Rule 57 Aquatic Values Data Sheet

2/4/2010

Chemical or product name: Nitrobenzene
Manufacturer (WTAs): -----
C.A.S #: 98-95-3

Developed by: Christopher Hull *FAV*: 2,100 ug/l* *(Tier: II)*
Approved by: D. Bush *AMV*: 1,000 ug/l* *(Tier: II)*
Approval date: 2/8/2010 *FCV*: 230 ug/l* *(Tier: II)*
CAS, AQUIRE: 11/25/09; QSAR: 12/11/09 *Acute CF: ----* *Chronic CF: ----*
Clearinghouse search date: 6/13/96

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
Water Flea	LC50	48	S,U	173	-----	27,000	27,000	27,000	1	1
(Daphnia magna)										
Fathead Minnow	LC50	96	FT,M	44.1	-----	119,000	117,996	117,996	2	2
(Pimephales promelas)	LC50	96	FT,M	44.9	-----	117,000				3

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
Fathead Minnow *(Pimephales promelas)*	LSG	7	FT,M	45.5	-----	48,375 [1]	48,375	48,375	1	4

*Value rounded to 2 significant figures.

[1] For MATC and ACR calculations, see Table 1.

9/21/04

Table 1. Nitrobenzene MATC and ACR calculations for Fathead Minnow from References #3 and 4*, 2/04/10 (Hull).

Acute data (Ref. #3):

96-hr. LC50 = 117,000 ug/l .

Chronic Data (Ref. #4):

7-d LSG $NOEC_{growth}$ = <10,200 ug/l; $LOEC_{growth}$ = <10,200 ug/l; $MATC_{growth}$ = Xg = ≤10,200 ug/l.

7-d LSG $NOEC_{survival}$ = 38,300 ug/l; $LOEC_{survival}$ = 61,100 ug/l; $MATC_{survival}$ = Xg = 48,375 ug/l.

ACR = 96-hr. LC50 / 7-d $MATC_{survival}$ = 117,000 ug/l / 48,375 ug/l = 2.4186047.

*Acute and chronic tests were conducted in different studies, by different investigators, but at the same lab (USEPA-ERL-Duluth). Both used Lake Superior water as diluent. Test organisms for acute tests were from in-house (USEPA-ERL-Duluth) cultures. Test organisms for chronic tests were from USEPA-Newtown, OH.

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: **Nitrobenzene**
CAS #: **98-95-3**
Developed by: **Christopher Hull**
Date: **2/04/10**

AQUATIC MAXIMUM VALUE CALCULATIONS

A. Minimum 8-species requirement for Tier I is not met (Tier II): **Yes**.

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

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

3. Acute Factor = 13.

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

   a. FAV calculation: Tier II FAV = Lowest GMAV / Acute Factor = 27,000 ug/l / 13 = **2,076.9231 ug/l**.

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

   a. Slope = _____ (Table_____).

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

6. Go to C.

B. Minimum 8-species requirement is met (Tier I): **No**.

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

   a. Tier I FAV calculation: ______ (_____).

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

   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 II AMV = Tier II FAV / 2 = 2,076.9231 ug/l / 2 = **1,038.4615 ug/l**.

RULE 57 AQUATIC VALUES WORK SHEET-CHRONIC

Chemical Name: **Nitrobenzene**
CAS #: **98-95-3**
Developed by: **Christopher Hull**
Date: **2/04/10**

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 = 1 (Table1).

   b. Tier II Acute-to-Chronic Ratio = Xg(Table 1 ACR (FHM), 18, 18) = Xg(2.4186047, 18, 18) = 9.2194136.

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

   Tier II FCV = Tier II FAV / Tier II ACR = 2,076.9231 ug/l / 9.2194136 = **225.27714 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 = ______ = ______ = ______.

