Rule 57 Aquatic Values Data Sheet

5/19/2010

Chemical or product name: 1,2,4-Trichlorobenzene *Developed by: Christopher Hull* *FAV*: 850 ug/l* *(Tier: I)*

Manufacturer (WTAs): ----- *Approved by: D. Bush* *AMV*: 420 ug/l* *(Tier: I)*

C.A.S #: 120-82-1 *Approval date: 6/2/2010* *FCV*: 130 ug/l* *(Tier: II)*

CAS, AQUIRE, QSAR: 1/12/10 *Acute CF: ----* *Chronic CF: ----*

Clearinghouse search date: 6/20/96

ACUTE DATA

Species	Endpoint (EC or LC50)	Duration (hours)	Test Type (FT,M, etc.)	Hardness mg/L	Test Chemical	LC50/EC50 ug/L	SMAV ug/L	GMAV ug/L	Rank	Reference
Midge	LC50	48	FT,M	44.7	-----	930	930	930	1	1
(Tanytarsus dissimilis)										
American Flagfish	LC50	96	FT,M	48	-----	1,217	1,217	1,217	2	2
(Jordanella floridae)	LC50	96	SR,U	48	-----	4,000 [1]				2
Rainbow Trout	LC50	96	FT,M	43-57	-----	1,520	1,453	1,453	3	3,4
(Oncorhynchus mykiss)	LC50	96	FT,M	44.7	-----	1,320				1,5
	LC50	96	FT,M	44.5	-----	1,530				6
Stonefly	LC50	96	S,U	-----	-----	1,800	1,800	1,800	4	7
(Peltoperla maria)										
Annelid	EC50	96	FT,?	-----	-----	2,140	2,140	2,140	5	8
(Lumbriculus variegatus)	LC50	96	FT,?	-----	-----	>3,370 [2]				8
Fathead Minnow	LC50	96	FT,M	44.0	-----	2,990	2,906	2,906	6	9
(Pimephales promelas)	LC50	96	FT,M	43-57	-----	2,760				4,7,10,11[3],12[3],13,14
	LC50	96	FT,M	44.7	-----	3,010				1, 5
	LC50	96	FT,M	56.3, 45.5	-----	2,870				6, 15[3], 16[3]
Bluegill Sunfish	LC50	96	FT,M	44.7	-----	3,020	3,020	3,020	7	1
(Lepomis macrochirus)										

Crayfish *(Orconectes immunis)*	LC50	96	FT,M	44.7	-----	3,020	3,020	3,020	8	1
Snail *(Aplexus hypnorum)*	LC50	96	FT,M	44.7	-----	3,160	3,160	3,160	9	1
Cnidarian	EC50	96	FT,?	-----	-----	>3,370	>3,370	>3,370	10	8
(Hydra oligactis)	LC50	96	FT,?	-----	-----	>3,370				8
Water Flea	EC50	48	FT,M	44.7	-----	3,390	3,390	3,390	11	1
(Daphnia magna)	EC50	48	S,M	160	-----	1090 [1]				17
	LC50	48	S,M	44.7	-----	2,090 [1]				3, 4, 6, 18[3]
	LC50	48	S,U	173	-----	50,000 [1]				19
Amphipod *(Gammarus minus)*	LC50	96	S,U	-----	-----	3,900	3,900	3,900	12	7
Midge *(Chironomus riparius)*	LC50	96	S,U	-----	-----	21,200	21,200	21,200	13	7
Snail *(Physa heterostropha)*	LC50	96	S,U	-----	-----	23,800	23,800	23,800	14	7

CHRONIC DATA

Species	Test type (ELS, etc.)	Duration (days)	Study Conditions (FT,M etc.)	Hardness mg/L	Test Chemical	MATC ug/L	SMCV ug/L	GMCV ug/L	Rank	Reference
Water Flea	LC	28	S,M	44.7	------	501.91832	501.91832	501.91832	1	3, 4, 6, 18
(Daphnia magna)										
Fathead Minnow	ELS	33	FT,M	44.5	------	678.233	697.22629	697.22629	2	11[3], 12[3], 13
(Pimephales promelas)	ELS	32	FT,M	-----	-----	704.63111				6
	ELS	32	FT,M	45	-----	709.21929				3, 4

*Value rounded to 2 significant figures.

[1] This value was not used to calculate the SMAV, because a FT,M value is preferred and available.

[2] This value was not used to calculate the SMAV, because an EC50 value from the same test is preferred and available.

[3] This reference reports a rounded version of the value shown here.

