

Rule 57 Aquatic Values Data Sheet

10/24/2005

Chemical or product name: Chlorobenzene

Manufacturer (WTAs): -----

C.A.S #: 108-90-7

Developed by: Christopher Hull FAV*: 450 ug/l

Approved by: D. Bush AMV*: 220 ug/l

Approval date: 3/27/07 FCV*: 25 ug/l

CAS, AQUIRE, QSAR: 8/29, 30/05 Acute CF: ----

Clearinghouse search date: 6/13/96

(Tier: II)

(Tier: II)

(Tier: II)

Chronic CF: ----

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 (<i>Daphnia magna</i>)	EC50	48	S,M	160	-----	3,600 ¹	3,600	3,600	1	1
	LC50	48	S,U	157-159.6	20 c	13,000				2,3,4
	LC50	48	S,U	157-159.6	20 c	10,700				2,3,4
	LC50	48	S,U	157-159.6	20 c	15,400				2,3,4
	LC50	48	S,U	159.6	24 c	20,600				2,3
	LC50	48	S,U	159.6	24 c	11,900				2,3
	LC50	48	S,U	159.6	24 c	21,300				2,3
	LC50	48	S,U	72	-----	86,000				5
Bluegill Sunfish (<i>Lepomis macrochirus</i>)	LC50	96	FT,M	31.2	-----	7,400 ²	7,400	7,400	2	6
	LC50	96	S,U	20	B.P.=130-132	24,000				7
Water Flea (<i>Ceriodaphnia affinis</i>)	LC50	48	S,U	90.3	20 c	7,900	9,933	9,933	3	2
	LC50	48	S,U	90.3	20 c	7,900				2
	LC50	48	S,U	90.3	20 c	11,400				2
	LC50	48	S,U	90.3	24 c	11,000				2
	LC50	48	S,U	90.3	24 c	11,800				2
	LC50	48	S,U	90.3	24 c	10,400				2
Fathead Minnow (<i>Pimephales promelas</i>)	EC50	96	FT,M	43.8	-----	16,900 ^{2,3}	16,900	16,900	4	8
	LC50	96	FT,M	43.8	-----	16,900				8
	LC50	96	S,U	20	B.P.=130-132	29,120				7
	LC50	96	S,U	20	B.P.=130-132	33,930				7
	LC50	96	S,U	360	B.P.=130-132	33,930		(cont'd.)		9/27/04

Guppy
(*Poecilia reticulata*)

LC50 96 S,U 20 B.P.=130-132 45,530 45,530 45,530 5

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Goldfish
(*Carassius auratus*)

LC50 96 S,U 20 B.P.=130-132 45,530 45,530 45,530 6

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(cont'd.)

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CHRONIC DATA

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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
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NO SUITABLE DATA WERE FOUND.

*Value rounded to 2 significant figures.

¹ This value only was used to calculate the SMAV because this chemical is hydrophobic and volatile, and BPJ dictates exerting preference for measured values from tests using recommended protocols for such chemicals when available. This value was measured and derived from a USEPA test using such protocols, while the others were not.

² Value used to calculate the SMAV because FT,M test data are preferred over data from other test types.

³ Value used to calculate the SMAV because EC50 data are preferred over LC50 data from the same test.

9/21/04

Rule 57 Aquatic Values Work Sheet

Chemical Name: Chlorobenzene
C.A.S. #: 108-90-7

Chris Hall

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

AQUATIC MAXIMUM VALUE CALCULATIONS

A. Minimum 8 species requirement is **not** met (Tier II). Minimum requirements met = 3
Minimum requirements missing for Tier I = 5 ($i, v, vi, vii, viii$).
Acute factor = 8

1. Toxicity is **not** dependent on a water characteristic

a. FAV calculation $FAV = \frac{\text{lowest AMAU}}{\text{Acute Factor}} = \frac{3,600 \mu\text{g/L}}{8} = \boxed{450 \mu\text{g/L}}$

2. ~~Toxicity is dependent on a water characteristic~~

a. Slope = (Table)

b. FAV equation:

3. Go to C.

B. ~~Minimum 8 species requirement is met (Tier I)~~

1. Toxicity is **not** dependent on a water characteristic

a. FAV calculation. Att.