NITROBENZENE REFERENCES, 2/10

References Used:
1.#007906 : LeBlanc, G. A. 1980. Acute toxicity of Priority Pollutants to water flea (*Daphnia magna*). Bull. Environ. Contam. Toxicol. 24(5): 684-91 .
2. #QL 638 .C94 A27 v.2: Geiger, D. L., Northcott, C. E., Call, D. J., and Brooke, L. T. 1985. Acute toxicities of organic chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 2. Center for Lake Superior Environmental Stud., Univ.of Wisconsin-Superior, Superior, WI I:326 .
3. #013384: Holcombe, G. W., Phipps, G. L., Knuth, M. L., and Felhaber, T. 1984. The acute toxicity of selected substituted phenols, benzenes and benzoic acid esters to Fathead Minnows *Pimephales promelas*. Environ Pollut Ser A Ecol Biol 35(4): 367-381.
4. #013649: Marchini, S. , Tosato, M. L., Norberg-King, T. J., Hammermeister, D. E., and Hoglund, M. D. 1992. Lethal and sublethal toxicity of benzene derivatives to the Fathead Minnow, using a short-term test. Environ.Toxicol.Chem. 11(2): 187-195.

References Reviewed, but Not Used*:
#013562: Abernethy, S. G., D. Mackay, and L. S. McCarty. 1988. Volume fraction correlation for narcosis in aquatic organisms: the key role of partitioning. Environ. Toxicol. Chem. 7(6): 469-81.
-SDO.
#ET&C 25(11): Ahlers, J., C. Riedhammer, M. Vogliano, R.-U. Ebert , R. Kuhne, and G. Schuumann. 2006. Acute to chronic ratios in aquatic toxicity variation across trophic levels and relationship with chemical structure. Environmental Toxicology and Chemistry 25(11): 2937-2945.
-SDO.
#V3103: Barata, C., P. Alanon, S. Gutierrez-Alonso, M. C. Riva, C. Fernandez, and J. V. Tarazona. 2008. A *Daphnia magna* feeding bioassay as a cost effective and ecological relevant sublethal toxicity test for Environmental Risk Assessment of toxic effluents. Sci Total Environ 405(1-3): 78-86.
-NUE; TM/CU; MDO).
#V1096: Bearden, A. P. and T. W. Schultz. 1998. Comparison of *Tetrahymena* and *Pimephales* toxicity based on mechanism of action. SAR QSAR Environ. Res. 9(3-4): 127-153.
-QSAR / SDO.
#V1097: Bearden, A. P. and T. W. Schultz. 1997. Structure-activity relationships for *Pimephales* and *Tetrahymena*: a mechanism of action approach. Environ. Toxicol. Chem. 16(6): 1311-1317.
-QSAR / SDO.
#V1001: Bermúdez-Saldaña, J. M., M. A. Garcia, M. J. Medina-Hernández, and M. L. Marina. 2004. Micellar electrokinetic chromatography with bile salts for predicting ecotoxicity of aromatic compounds. J Chromatogr A 1052(1-2): 171-80.
-NUE; SDO.
#V1018: Bringmann, G. and Kuhn, R. 1959. Comparative water-toxicological investigations on bacteria, algae, and *Daphnia*. Gesundheitsingenieur 80(4): 115-120.
-TONS, NUE.
#V1006: Bringmann, G. and Kuhn, R. 1981. Comparison of the effect of toxic substances on the flagellate organisms such as ciliates and the holozoic bacteria-devouring organisms such as saprozoic protozoans (Vergleich der Wirkung von Schadstoffen auf Flagellate). Gwf-Wasser Abwasser 122(7): 308-313.
-NUE; TONS.
#V1005: Bringmann, G. and Kuhn, R. 1980. Determination of the biological effect of water pollutants in protozoa. II. Bacteriovorous ciliates (Bestimmung der Biologischen Schadwirkung Wassergefahrdender Stoffe Gegen Protozoen. II. Bakterienfressende Ciliaten. Z. Wasser-Abwasser-Forsch 13(1): 26-31.
-REJECT: No useable endpoint: Test organisms not suitable.
#005672: Bringmann, G. and Kuhn, R. 1977. Results of the damaging effect of water pollutants on *Daphnia magna* (Befunde der Schadwirkung Wassergefahrdender Stoffe Gegen Daphnia magna). Z. Wasser-Abwasser-Forsch 10(5): 161-166.
-REJECT: (test duration inappropriate).
#V1018: Bringmann, G. and Kuhn, R. 1959. The toxic effects of waste water on aquatic bacteria, algae, and small