Min. Data Req. met	Acute Factor
2	13
3	8
4	7
5	6.1
6	5.2
7	4.3

RULE 57 AQUATIC VALUES WORK SHEET-ACUTE

Chemical Name: **1,2,4-Trichlorobenzene**
CAS #: **120-82-1**
Developed by: **Christopher Hull**
Date: **5/19/10**

AQUATIC MAXIMUM VALUE CALCULATIONS

A. Minimum 8-species requirement for Tier I is **not** met (Tier II): **No**.

1. Minimum requirements met = _____.

2. Minimum requirements missing for Tier I = _____.

3. Acute Factor = _____.

4. Toxicity is not dependent upon a water quality characteristic: _____.

   a. FAV calculation: Tier II FAV = Lowest GMAV / Acute Factor = _____ / _____ = _____.

5. Toxicity is dependent upon a water quality characteristic: _____.

   a. Slope = _____ (Table_____).

   b. FAV equation: Tier II FAV = _____ = _____ = _____.

6. Go to C.

B. Minimum 8-species requirement is met (Tier I): **Yes**.

1. Toxicity is not dependent upon a water quality characteristic: **Yes**.

   a. Tier I FAV calculation: **848.572 ug/l** (Fig. 1).

2. Toxicity is dependent upon a water quality characteristic: **No**.

   a. Slope = _____ (Table_____).

   b. Ranked genus mean acute intercepts: Table _____.

   c. Final acute intercept = _____ (_____).

   ln of final acute intercept = _____.

   d. FAV equation: Tier I FAV = _____ = _____ = _____.

C. Aquatic Maximum Value (AMV) calculation: Tier I AMV = Tier I FAV / 2 = 848.572 ug/l / 2 = **424.286 ug/l**.

RULE 57 AQUATIC VALUES WORK SHEET-CHRONIC

Chemical Name: **1,2,4-Trichlorobenzene**
CAS #: **120-82-1**
Developed by: **Christopher Hull**
Date: **5/19/10**

FINAL CHRONIC VALUE CALCULATIONS

A. Minimum 8-species requirement for GMCV-based Tier I is **not** met: **Yes**.

1. Minimum requirements met = 2 (iii, iv).

2. Minimum requirements missing = 6 (i, ii, v, vi, vii, viii).

B. Minimum 8-species requirement for GMCV-based Tier I **is** met: **No**.

1. Toxicity is **not** dependent upon a water quality characteristic: _____.

a. Tier I FCV = _____ (Fig. _____).

2. Toxicity **is** dependent upon a water quality characteristic: _____.

a. Slope = _____ (Table_____).

b. Ranked Genus Mean Chronic Intercepts: Table _____.

c. Final Chronic Intercept = _____ (Fig. _____).

d. ln of Final Chronic Intercept = _____.

e. FCV equation = Tier I FCV = _____ = _____ = _____.

C. Acute-to-Chronic-Ratio method: **Yes**.

1. Acute-to-Chronic Ratio:

a. Number of ACRs meeting minimum data requirements = 2 (Tables 1-2).

b. Tier II Acute-to-Chronic Ratio = Xg(D. magna ACR, FHM SMACR, Default Value) = Xg(4.1640241, 4.0104484, 18) = **6.6987364**.

2. Toxicity is **not** dependent upon a water quality characteristic: **Yes**.

Tier II FCV = Tier I FAV / Tier II ACR = 848.572 ug/l / 6.6987364 = **126.67643 ug/l**.

3. Toxicity **is** dependent upon a water quality characteristic: **No**.

a. Slope = _____ (Table_____).

b. Aquatic Chronic Intercept = _____ (Table _____).

c. ln of Aquatic Chronic Intercept = _____.

d. FCV equation = Tier _____ FCV = _____ = _____ = _____.

Figure 1. 1,2,4-Trichlorobenzene FAV calculation, 5/10 (Hull).