2. ~~Toxicity is dependent on a water characteristic~~

a. Slope = (Table)

b. Ranked genus mean acute intercepts: Table

c. Final acute intercept = (Att.)

ln of final acute intercept =

d. FAV equation =

C. Aquatic Maximum Value (AMV) calculation:

$AMV = \frac{FAV}{2} = \frac{450 \mu\text{g/L}}{2} = \boxed{225 \mu\text{g/L}}$

CALCULATIONS:

CHARLES HULL

FINAL CHRONIC VALUE CALCULATIONS

A. Minimum 8 species requirement is **not** met (Tier II). Minimum requirements met = 0

Minimum requirements missing for Tier I = AMCV Route: 8

ACR Route: 3

1. Acute to chronic ratio

a. Number ACRs meeting minimum data requirements = 0 (Table —)

b. Acute to chronic ratio = 18

2. Toxicity **is not** dependent on a water characteristic

$$FCV = \frac{FAV}{ACR} = \frac{450 \mu\text{g/l}}{18} = \boxed{25 \mu\text{g/l}}$$

3. Toxicity **is** dependent on a water characteristic

a. Slope = (Table —)

b. Aquatic chronic intercept = (Table —)

ln of aquatic chronic intercept =

c. FCV equation =

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

1. Toxicity **is not** dependent on a water characteristic

a. FCV = — (Att. —)

2. Toxicity **is** dependent on a water characteristic

a. Slope = (Table —)

b. Ranked genus mean chronic intercepts: Table —

c. Final chronic intercept = — (Att. —); ln of final chronic intercept =

d. FCV equation =

CHLOROBENZENE REFERENCES, 10/05

References Used:

1. #016578: Marchini, Silvia, Passerini, Laura, Hoglund, Marilyn D., Pino, Anna, and Nendza, Monika. 1999. Toxicity of aryl- and benzylhalides to *Daphnia magna* and classification of their mode of action based on quantitative structure-activity relationship. Environ. Toxicol. Chem. 18(12): 2759-2766.
2. #013380: Cowgill, U. M., Takahashi, I. T., and Applegath, S. L. 1985. A comparison of the effect of four benchmark chemicals on *Daphnia magna* and *Ceriodaphnia dubia affinis* tested at two different temperatures. Environ. Toxicol. Chem. 4(3): 415-422.
3. #OTS0515905: A comparison of the effect of four benchmark chemicals on *Daphnia magna* and *Ceriodaphnia dubia affinis* tested at two different temperatures: static acute toxicity test results. Dow Chemical Co. Rept.#86-870002116.
4. #013168: Gersich, F. M., Blanchard, F. A., Applegath, S. L., and Park, C. N. 1986. The precision of Daphnid (*Daphnia magna* Straus, 1820) static acute toxicity tests. Arch.Environ.Contam.Toxicol. 15(6): 741-749.
5. #007906: LeBlanc, Gerald A. 1980. Acute toxicity of Priority Pollutants to water flea (*Daphnia magna*). Bull. Environ. Contam. Toxicol. 24(5): 684-91.
6. #010847, #QH 545 .W3 S95 1984: Bailey, H. C., Liu, D. H. W., and Javitz, H. A. 1985. Time/toxicity relationships in short-term static, dynamic, and plug-flow bioassays. R.C.Bahner and D.J.Hansen (Eds.), Aquatic Toxicology and Hazard Assessment, 8th Symposium, ASTM STP 891, Philadelphia, PA : 193-212.
7. #004630: Pickering, Q. H. and Henderson, C. 1966. Acute toxicity of some important petrochemicals to fish. J.Water Pollut.Control Fed. 38(9): 1419-1429.
8. #QL 638 .C94 A27 v.5: Geiger, D. L., Brooke, L. T., and Call, D. J. 1990. Acute toxicities of organic chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 5. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI:332.