crustaceans. Gesund. Ing 80: 115-120.
-TONS, NUE
#V1030: Bringmann, G. and Kuhn, R. 1959. Water toxicological studies with protozoa as test organisms. Gesund. - Ing. TR-80-0058 80: 239-242.
-NUE
#005672: Bringmann, G. and R. Kuhn. 1977. Results of the damaging effect of water pollutants on *Daphnia magna*. Z. Wasser Abwasser Forsch. 10(5): 161-6.
-TDI
#011330: Bringmann, G. and Kuhn, R. 1982. Results of toxic action of water pollutants on *Daphnia magna* Straus tested by an improved standardized procedure. Z. Wasser Abwasser Forsch. 15(1): 1-6.
-TDI; test volume loading violate ASTM standards
#007905: Buccafusco, R. J., Ells, S. J., and Leblanc, G. A. 1981. Acute toxicity of Priority Pollutants to Bluegill (*Lepomis macrochirus*). Bull Environ Contam Toxicol 26(4): 446-452.
-REJECT (low D.O. in undetermined test runs; also, solubility problems coupled with unmeasured concentrations in some tests)
#014745: Canton, J. H., W. Slooff, H. J. Kool, J. Struys, T. J. M. Pouw, R. C. C. Wegman, and G. J. Piet. 1985. Toxicity, biodegradability, and accumulation of a number of chlorine/nitrogen containing compounds for classification and establishing water quality criteria. Regul. Toxicol. Pharmacol. 5(2): 123-31.
-REJECT (insufficient information on test methodology/conditions).
#014745: Canton, J. H., Slooff, W., Kool, H. J., Struys, J., Th. Pouw, J. M., Wegman, R. C. C., and Piet, G. J. 1985. Toxicity, biodegradability and accumulation of a number of Cl/N-containing compounds for classification and establishing Water Quality Criteria. Regul. Toxicol. Pharmacol 5: 123-131 .
-IITM/C
#014779: Castano, A., Cantarino, M. J., Castillo, P., and Tarazona, J. V. 1996. Correlations between the RTG-2 cytotoxicity test EC50 and in vivo LC50 rainbow trout bioassay. Chemosphere 32(11): 2141-2157.
-REJECT (all data are either secondary, or insufficiently described).
#V1123: Chen, J., L. Feng, Y. Zhao, and L. Wang. 1996. Using theoretical solvatochromic parameters in prediction of acute toxicity of substituted aromatic compounds to aquatic organisms. Chin. Sci. Bull. 41(9): 740-743.
-QSAR / SDO.
#V3104: Cheng, Q. 1999. Effect of nitrobenzene derivatives on the toxicity of *Daphnia carinata* and QSAR. Liaoning Shifan Daxue Xuebao, Ziran Kexueban 22(2): 148-152.
-NA; FLO.
#V1124: Cocchi, M., M. C. Menziani, and P. G. De Benedetti. 1993. A quantitative structure-toxicity relationship study of substituted benzenes on aquatic organisms using theoretical molecular descriptors. Trends Ecol. Phys. Chem., Proc. Int. Workshop Ecol. Phys. Chem., 2nd Meeting Date 1992, 39-56. Editor(s): Bonati, Laura. Publisher: Elsevier, Amsterdam, Neth.
-QSAR / SDO.
#V3094: Colombo, A., E. Benfenati, M. Karelson, and U. Maran. 2008. The proposal of architecture for chemical splitting to optimize QSAR models for aquatic toxicity. Chemosphere 72(5): 772-780.
-NUE: MOD/QSAR/SDO.
#V3105: Deneer, J., T. Sinnige, and J. Hermens. 1987. A QSAR study of fish toxicity data of nitroaromatic compounds. QSAR in Drug Design and Toxicology 10: 352-354.
-QSAR / SDO.
#V3106: Deneer, J., C. Van Leeuwen, W. Seinen, J. Maas-Diepeveen, and J. Hermens. 1989. QSAR study of the toxicity of nitrobenzene derivatives towards *Daphnia magna*, *Chlorella pyrenoidosa* and *Photobacterium phosphoreum*. Aquatic Toxicology 15(1): 83-98.
-QSAR / SDO.
#V1208: Devillers, J. , A. Elmouaffek, D. Zakarya, and M. Chastrette. 1987. Comparison of ecotoxicological data by means of an approach combining cluster and correspondence factor analyses. Chemosphere 17(4): 633-46.
-NUE; TONS.
#V1173: Dierickx, P. J. 1993. Comparison between fish lethality data and the in vitro cytotoxicity of lipophilic solvents to cultured fish cells in a two-compartment model. Chemosphere 27(8): 1511-18.
-NUE; SD.
#V1236: Eldred, D. V. , C. L. Weikel, P. C. Jurs, and K. L. E. Kaiser. 1999. Prediction of Fathead Minnow acute toxicity of organic compounds from molecular structure. Chem. Res. Toxicol. 12(7): 670-678.
-NUE; QSAR / SDO.

