GLI) are 1.007 for trophic level 3 (warm waters) and 1.001 for trophic level 4 (cold waters).

a) Cold Water

Baseline BAF = (FCM)(Kow)

= (1.001)(151.3561)

= **151.5074**

b) Warm Waters

Baseline BAF = (FCM)(Kow)

= (1.007)(151.3561)

= 152.4156

3) Calculation of the human health BAF

a) Cold Water

$BAF^{HH}_{TL4} = \{[(\text{baseline BAF})(0.044)] + 1\}\ (f_{fd})$

where

BAF^{HH}_{TL4} = Human health BAF for trophic level 4 (cold water)

baseline BAF = the baseline BAF (for cold waters) calculated in 2)

0.044 = fraction lipid value for cold water fish and aquatic life communities

f_{fd} = fraction freely dissolved

$BAF^{HH}_{TL4} = \{[(\mathbf{151.5074})(0.044)] + 1\}\ (1.0000)$

= **7.6663**

b) Warm Waters

$BAF^{HH}_{TL3} = \{[(\text{baseline BAF})(0.013)] + 1\}\ (f_{fd})$

where

BAF^{HH}_{TL3} = Human health BAF for trophic level 3 (warm waters)

baseline BAF = the baseline BAF (for warm waters) calculated in 2)

0.013 = fraction lipid value for warm water fish and aquatic life communities

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL3} = {[(**152.4156**)(0.013)] + 1} (1.0000)

= **2.9814**

4) Calculation of the human threshold secondary value

Human Threshold Secondary Value = [(ADE)(70 Kg)(RSC)]/[W_H + (F_H)(BAF)]

where

ADE = acceptable daily exposure (= oral reference dose, or RfD; = 0.005 mg/Kg/day for simazine (IRIS 2003))

70 Kg = average weight of an adult

RSC = relative source contribution to account for other routes of exposure (= 0.8 in the absence of other data)

W_H = average per capita daily water consumption (= 2 L/d for public water supplies, and 0.01 L/d for non-public water supplies)

F_H = average consumption of sport-caught fish in Wisconsin (= 0.02 Kg/d)

BAF = appropriate (cold or warm) human health BAF calculated in 3).

a) Public Water Supply/Cold Water

Human Threshold Secondary Value = [(ADE)(70 Kg)(RSC)]/[W_H + (F_H)(BAF)]

= [(0.005 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(7.6663 L/Kg)]

= 0.1300 mg/L

= 130 µg/L

b) Public Water Supply/Warm Water Sportfish

Human Threshold Secondary Value = [(ADE)(70 Kg)(RSC)]/[W_H + (F_H)(BAF)]

= [(0.005 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(2.9814 L/Kg)]

= 0.1359 mg/L

= 135.9 µg/L

c) Non-Public Water Supply/Cold Water

Human Threshold Secondary Value = [(ADE)(70 Kg)(RSC)]/[W_H + (F_H)(BAF)]

= [(0.005 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(7.6663 L/Kg)]

= 1.7146 mg/L

= 1,714.6 µg/L

d) Non-Public Water Supply/Warm Waters (Warm Water Sportfish, Warm Water Forage Fish, and Limited Forage Fish designated waters)

Human Threshold Secondary Value = [(ADE)(70 Kg)(RSC)]/[W_H + (F_H)(BAF)]

= [(0.005 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(2.9814 L/Kg)]

= 4.0230 mg/L

= 4,023 µg/L

e) Non-Public Water Supply/Limited Aquatic Life

Note: The Limited Aquatic Life classification applies to water bodies with no (or very few) fish present. Therefore, calculation of a human health threshold value for water bodies with this classification does not include a human health BAF since it is assumed that humans will not be exposed to simazine through consumption of fish in these areas.

Human Threshold Secondary Value = [(ADE)(70 Kg)(RSC)]/[W_H + (F_H)(BAF)]

= [(0.005 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0)]

= 28 mg/L

= 28,000 µg/L

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
Simazine	122-34-9	Fish and Aquatic	Acute	Cold/WWSF/WWFF/ LFF/LAL	301
Simazine	122-34-9	Fish and Aquatic	Chronic	Cold/WWSF/WWFF/ LFF/LAL	17
Simazine	122-34-9	Human Health	Human Threshold	Public Water Supply/Cold	130
Simazine	122-34-9	Human Health	Human Threshold	Public Water Supply/WWSF	136
Simazine	122-34-9	Human Health	Human Threshold	Non-Public Water Supply/Cold	1,715
Simazine	122-34-9	Human Health	Human Threshold	Non-Public Water Supply/WWSF, WWFF, LFF	4,023
Simazine	122-34-9	Human Health	Human Threshold	Non-Public Water Supply/LAL	28,000

Cold = cold water designated water bodies
WWSF = warm water sportfish designated water bodies
WWFF = warm water forage fish designated water bodies
LFF = limited forage fish designated water bodies
LAL = limited aquatic life designated water bodies (includes wetlands)