References Reviewed, but Not Used*:

- #003175: Abernethy, S., Bobra, A. M., Shiu, W. Y., Wells, P. G., and MacKay, D. 1986. Acute lethal toxicity of hydrocarbons and chlorinated hydrocarbons to two planktonic crustaceans: the key role of organism-water partitioning. Aquat.Toxicol. 8(3): 163-174.
-TM/CU.
- #013562: Abernethy, S. G., Mackay, D., and McCarty, L. S. 1988. Volume fraction correlation for narcosis in aquatic organisms: the key role of partitioning. Environ. Toxicol. Chem. 7(6): 469-81.
-SDO.
- NIL: Babich, H. and Borenfreund, E. 1988. Structure-activity relationships for diorganotin, chlorinated benzenes, and chlorinated anilines established with Bluegill Sunfish BF-2 cells. Fundam. Appl. Toxicol. 10(2): 295-301.
-QSAR / SDO.
- NIL: Basak, S. C., Grunwald, G. D., Gute, B. D., Balasubramanian, K., and Opitz, D. 2000. Use of statistical and neural net approaches in predicting toxicity of chemicals. J Chem Inf Comput Sci 40(4): 885-90.
-MOD.
- NIL: Bazin, C., Chambon, P., Bonnefille, M., and Larbaigt, G. 1987. Compared sensitivity of luminescent marine bacteria (*Photobacterium phosphoreum*) and *Daphnia* bioassays. Sci.Eau. 6: 403-413.
-TONS, SW.
- NIL: Bearden, Anna P. and Schultz, T. Wayne. 1997. Structure-activity relationships for *Pimephales* and *Tetrahymena*: a mechanism of action approach. Environ. Toxicol. Chem. 16(6): 1311-1317.
-QSAR / SDO; TONS.
- NIL: Benoit-Guyod, J. L., Andre, C., and Clavel, A. K. 1984. Chlorophenols: degradation and toxicity (chlorophenols: degradation et toxicite). J Fr Hydrol 15(3): 249-266.
-NUE.
- NIL: Bermúdez-Saldaña, J. M., Escuder-Gilabert, L., Medina-Hernández, M. J., Villanueva-Camañas, R. M., and Sagrado, S. 2005. Chromatographic evaluation of the toxicity in fish of pesticides. J Chromatogr B Analyt Technol Biomed Life Sci 814(1): 115-25.
-NUE; SDO.
- NIL: Bermúdez-Saldaña, J. M., Garcia, M. A., Medina-Hernández, M. J., and Marina, M. L. 2004. Micellar electrokinetic chromatography with bile salts for predicting ecotoxicity of aromatic compounds. J Chromatogr A

1052(1-2): 171-80.

-NUE.

NIL: Binet, M. T., Adams, M. A., Stauber, J. L., King, C. K., Doyle, C. J., Lim, R. P., and Laginestra, E. 2003. Toxicity assessment of leachates from Homebush Bay landfills. *Australasian Journal of Ecotoxicology* 9(1): 7-18.

-LDO, TONNA.

#018002: Birge, W. J., Black, J. A., Hudson, J. E., and Bruser, D. M. 1979. Embryo-larval toxicity tests with organic compounds. L. L. Marking and R. A. Kimerle (Eds.), *Aquatic Toxicology and Hazard Assessment*, 2nd Symposium, ASTM STP 667, Philadelphia, PA:131-147.

-NUE: TDI. Same tests and results as #RA 1235 .T6 B5 and #PB 80 101637.

#RA 1235 .T6 B5: Birge, Wesley J., Black, Jeffrey A., and Bruser, Donald M. 1979. Toxicity of organic chemicals to embryo-larval stages of fish. Report #EPA/560/11-79/007. USEPA-OTS.

-TDI; tests and data same as those in #018002 and #PB 80 101637.

#PB 80 101637 (Fiche): Birge, Wesley J., Black, Jeffrey A., and Bruser, Donald M. 1979. Toxicity of organic chemicals to embryo-larval stages of fish. Report #EPA/560/11-79/007. USEPA-OTS: 72 pp.

-TDI; tests and data same as those in #018002 and #RA 1235 .T6 B5 .

#015334: Blondin, George A., Knobeloch, Lynda M., Read, Harry W., and Harkin, John M. 1988. An in vitro submitochondrial bioassay for predicting acute toxicity in fish. *ASTM Spec. Tech. Publ.* 1007(Aquat. Toxicol. Environ. Fate: 11th Vol.): 551-63.

-SDO.