#014615: Enslein, K., T. M. Tuzzeo, H. H. Borgstedt, B. W. Blake, and J. B. Hart. 1987. Prediction of rat oral LD50 from *Daphnia magna* LC50 and chemical structure. QSAR Environ. Toxicol., Proc. Int. Workshop, 2nd Meeting Date 1986, 91-106. Editor(s): Kaiser, Klaus L. E. Publisher: Reidel, Dordrecht, Neth..
-QSAR/SDO.
#V1237: Espinosa, G., A. Arenas, and F. Giralt. 2002. An Integrated SOM-Fuzzy ARTMAP Neural System for the Evaluation of Toxicity. Journal of Chemical Information and Computer Sciences 42(2): 343-359.
-NUE; SDO.
#015326: Fiedler, H., O. Hutzinger, and J. P. Giesy. 1990. Utility of the QSAR modeling system for predicting the toxicity of substances on the European inventory of existing commercial chemicals. Toxicological and Environmental Chemistry 28(2/3): 167-188.
-QSAR / SDO.
#V2152: Freidig, A. P. and J. L. M. Hermens. 2001. Narcosis and chemical reactivity QSARs for acute fish toxicity. Quant. Struct.-Act. Relat. 19(6): 547-553.
-QSAR / SDO.
#V2154: Freitag, D., Geyer, H., Kraus, A., Viswanathan, R., Kotzias, D., Attar, A., Klein, W., and Korte, F. 1982. Ecotoxicological Profile Analysis VII. Screening chemicals for their environmental behavior by comparative evaluation. Ecotoxicol. Environ. Saf. 6: 60-81.
-NUE.
#005191: Freitag, D., Lay, J. P., and Korte, F., 1984.
- QSAR/SDO.
#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.
#V3107: Hattori, M., Senoo, K., Harada, S., Ishizu, Y., and Goto, M. 1984. The *Daphnia* Reproduction Test of some environmental chemicals. Aquat. Ecol. Chem.(Seitai Kagaku) 6(4): 23-27.
-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), if suitable chronic data from #007902 or other studies by this lab can be found.
#V1385: Hendricks, A. J., J. L. Maas-Diepeveen, A. Noordsij, and M. A. van der Gaag. 1994. Monitoring response of XAD-concentrated water in the Rhine delta: a major part of the toxic compounds remains unidentified. Water Res. 28(3): 581-98.
-RWDO.
#008079: Juhnke, I. and Luedemann, D. 1978. Results of the investigation of 200 chemical compounds for acute fish toxicity with the Golden Orfe Test (Ergebnisse der Untersuchung von 200 Chemischen Verbindungen auf Akute Fischtoxizitat mit dem Goldorfentest). Z.Wasser-Abwasser-Forsch. 11(5): 161-164.
-SDO; TONNA; TDI. Methods for this study are in Mann (1976), attached to this paper under the same library number.
#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.
#V1420: Kamlet, M. J. , R. M. Doherty, M. H. Abraham, and R. W. Taft. 1988. Solubility properties in biological media. 12. Regarding the mechanism of nonspecific toxicity or narcosis by organic nonelectrolytes. Quant. Struct.-Act. Relat. 7(2): 71-8.
-NUE.
#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.
#V1432: Kuhn, R. 1988. Schadstoffwirkungen von Umweltchemikalien im Daphnien-Reproduktions-Test als