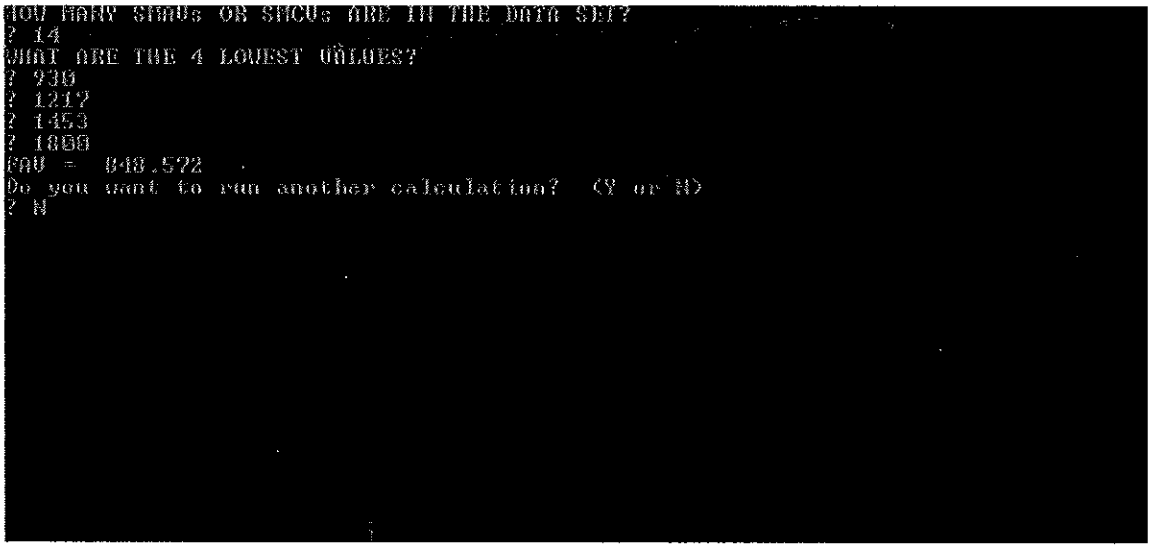

Table 1. 1,2,4-Trichlorobenzene MATC and ACR calculations for *Daphnia magna*, 5/10 (Hull).

Acute Data (Refs. #3, 4, 6, 18):

48-hr. LC50 = 2,090 ug/l.

Chronic Data (Refs. #3, 4, 6, 18):

28-d LC $NOEC_{(reprod., gr.)}$ = 363 ug/l; $LOEC_{(reprod., gr.)}$ = 694 ug/l; $MATC_{(reprod., gr.)}$ = Xg = 501.91832 ug/l.

ACR = 48-hr. LC50 / 28-d $MATC_{(reprod., gr.)}$ = 2,090 ug/l / 501.91832 ug/l = 4.1640241.

Table 2. 1,2,4-Trichlorobenzene MATC and ACR calculations for Fathead Minnow, 5/10 (Hull).

FHM MATC, ACR #1:

Acute Data (Refs. #4, 7, 10, 11, 12, 13, 14):
96-hr. LC50 = 2,760 ug/l.

Chronic Data (Refs. #11, 12, 13):
33-day ELS $NOEC_{(surv., gr.)}$ = 500 ug/l; $LOEC_{(surv., gr.)}$ = 920 ug/l; $MATC_{(surv., gr.)}$ = Xg = 678.233 ug/l.

ACR = 96-hr. / 33-day ELS MATC = 2,760 ug/l / 678.233 ug/l = 4.069398.

FHM MATC, ACR #2:

Acute Data (Refs. #6, 15, 16):
96-hr. LC50 = 2,870 ug/l.

Chronic Data (Ref. #6):
32-day ELS $NOEC_{(reprod., gr.)}$ = 499 ug/; $LOEC_{(reprod., gr.)}$ = 995 ug/l; $MATC_{(reprod., gr.)}$ = Xg = 704.63111 ug/l.

ACR = 96-hr. LC50 / 32-day ELS MATC = 2,870 ug/l / 704.63111 ug/l = 4.0730532.

FHM MATC, ACR #3:

Acute Data (Refs. #4, 7, 10, 11, 12, 13, 14):
96-hr. LC50 = 2,760 ug/l.

Chronic Data (Refs. #3, 4):
32-day ELS $NOEC_{(growth)}$ = 499 ug/l; $LOEC_{(growth)}$ = 1,008 ug/l; $MATC_{(growth)}$ = Xg = 709.21929 ug/l.

ACR = 96-hr. LC50 / 32-day MATC = 2,760 ug/l / 709.21929 ug/l = 3.8916031.

FHM SMACR:
FHM ACR = Xg(FHM ACR #1, FHM ACR #2, FHM ACR #3)
= Xg(4.069398, 4.0730532, 3.8916031)
= 4.0104484.

1,2,4-TRICHLOROBENZENE REFERENCES, 5/10

References Used:

1. #009917: Holcombe, G. W., Phipps, G. L., Sulaiman, A. H., and Hoffman, A. D. 1987. Simultaneous multiple species testing: acute toxicity of 13 chemicals to 12 diverse freshwater amphibian, fish, and invertebrate families. Arch. Environ. Contam. Toxicol. 16(6): 697-710.
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#016600: Gao, C., R. Govind, and H. H. Tabak. 1992. Application of the group contribution method for predicting the toxicity of organic chemicals. Environ. Toxicol. Chem. 11(5): 631-6.
-REJECT (IITM/C; TM/CU e.g. no controls)
#V3118: Hahn, J., Hansen, H. P., Rotard, W., Pattard, M., Bock, R., and Pluta, W. 1989. 1,2-Dichloroethane. Bundesgesundheitsamt, Unveroffentlicht (OECDG Data File) .
-NUE.
#V1340: Hall, L. W., W. S. Hall, S. J. Bushong, and R. L. Herman. 1987. *In situ* Striped Bass (*Morone saxatilis*) contaminant and water quality studies in the Potomac River. Aquat. Toxicol. 10(2-3): 73-99.
-ISDO.
#009690: Hall, L. H., L. B. Kier, and G. Phipps. 1984. Structure-activity relationship studies on the toxicities of benzene derivatives: I. An additivity model. Environ. Toxicol. Chem. 3(3): 355-65.
-NUE: TDI.
#007904: Heitmuller, P. T., T. A. Hollister, and P. R. Parrish. 1981. Acute toxicity of 54 industrial chemicals to Sheepshead Minnows (Cyprinodon variegatus). Bull. Environ. Contam. Toxicol. 27(5): 596-604.
-ACCEPT only for ACR calculation (SW), no suitable chronic available.
#V1349: Hendriks, A. J. 1995. Modeling response of species to microcontaminants: comparative ecotoxicology by (sub)lethal body burdens as a function of species size and partition ratio of chemicals. Ecotoxicol Environ Saf 32(2): 103-30.
-NUE.
#009663: Hermens, J., H. Canton, P. Janssen, and R. De Jong. 1984. Quantitative structure-activity relationships and toxicity studies of mixtures of chemicals with anesthetic potency: acute lethal and sublethal toxicity to *Daphnia magna.* Aquat. Toxicol. 5(2): 143-54.
-TATO; IITM/C.
#000473: Hodson, P. V., Dixon, D. G., and Kaiser, K. L. E. 1984. Measurement of median lethal dose as a rapid indication of contaminant toxicity to fish. Environ. Toxicol. Chem. 3(2): 243-54.
-REJECT: TM/CU; IITM/C these data are later reported in 012010 & 013981.
#016610: Hodson, P. V., Parisella, R., Blunt, B., Gray, B., and Kaiser, K. L. E. 1991 . Quantitative Structure-Activity Relationships for chronic toxicity of phenol, p-chlorophenol, 2,4-dichlorophenol, pentachlorophenol, p-nitrophenol, and 1,2,4-trichlorobenzene to early life stages of Rainbow Trout (Oncorh. Can. Tech.Rep. Fish. Aquat. Sci. 1784: 55 p.
-TDI.
#013981: Hodson, P. V., D. G. Dixon, and K. L. E. Kaiser. 1988. Estimating the acute toxicity of waterborne chemicals in trout from measurements of median lethal dose and the octanol-water partition coefficient. Environ. Toxicol. Chem. 7(6): 443-54.
-ACCEPT on a per-test basis, only. Some data are original here, if acceptable. Most, however are SD, from 012010 or 000473.
#V1342: Hoke, R A, Giesy, J P, Zabik, M, and Unger, M, 1994. Toxicity of Sediments and Sediment Pore Waters from the Grand Calumet River-Indiana Harbor, Indiana Area of Concern.
- SED.
#013167: Holcombe, Gary W., Phipps, Gary L., and Veith, Gilman D., 1988. Use of aquatic lethality tests to estimate safe toxicant concentrations for initial ecological risk assessments Aquat. Toxicol. Environ. Fate STP 1007. ASTM.
- SDO.
#V2998: Hsieh, S. H., C. H. Hsu, D. Y. Tsai, and C. Y. Chen. 2006. Quantitative structure-activity relationships for toxicity of nonpolar narcotic chemicals to *Pseudokirchneriella subcapitata.* Environ Toxicol Chem 25(11): 2920-6.
-QSAR / SDO, PDO.
#V1416: Kaiser, K. L. E., D. G. Dixon, and P. V. Hodson. 1984. QSAR studies on chlorophenols, chlorobenzenes and para-substituted phenols. Proc. Workshop Quant. Struct.-Act. Relat. QSAR Environ. Toxicol. 189-206.
-QSAR / SDO.