#013295: Bobra, A., Shiu, W. Y., and MacKay, D. 1985. Quantitative structure-activity relationships for the acute toxicity of chlorobenzenes to *Daphnia magna*. *Environ. Toxicol. Chem.* 4(3): 297-305.

-TM/CU, TATO.

#017541: Botsford, J. L. 2002. A comparison of ecotoxicological tests. *Altern Lab Anim* 30(5): 539-50.

-TONS.

NIL: Bragadin, Marcantonio, Argese, Emanuele, Nicolli, Annamaria, and Bernardi, Paolo. 1992. A simple in vitro test to monitor trace metal toxicity in aqueous samples. *Environ. Technol.* 13(8): 779-84.

-NUE.

NIL: Breck, James E. 1988. Relationships among models for acute toxic effects: applications to fluctuating concentrations. *Environ. Toxicol. Chem.* 7(9): 775-8.

-MOD.

NIL: 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 ... *GWF-Wasser Abwasser* 122(7): 308-313.

-TONS.

NIL: Bringmann, G. and Kuhn, R. 1980. Determination of the harmful biological effect of water pollutants to bacteria, algae, and protozoa in the Cell Multiplication Inhibition Test. *Z. Wasser-Abwasser-Forsch.* 13(1): 26-31.

-TONS.

#005672: Bringmann, G. and Kuhn, R. 1977. The effects of water pollutants on *Daphnia magna*. *Z. Wasser-Abwasser-Forsch.* 10(5): 161-166.

-TDI.

#011330: Bringmann, Gottfried 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.

-TM/CU; TDI.

#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.

-TM/CU.

NIL: Burton, D. T., Dilorenzo, J. L., Shedd, T. R., and Wrobel, J. G. 2002. Aquatic hazard assessment of a contaminated surficial aquifer discharge into the Bush River, Maryland (U.S.A.). *Water, Air, and Soil Pollution* 139(1-4): 159-182.

-GWDO.

#005488: Calamari, D., Galassi, S., Setti, F., and Vighi, M. 1983. Toxicity of selected chlorobenzenes to aquatic organisms. *Chemosphere* 12(2): 253-262.

-NUE.

#PB 83 263665: Call, Daniel J., Brooke, Larry T., Ahmad, Nasim, and Richter, Joseph E. 1983. Report EPA-600/3-83-095(1983): 6472.

-ND for this chemical.

NIL: Chen, Jingwen, Feng, Liu, Zhao, Yuanhui, and Wang, Liansheng. 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; LSER; MOD.

NIL: Cocchi, M., Menziani, M. C., and De Benedetti, P. G. 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.

#013379: Cowgill, U. M. and Milazzo, D. P. 1991. The sensitivity of *Ceriodaphnia dubia* and *Daphnia magna* to seven chemicals utilizing the Three-Brood Test. *Arch. Environ. Contam. Toxicol.* 20(2): 211-217.

-TM/CU; TDI; NUE.

NIL: Cronin, Mark T. D. and Schultz, T. Wayne. 1997. Validation of *Vibrio fischeri* acute toxicity data: mechanism of action-based QSARs for non-polar narcotics and polar narcotic phenols. *Sci. Total Environ.* 204(1): 75-88.

-QSAR / SDO.

NIL: Dalich, G. M. and R. E. Larson. 1985. A comparative study of the hepatotoxicity of monochlorobenzene in the Rainbow Trout (*Salmo gairdnerii*) and the Sprague-Dawley Rat. *Comp. Biochem. Physiol. C* 80(1): 115-122.

-NUE.

NIL: Dalich, G. M. and R. E. Larson. 1980. The effects of monochlorobenzene on hepatic glutathione and liver function in Rainbow Trout and rats. *Fed. Proc.* 39(3): 621.

-NUE.

#007482: Dalich, G. M., Larson, R. E., and Gingerich, W. H. 1982. Acute and chronic toxicity studies with monochlorobenzene in Rainbow Trout. *Aquatic Toxicology* 2: 127-142.

-TM/CU; IITM/C.

#014420: De Wolf, W., Canton, J. H., Deneer, J. W., Wegman, R. C. C., and Hermens, J. L. M. 1988. Quantitative structure-activity relationships and mixture-toxicity studies of alcohols and chlorohydrocarbons: reproducibility of effects on growth and reproduction of *Daphnia magna*. *Aquat. Toxicol.* 12(1): 39-49.