Grundlage fr die Bewertung der Umweltgefhrlichkeit in Aquatischen Sys... Forschungsbericht .
-NUE.
#010310: Kuhn, R., Pattard, M., Pernak, K. D., and Winter, A. 1989. Results of the harmful effects of water pollutants to *Daphnia magna* in the 21 day reproduction test. Water Res. 23(4): 501-10.
-TM/CU.
#009664: LeBlanc, G. A. 1984. Interspecies relationships in acute toxicity of chemicals to aquatic organisms. Environ. Toxicol. Chem. 3(1): 47-60.
-REJECT (SW; IITM/C). Possibly the same tests described in #OTS0517186.
#V2822: Liu, Z., L. Wang, H. Ni, and Z. Kong. 1997. QSAR for biotoxication of aromatic compounds. Chin. Sci. Bull. 42(5): 380-384.
-NUE.
#014901: Maas-Diepeveen, J. L. and van Leeuwen, C. J., 1987? Aquatic Toxicity of Aromatic Nitro Compounds and Anilines to Several Freshwater Species .
- REJECT (test animals fed during test).
#013650: Marchini, S. , Hoglund, M. D., Borderius, S. J., and Tosato, M. L. 1993. Comparison of the susceptibility of daphnids and fish to benzene derivatives . Sci.Total Environ. (Suppl.): 799-808.
-REJECT (*C. dubia:* TDI; FHM: fed test; *D. magna*: SDO).
#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.
#011527: McKim, J., Schmieder, P., and Veith, G. 1985. Absorption dynamics of organic chemical transport across trout gills as related to octanol-water partition coefficient. Toxicoloy and Applied Pharmacology 77: 1-10.
-NUE.
#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.
#015384: Nishiuchi, Y. 1981. Toxicity of pesticides to some aquatic animals. II. Toxicity of several solvents to carp and *Daphnia*. Seitai Kagaku 4(3): 45-7.
-TDI.
#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.
#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.
#V3108: Qin, Z. and Z. Jiang. 2007. Quantitative relationship between acute toxicities of aromatic compounds to aquatic organisms and molecular structures of the compounds. Huanan Ligong Daxue Xuebao, Ziran Kexueban 35(6): 97-100.
-QSAR / SDO; NA; FLO.
#V3109: Ramos, E. U., W. H. Vaes, H. J. Verhaar, and J. L. Hermens. 1997. Polar narcosis: Designing a suitable training set for QSAR studies. Environ Sci Pollut Res Int 4(2): 83-90.
-MOD / QSAR / SDO.
#015402: Ramos, E. U. , Vermeer, C., Vaes, W. H. J., and Hermens, J. L. M. 1998. Acute Toxicity of Polar Narcotics to Three Aquatic Species (Daphnia magna, Poecilia reticulata and Lymnaea stagnalis) and Its Relation to Hydrophobicity. Chemosphere 37(4): 633-650.
-IITM/C especially regarding D.O. and controls; Daphnia magna test also violated ASTM loading standards; guppy