#V1417: Kaiser, K. L. E., S. P. Niculescu, and G. Schuurmann. 1997. Feed forward back-propagation neural networks and their use in predicting the acute toxicity of chemicals to the Fathead Minnow. [Erratum to document cited in CA127:132092]. Water Qual. Res. J. Can. 32(4): 855.
-NUE.
#V1418: Kaiser, K. L. E., S. P. Niculescu, and G. Schuurmann. 1997. Feed forward backpropagation neural networks and their use in predicting the acute toxicity of chemicals to the Fathead Minnow. Water Qual. Res. J. Can. 32(3): 637-657.
-NUE; SDO.
#V1422: Karabunarliev, S., O. G. Mekenyan, W. Karcher, C. L. Russom, and S. P. Bradbury. 1996. Quantum-chemical descriptors for estimating the acute toxicity of substituted benzenes to the guppy (Poecilia reticulata) and Fathead Minnow (*Pimephales promelas*). Quant. Struct.-Act. Relat. 15(4): 311-320.
-QSAR / SDO.
#003169: Kenaga, E. E. 1982. Predictability of chronic toxicity from acute toxicity of chemicals in fish and aquatic invertebrates. Environ. Toxicol. Chem. 1(4): 347-58.
-SDO.
#017447: Klein, W., H. Geyer, D. Freitag, and H. Rohleder. 1984. Sensitivity of schemes for ecotoxicological hazard ranking of chemicals. Chemosphere 13(1): 203-211.
-SDO.
#V2295: Knezovich, J. P. and Harrison, F. L. 1988. The bioavailability of sediment-sorbed chlorobenzenes to larvae of the midge, *Chironomus decorus*. Ecotoxicol. Environ. Saf. 15: 226-241.
-TATO.
#015583: Knie, J., Halke, A., Juhnke, I., and Schiller, W. 1983. Results of studies on chemical substances with four biotests. (Ergebnisse Der Untersuch-Ungen Von Chemischen Stoffen Mit Vier Biotests). Dtsch. Gewaesserkd. Mitt 27(3): 77-79.
-REJECT (No test duration given; IITM/C).
#015583: Knie, J., A. Haelke, I. Juhnke, and W. Schiller. 1983. Results of studies of chemical substances using four biotests. Dtsch. Gewaesserkd. Mitt. 27(3): 77-9.
-No test duration given; IITM/C.
#006060: Konemann, H. 1981. Quantitative structure-activity relationships (QSARs) in fish toxicity studies. Part 1: relationship for industrial pollutants. Toxicology 19(3): 209-21.
-TM/CU
#V3119: Kosian, P., Lemke, A., Studders, K., and Veith, G., 1981. The precision of the ASTM Bioconcentration Test . U.S.EPA, Duluth, MN.
-NUE: BCF / UDO.
#V3120: Lay, J. P., Schauerte, W., Muller, A., Klein, W., and Korte, F. 1985. Long-term effects of 1,2,4-trichlorobenzene on freshwater plankton in an outdoor-model-ecosystem. Bull. Environ. Contam.Toxicol 34(5): 761-769.
-MED.
#013840: Leblanc, G. A. 1984. Comparative structure- toxicity relationships between acute and chronic effects to aquatic organisms. QSAR in environmental toxicology. Proc. workshop, Hamilton, Ont., 1983 : 235-260.
-IITM/C; analysis & results questionalble; no acute data so no ACR possible.
#SH 157.7 .M241: MacPhee, C. and Ruelle, R. 1969. Lethal effects of 1888 chemicals upon four species of fish from Western North America : 112p.
-TDI.
#V1535: Martin, T. M. and D. M. Young. 2001 . Prediction of the acute toxicity (96-h LC50) of organic compounds to the Fathead Minnow (*Pimephales promelas*) using a group contribution method. Chem Res Toxicol 14(10): 1378-85.
-NUE; QSAR / SDO.
#013104: McGowan, J. C. and A. Mellors. 1986. Molecular volumes and the toxicities of chemicals to fish. Bull. Environ. Contam. Toxicol. 36(6): 881-7.
-SDO.
#007382: Melancon, M. J. J., Branson, D. R., and Lech, J. J. 1979. The Uptake, Elimination and metabolism of 1,2,4-trichlorobenzene in Rainbow Trout. Toxicol. Appl. Pharmacol. 48(1 Pt. 2): A170.
-NUE: UDO.
#019100, #V1617: Neely, W. B. 1984. An Analysis of Aquatic Toxicity Data: Water Solubility and Acute Lc50 Fish Data. Chemosphere 13(7): 813-820.