-NUE.

NIL: DeJongh, J., Verhaar, H. J. M., and Hermens, J. L. M. 1998. Role of kinetics in acute lethality of nonreactive volatile organic compounds (VOCs). *Toxicol. Sci.* 45(1): 26-32.

-NUE: MOD.

#015330: Deneer, J. W., Sinnige, T. L., Seinen, W., and Hermens, J. L. M. 1988. The joint acute toxicity to *Daphnia magna* of industrial organic chemicals at low concentrations. *Aquat. Toxicol.* 12(1): 33-8.

-QSAR / SD; MD; IITM/C.

#006950: Devillers, J., Chambon, P., Zakarya, D., Chastrette, M., and Chambon, R. 1987. A predictive structure-toxicity model with *Daphnia magna*. *Chemosphere* 16(6): 1149-63.

-QSAR / SDO.

NIL: Devillers, James, Chambon, Paul, Zakarya, Driss, and Chastrette, Maurice. 1986. Quantitative structure-activity relations of lethal effects of 38 halogenated compounds on *Lepomis macrochirus*. *C. R. Acad. Sci., Ser. 3* 303(14): 613-16.

-QSAR / SDO.

NIL: Eldred, Donald V., Weikel, Cara L., Jurs, Peter C., and Kaiser, Klaus L. E. 1999. Prediction of Fathead Minnow acute toxicity of organic compounds from molecular structure. *Chem. Res. Toxicol.* 12(7): 670-678.

-QSAR / SDO.

NIL: Espinosa, G., Arenas, A., and Giralt, Francesc. 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: QSAR / SD; MOD.

NIL: Feng, Liu, Han, Shuokui, Zhao, Yuanhui, Wang, Liangsheng, and Chen, Jingwen. 1996. Toxicity of organic chemicals to Fathead Minnow: A United Quantitative Structure-Activity Relationship Model and its application. *Chem. Res. Toxicol.* 9(3): 610-13.

-QSAR / SDO.

#015326: Fiedler, H., Hutzinger, O., and Giesy, J. P. 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.

(4)

#005191: Freitag, D., Lay, J. P., and Korte, F. 1984. Environmental Hazard Profile - Test results as related to structures and translation into the environment. QSAR in Environmental Toxicology, Proc. of the Workshop held at McMaster University, Hamilton, Ont., Aug. 16-18, 1983, D.Reidel Publ. Co., Dordrecht, Netherlands: 111-131.
-QSAR / SDO.

NIL: Furay, V. J. and Smith, S. 1995. Toxicity and QSAR of chlorobenzenes in two species of benthic flatfish, Flounder (*Platichthys flesus* L.) and Sole (*Solea solea* L.). Bull. Environ. Contam. Toxicol. 54(1): 36-42.
-SW.

#016600: Gao, Chao, Govind, Rakesh, and Tabak, Henry H. 1992. Application of the group contribution method for predicting the toxicity of organic chemicals. Environ. Toxicol. Chem. 11(5): 631-6.
-TM/CU; IITM/C.

NIL: Gingerich, W. H. and G. M. Dalich. 1978. An evaluation of liver toxicity in Rainbow Trout following treatment with monochlorobenzene. Proc. West. Pharmacol. Soc. Calif. 21: 475-480.
-NUE.

#017473: Gingerich, W.H.; W.K. Seim; and R.D. Schonbrod. 1979. An apparatus for the continuous generation of stock solutions of hydrophobic chemicals. Bull. Environ. Contam. Toxicol. 23: 685-689.
-NUE; methodology, only.

NIL: Hall, Lenwood W, Hall, W. Scott, Bushong, Steven J., and Herman, Roger L. 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, Lowell H., Kier, Lemont B., and Phipps, Gary. 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., Hollister, T. A., and Parrish, P. R. 1981. Acute toxicity of 54 industrial chemicals to Sheepshead Minnows (*Cyprinodon variegatus*). Bull. Environ. Contam. Toxicol. 27(5): 596-604.
-SW.