and snail tests had D.O. problems; snail species may not have been North American.
#V1704: Ramos, E. U., M. A. Vaal, and J. L. M. Hermens. 2002. Interspecies sensitivity in the aquatic toxicity of aromatic amines. Environmental Toxicology and Pharmacology 11(3-4): 149-158.
-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.
#V3110: Roberts, D. W. 1987. An analysis of published data on fish toxicity of nitrobenzene and aniline derivatives. QSAR Environ. Toxicol., Proc. Int. Workshop, 2nd : 295-308.
-QSAR / SDO.
#V2826: Robinson, P. W. 1999. The toxicity of pesticides and organics to Mysid shrimps can be predicted from *Daphnia* spp. toxicity data. Water Research 33(6): 1545-1549.
-SD; SW.
#V1687: Roderer, G. 1990 . Testung Wassergefahrdender Stoffe als Grundlage fur Wasserqualitatsstandards. Testbericht: Wassergefahrdende Stoffe.
-NA.
#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.
#V3111: Schultz, T. W., 1981. Structure-activity correlations of synthetic fuel related nitrogenous compounds . Oak Ridge Natl.Lab.
-TONS; NUE.
#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.
#V1798: Schultz, T. W., Cajina-Quezada, M., Chang, M., Lin, D. T., and Jain, R. 1989 : 410-423.
-QSAR / ND (on this chemical).
#V3112: Schultz, T. W. and Moulton, B. A., 1984. Structure-activity correlations of selected azaarenes, aromatic amines, and nitro aromatics IN:QSAR in Environmental Toxicology, Proc.of the Workshop held at McMaster University, Hamilton, Ont., Aug.16-18, 1983 . D.Reidel Publ.Co.
-TONS; NUE.
#ET&C v4: Schultz, T. W. and Moulton, B. A. 1985. Structure-activity relationships for nitrogen-containing aromatic molecules. Environ. Toxicol. Chem 4: 353-359.
-TONS; NUE.
#013971: Schultz, T., D. Dawson, and D. Lin. 1989. Comparative toxicity of selected nitrogen-containing aromatic compounds in the *Tetrahymena pyriformis* and *Pimephales promelas* test systems. Chemosphere 18(11): 2283-2291.
-NUE; SDO.
#V1739: Solari, P. and P. J. Dierickx. 1994 . Correlation between fish lethality data and the cytotoxicity to cultured fish cells of lipophilic solvents emulsified by ultrasonication. Chemosphere 28(8): 1495-501.
-NUE; TONNA; SD.
#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.
#V2997: Tichy, M., M. Rucki, I. Hanzlikova, and Z. Roth. 2007. The *Tubifex tubifex* assay for the determination of acute toxicity. Altern Lab Anim 35(2): 229-37.
-NUE; TDI.
#000819: Tonogai, Y., Ogawa, S., Ito, Y., and Iwaida, M. 1982. Actual survey on TLM (Median Tolerance Limit) values of environmental pollutants, especially on amines, nitriles, aromatic nitrogen compounds. J.Toxicol.Sci. 7(3): 193-203.
-TONS.
#V2730: Tonogai, Y. and Y. Ito. 1984. Toxicity of organic nitrogen compounds to fish. Syncopic effect of aniline derivatives on fish. Seitai Kagaku 7(1): 17-26.
-TONNA.
#V1837: Tosato, M. L. , Vigano, L., Skagerberg, B., and Clement, S. 1991. A new strategy for ranking chemical hazards. Framework and Application. Environ. Sci. Technol. 25: 695-702.