-SDO.
#V3124: Nendza, M. and A. Wenzel. 2006-. Discriminating toxicant classes by mode of action - 1. (Eco)toxicity profiles. Environmental Science and Pollution Research 13(3): 192-203.
-QSAR / SDO.
#V1618: Netzeva, T. I., A. O. Aptula, E. Benfenati, M. T. Cronin, G. Gini, I. Lessigiarska, U. Maran, M. Vracko, and G. Schüürmann. 2005. Description of the electronic structure of organic chemicals using semiempirical and *ab initio* methods for development of toxicological QSARs. J Chem Inf Model 45(1): 106-14.
-NUE; QSAR / SDO.
#V1616: Niculescu, S. P., A. Atkinson, G. Hammond, and M. Lewis. 2004. Using fragment chemistry data mining and probabilistic neural networks in screening chemicals for acute toxicity to the fathead minnow. SAR QSAR Environ Res 15(4): 293-309.
-NUE; QSAR / SDO.
#V2433: Niinomi, J., Y. Nakagawa, K. Araki, S. Hayakawa, and T. Kanamaru. 1989. Studies on water pollution by chemicals - microbial degradation and acute himedaka killifish toxicity. Mie-Ken Kankyo Kagaku Senta Kenkyu Hokoku (9): 53-60.
-NUE; TONNA.
#V1620: Nouwen, J., F. Lindgren, B. Hansen, and W. Karcher. 1996. Fast screening of large databases using clustering and PCA based on structure fragments. J. Chemom. 10(5 & 6): 385-398.
-QSAR / SDO.
#013826: Oikari, A., Kukkonen, J., and Virtanen, V. 1992. Acute toxicity of chemicals to *Daphnia magna* in humic waters. Science of the Total Environment 117-118: 367-377.
-TM/CU; IITM/C.
#009689: Oliver, B. G. and Niimi, A. J. 1985. Bioconcentration factors of some halogenated organics for Rainbow Trout: limitations in their use for prediction of environmental residues. Environ.Sci.Technol. 19(9): 842-849.
-NUE; BCF.
#V2801: Papa, E., F. Villa, and P. Gramatica. 2005. Statistically validated QSARs, based on theoretical descriptors, for modeling aquatic toxicity of organic chemicals in *Pimephales promelas* (Fathead Minnow). Journal of Chemical Information and Modeling 45(5): 1256-66.
-QSAR/SDO.
#V2857: Pavan, M., T. I. Netzeva, and A. P. Worth. 2006. Validation of a QSAR model for acute toxicity. SAR and QSAR in Environmental Research 17(2): 147-171.
-QSAR/SDO.
#015358: Pawlisz, A. V. and Peters, R. H. 1993. A radioactive tracer technique for the study of lethal body burdens of narcotic organic chemicals in *Daphnia magna*. Environmental Science & Technology 27(13): 2795-2800.
-NUE.
#V1661: Pawlisz, A. V. and R. H. Peters. 1993. A test of the equipotency of internal burdens of nine narcotic chemicals using *Daphnia magna*. Environmental Science & Technology 27(13): 2801-2806.
-BCF/UDO.
#V1662: Pawlisz, A. V. and Peters, R. H. 1995. Effects of sublethal exposure on lethal body burdens of narcotic organic chemicals in *Daphnia magna*. Environ.Sci.Technol. 29(3): 613-621.
-NUE; BCF/UDO.
#015353: Protic, M. and A. Sabljic. 1989. Quantitative structure-activity relationships of acute toxicity of commercial chemicals on Fathead Minnows: effect of molecular size. Aquatic Toxicology 14(1): 47-64.
-QSAR/SDO.
#V3121: Raevsky, O. A., V. Y. Grigor'ev, E. E. Weber, and J. C. Dearden. 2008. Classification and quantification of the toxicity of chemicals to Guppy, Fathead Minnow and Rainbow Trout: Part 1. Nonpolar narcosis mode of action. QSAR & Combinatorial Science 27(11-12): 1274-1281.
-QSAR / SDO.
#015771: Ramos, E. U. , W. H. J. Vaes, H. J. M. Verhaar, and J. L. M. Hermens. 1998. Quantitative Structure-Activity Relationships for the aquatic toxicity of polar and nonpolar narcotic pollutants. Journal of Chemical Information and Computer Sciences 38(5): 845-852.
-QSAR/SDO.
#009495: Rawlings, G. D. and M. Samfield. 1979. U. S. Environ. Prot. Agency, Off. Res. Dev., [Rep.] EPA EPA-600/7-78-168, Symp. Proc. Process Meas. Environ. Assess., 1978; PB-290 331, 153-69 .
-WETO.
#015324: Ribo, J. M. and K. L. E. Kaiser. 1983. Effects of selected chemicals to photoluminescent bacteria and

their correlations with acute and sublethal effects on other organisms. Chemosphere 12(11/12): 1421-1442.
-SDO.
#V1690: Roex, E. W. M., C. A. M. Van Gestel, A. P. Van Wezel, and N. M. Van Straalen. 2000. Ratios between acute aquatic toxicity and effects on population growth rates in relation to toxicant mode of action. Environ. Toxicol. Chem. 19(3): 685-693.
-SDO.
#V2610: Rose, R. M., Warne, M. S. J., and Lim, R. P. 1998. Quantitative structure-activity relationships and volume fraction analysis for nonpolar narcotic chemicals to the Australian cladoceran *Ceriodaphnia cf. dubia*. Arch. Environ. Contam. Toxicol. 34(3): 248-252.
-QSAR; TONNA.
#V1726: Sabljic, Aleksandar, 1987. Nonempirical modeling of environmental distribution and toxicity of major organic pollutants QSAR Environ. Toxicol., Proc. Int. Workshop, 2nd, 2.
-QSAR / SDO.
#015372: Saito, H., J. Koyasu, K. Yoshida, T. Shigeoka, and S. Koike. 1993. Cytotoxicity of 109 chemicals to goldfish GFS cells and relationships with 1-octanol/water partition coefficients. Chemosphere 26(5): 1015-28.
-NUE.
#V1727: Santiago, S., R. L. Thomas, G. Larbaigt, D. Rossel, M. A. Echeverria, J. Tarradellas, J. L. Loizeau, L. McCarthy, C. I. Mayfield, and C. Corvi. 1993. Comparative ecotoxicity of suspended sediment in the lower Rhone River using algal fractionation, Microtox and *Daphnia magna* bioassays. Hydrobiologia 252(3): 231-44.
-SED.
#V3101: Schirmer, K., K. Tanneberger, N. I. Kramer, D. V÷lker, S. Scholz, C. Hafner, L. E. J. Lee, N. C. Bols, and J. L. M. Hermens. 2008. Developing a list of reference chemicals for testing alternatives to whole fish toxicity tests. Aquatic Toxicology 90(2): 128-137.
-MOD; QSAR; SDO.
#V3122: Schramm, K. W., Behechti, A., Beck, B., and Kettrup, A. 1998. Influence of an aquatic humic acid on the bioconcentration of selected compounds in *Daphnia magna*. Ecotoxicol. Environ. Saf 41(1): 73-76.
-NUE: BCF / UDO.
#V1797: Schultz, T. W. 1997. Tetratox: *Tetrahymena pyriformis* population growth impairment endpoint-a surrogate for fish lethality. Toxicol. Methods 7(4): 289-309.
-NUE; TONS.
#V1747: Sinks, G. D. and T. W. Schultz. 2001. Correlation of *Tetrahymena* and *Pimephales* toxicity: evaluation of 100 additional compounds. Environ Toxicol Chem 20(4): 917-21.
-TONS; SD.
#V1748: Sixt, Stefan and Altschuh, Joachim, 1997. Prediction of luminescent bacteria toxicity using quantum chemical descriptors: test of a classification scheme Quantitative Structure-Activity Relationships in Environmental Sciences-VII, Proceedings of QSAR 96, Elsinore, Den., June 24-28, 1996.
- QSAR; SD; TONS.
#V1750: Sixt, S., J. Altschuh, and R. Brueggemann. 1995. Quantitative structure-toxicity relationships for 80 chlorinated compounds using quantum chemical descriptors. Chemosphere 30(12): 2397-414.
-NUE; QSAR / SDO.
#013084: Smith, A. D., Bharath, A., Mallard, C., Orr, D., McCarty, L. S., and Ozburn, G. W. 1990. Bioconcentration kinetics of some chlorinated benzenes and chlorinated phenols in American Flagfish, *Jordanella floridae* (Goode and Bean). Chemosphere 20(4-Mar): 379-386.
-NUE: BCF/UDO.
#V1745: Smith, I. R. and G. R. Craig. 1983. Prediction of organic contaminant aquatic toxicity utilizing intraperitoneal injections and structure-activity relationships. Can. Tech. Rep. Fish. Aquat. Sci. 1151: 122-35.
-NUE; QSAR / ND (on this chemical only).
#V2858: Sánchez-Bayo, F. 2006. Comparative acute toxicity of organic pollutants and reference values for crustaceans. I. Branchiopoda, Copepoda and Ostracoda. Environmental Pollution 139(3): 385-420.
-QSAR / SDO.
#015502: Thebeau, L. C., M. Ellis, J. Paul, and J. Wrobel. 1995. Ecological risk assessment for the Canal Creek area of Aberdeen Proving Ground, a case study. Hydrocarbon Contam. Soils 5: 273-294.
-SED, AMDO.
#V1856: Trenel, J. and Kuhn, R. 1982. Bewertung Wassergefahrdender Stoffe im Hinblick auf Lagerung, Umschlag und Transport. Umweltforschungsplan des Bundesministers des Innern .
-NUE.