-NUE.
#V1838: Tosato, M. L., A. Pino, L. Passerini, S. Marchini, L. Vigano, and M. D. Hoglund. 1993. Updating and validation of a daphnia toxicity model for benzene derivatives. Sci. Total Environ. (Suppl., Pt. 2): 1479-90.
-QSAR / SDO.
#V2740: Vaes, W. H. J., E. Urrestarazu Ramos, H. J. M. Verhaar, and J. L. M. Hermens. 1998. Acute toxicity of nonpolar versus polar narcosis: is there a difference? Environmental Toxicology and Chemistry 17(7): 1380-84.
-NUE
#015458: Van der Schalie, W. H., 1983. Acute and chronic toxicity of 3,5-dinitroaniline, 1,3-dinitrobenzene, and 1,3,5-trinitrobenzene to freshwater aquatic organisms.
- Not reviewed.
#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.
#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.
#018001: Wang, H., Y. Shen, L. Lu, H. Zhu, H. Chen, Y. Xu, and S. Gao. 2003. Acute toxicity of typical hazard chemicals to three kinds of aquatic organisms. Yingyong Yu Huanjing Shengwu Xuebao 9(1): 49-52.
-IITM/C; TM/CU; Good SRM study but no info on solvent controls. Could use for Tier III.
#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.
#V2856: Wang, Y.-F. and Y.-X. Lu. 2004. Assessment of acute toxicity of 13 kinds of nitrobenzol compound by aquatic ecological toxicological assay. Journal of Xinxiang Medical College (Chinese) 21(6): 456-457.
-ND.
#014578: Wellens, H. 1982. Comparison of the sensitivity of *Brachydanio rerio* and *Leuciscus idus* by testing the fish toxicity of chemicals and wastewaters. Z.Wasser-Abwasser-Forsch. 15(2): 49-52.
-TM/CU; IITM/C.
#V3113: Yan, X.-F., H.-M. Xiao, X.-D. Gong, and X.-H. Ju. 2006. A comparison of semiempirical and first principle methods for establishing toxicological QSARs of nitroaromatics. Journal of Molecular Structure: THEOCHEM 764(1-3): 141-148.
-MOD / QSAR / SDO.
#V3114: Yan, X.-F., H.-M. Xiao, X.-H. Ju, and X.-D. Gong. 2005. DFT study on the QSAR of nitroaromatic compound toxicity to the Fathead Minnow. Chinese Journal of Chemistry 23(8): 947-952.
-MOD / QSAR / SDO.
#V1884: Yang, W.-H. and C.-J. Feng. 2003. QSAR study o the acute toxicities of substituted aromatics to sword fish (*Xiphophorus helleri*) and rare minnow (*Gobiocypris rarus*). Youji Huaxue 23(11): 1267-1270.
-QSAR; SDO; TONNA.
#018068, #V2806 : Yen, J. H., K. H. Lin, and Y. S. Wang. 2002. Acute lethal toxicity of environmental pollutants to aquatic organisms. Ecotoxicology and Environmental Safety 52(2): 113-6.
-NUE; TDI; TM/CU; IITM/C; PD.
#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
#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.
#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.
#V3115: Zhang, Z. and X. Fan. 2008. Quantitative Structure-Activity Relationship study on fish toxicity of substituted benzenes. QSAR & Combinatorial Science 27(8): na.
-MOD / QSAR / SDO.
#014780: Zhao, Y.-H., X. Yuan, G.-D. Ji, L.-X. Sheng, and L.-S. Wang. 1997. Quantitative Structure-Activity Relationships of nitroaromatic compounds to four aquatic organisms. Chemosphere 34(8): 1837-1844.
-MOD / QSAR / SDO.
#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.
#V3116: Zhou, Q., J. Fu, H. Meng, X. Zhu, G. Jiang, J. Zhang, J. Liu, and G. Shi. 2007-. Subchronic toxicological effects of aquatic nitrobenzene on Medaka and Chinese rare minnow. Science in China Series B: Chemistry 50(5): 707-717.
-TONNA.

*For abbreviations used, see Appendix, attached.

APPENDIX: REFERENCE ABBREVIATIONS USED, 2/10

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.
FLO = foreign language, only.
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.