#V2742: Van Wezel, A. P., De Vries, D. A. M., Kostense, S., Sijm, D. T. H., and Opperhuizen, A. 1995. Intraspecies variation in lethal body burdens of narcotic compounds. Aquat. Toxicol. 33(4-Mar): 325-342 .
-NUE.
##V3123: Van Wezel, A. P. and Jonker, M. T. O. 1998. Use of the lethal body burden in the risk quantification of field sediments; influence of temperature and salinity. Aquat. Toxicol 42: 287-300.
-NUE: BCF / UDO, SED.
#005576: Veith, G. D., Defoe, D. L., and Bergstedt, B. V. 1979. Measuring and estimating the bioconcentration factor of chemicals in fish. J. Fish. Res. Board Can. 36(9): 1040-1048.
-NUE: BCF / UDO.
#V1883: Veith, G. D. and O. G. Mekenyan. 1993. A QSAR Approach for estimating the aquatic toxicity of soft electrophiles qsar for soft electrophiles. Quantitative Structure-Activity Relationships 12(4): 349-356.
-QSAR / SDO.
#V1874: Verhaar, H. J. M., E. U. Ramos, and J. L. M. Hermens. 1996. Classifying environmental pollutants. 2: separation of class 1 (baseline toxicity) and class 2 ('polar narcosis') type compounds based on chemical descriptors. J. Chemom. 10(2): 149-62.
-NUE; QSAR / SDO.
#V1875: Verhaar, H. J. M., J. Solbe, J. Speksnijder, C. J. Van Leeuwen, and J. L. M. Hermens. 2000. Classifying environmental pollutants: Part 3. External validation of the classification system. Chemosphere 40(8): 875-883.
-NUE; QSAR / SDO.
#V1953: von der Ohe, P. C., R. Kühne, R. U. Ebert, R. Altenburger, M. Liess, and G. Schüürmann. 2005. Structural alerts--a new classification model to discriminate excess toxicity from narcotic effect levels of organic compounds in the acute daphnid assay. Chem Res Toxicol 18(3): 536-55.
-NUE; MOD.
#V1876: Wang, G. and N. Bai. 1997. Study on QSAR for general pollutants in organic industrial waste. Toxic Subst. Mech. 16(4): 315-326.
-QSAR / SDO.
#V2766: Wang, L., Z. Liu, F. Zhou, H. Yu, and H. Gao. 1994. QSAR model parameters research on substituted aromatic compounds. Huanjing Kexue 15(3): 7-10.
-SW; UDO; TATO.
#016611: Wei, L., W. Zhang, S. Han, L. Wang, and Y. Zhao. 1999. Acute/chronic ratios to estimate chronic toxicity from acute data. Toxicol. Environ. Chem. 69(3-4): 395-401.
-TDI; QSAR/SDO.
#V2779: Williams, D. and R. Fulthorpe. 2003 . Using invertebrate and microbial communities to assess the condition of the hyporheic zone of a river subject to 80 years of contamination by chlorobenzenes. Canadian Journal of Zoology 81: 789-802.
-NUE: COM.
#010088: Yoshioka, Y. , Ose, Y., and Sato, T. 1985. Testing for the toxicity of chemicals with *Tetrahymena pyriformis*. Sci.Total Environ. 43(2-Jan): 149-157.
-TONS.
#V1881: Yoshioka, Y., Ose, Y., and Sato, T. 1986. Correlation of the five test methods to assess chemical toxicity and relation to physical properties. Ecotoxicol.Environ.Saf. 12(1): 15-21.
-TONNA.
#V1882: Yoshioka, Y. and Y. Ose. 1993. A quantitative structure-activity relationship study and ecotoxicological risk quotient for the protection from chemical pollution. Environ. Toxicol. Water Qual. 8(1): 87-101.
-QSAR / SDO.
#V1910: Zaroogian, G. , J. F. Heltshe, and M. Johnson. 1985. Estimation of toxicity to marine species with structure-activity models developed to estimate toxicity to freshwater fish. Aquat. Toxicol. 6(4): 251-70.
-QSAR / SDO; SW.
#013103: Zhao, Y., L. Wang, H. Gao, and Z. Zhang. 1993. Quantitative structure-activity relationships-relationship between toxicity of organic chemicals to fish and to *Photobacterium phosphoreum*. Chemosphere 26(11): 1971-9.
-TDI; SDO; IITM/C.

*For abbreviations used, see Appendix, attached.

APPENDIX: REFERENCE ABBREVIATIONS USED, 5/10

AMD = ambient monitoring data.
BCF = bioconcentration factor.
D = data (as a suffix to other abbreviations listed here).
DEP = depuration data.
DO = data only (as a suffix to other abbreviations listed here).
EF = environmental fate.
GWD = groundwater data.
IITM/C = insufficient information on test methods / conditions.
ISD = *in situ* data.
LD = leachate data.
LSER = Linear Solvation Energy Relationship.
MCD = microcosm data.
MIX = mixture (not chemical-specific) test data.
MED = model ecosystem data.
MET = metabolism
MOD = model (theoretical) data / analysis.
NA = not available at this time.
ND = no data (on this chemical).
NIL = not in (MDEQ) Library.
NR = not reviewed.
NUE = no useable endpoint.
O = only (as a suffix to other abbreviations listed here).
PD = phytotoxicity data.
PHYS = physiological data.
QSAR = Quantitative Structure-Activity Relationship.
RWD = receiving water data.
SD = secondary data.
SED = sediment data or testing.
SW = saltwater.
TATO = test animals too old.
TDI = test duration inappropriate.
TM/CU = test methods / conditions unacceptable.
TONNA = test organisms not North American.
TONS = test organisms not suitable.
TTD = time-toxicity data.
UD or UP = uptake data.
WET = whole-effluent testing.