#009663: Hermens, Joop, Canton, Hans, Janssen, Peter, and De Jong, Rob. 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.

#012010: Hodson, P.V. 1985. A comparison of the acute toxicity of chemicals to fish, rats and mice. Journ. Appl. Toxicol. 5(4): 220-226.
-SDO.

#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.
-TM/CU; IITM/C.

#013981: Hodson, Peter V., Dixon, D. George, and Kaiser, Klaus L. E. 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.
-SDO.

NIL: 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. NTIS/PB94-163557.
-SED.

#008079: Juhnke, Ingolf and Luedemann, Dietrich. 1978. Results of the study of 200 chemical compounds on acute fish toxicity using the Golden Orfe test. Z. Wasser Abwasser Forsch. 11(5): 161-4.
-SD; TDI; TONNA.

#017386: Kahl, M. D., Russom, C. L., DeFoe, D. L., and Hammermeister, D. E. 1999. Saturation units for use in aquatic bioassays. Chemosphere 39(3): 539-51.
-NUE.

NIL: Kaiser, Klaus L. E., Dixon, D. George, and Hodson, Peter V. 1984. QSAR studies on chlorophenols, chlorobenzenes and para-substituted phenols. Proc. Workshop Quant. Struct.-Act. Relat. QSAR Environ. Toxicol. 189-206.
-QSAR / SDO.

NIL: Kaiser, Klaus L. E., Niculescu, Stefan P., and Schuurmann, Gerrit. 1997. Feed forward back-propagation neural networks and their use in predicting the acute toxicity of chemicals to the Fathead Minnow. [Erratum to

(5)

document cited in CA127:132092]. Water Qual. Res. J. Can. 32(4): 855.

-NUE.

NIL: Kaiser, Klaus L. E., Niculescu, Stefan P., and Schuurmann, Gerrit. 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.

NIL: Kamlet, M J, Doherty, R M, Veith, G D, Taft, R W, and Abraham, M H. 1987. Solubility properties in polymers and biological media. 7. An analysis of toxicant properties that influence inhibition of bioluminescence in '*Photobacterium phosphoreum*' (The Microtox Test). NTIS/PB87-168126 .

-NUE: TONS, MOD.

NIL: Karabunarliev, Stoyan, Mekenyan, Ovanes G., Karcher, Walter, Russom, Christine L., and Bradbury, Steven P. 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.

NIL: Kasokat, Thomas, Nagel, Roland, and Ulrich, Klaus. 1989. Metabolism of chlorobenzene and hexachlorobenzene by the Zebra Fish, *Brachydanio rerio*. Bull. Environ. Contam. Toxicol. 42(2): 254-61.

-METDO.

#007313: Kerster, H. W. and Schaeffer, D. J. 1983. Brine shrimp (*Artemia salina*) nauplii as a teratogen test system. Ecotoxicol. Environ. Saf. 7(3): 342-349.

-NUE; SW.

NIL: 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.

-TONNA.

#000816: Koch, R. 1982. Molecular connectivity and acute toxicity of environmental pollutants. Chemosphere 11(9): 925-31.

-NUE; SD.

#006060: Konemann, Hans. 1981. Quantitative structure-activity relationships (QSARs) in fish toxicity studies. Part 1: Relationship for industrial pollutants. Toxicology 19(3): 209-21.

-TM/CU.

NIL: Liu, Zhengtao, Wang, Liansheng, Ni, Hong, and Kong, Zhiming. 1997. QSAR for biotoxication of aromatic compounds. Chin. Sci. Bull. 42(5): 380-384.

-QSAR / SDO.

#011509: Lu, P. Y. and R. L. Metcalf. 1975. Environmental fate and biodegradability of benzene derivatives as studied in a model aquatic ecosystem. Environ. Health Perspect. 10: 269-284.

-NUE: UP / MED.

NIL: MacKenzie, C. L. and Shearer, L. W. 1959. Chemical control of *Polydora websteri* and other annelids inhabiting oyster shells. Proc. Natl. Shellfish Assoc. 50: 105-111.

-SW.

#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.

-TM/CU; TDI; SD.

NIL: Martin, T. M. and Young, D. M. 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.

-QSAR / SDO.

#007917: Mayes, M. A. , Alexander, H. C., and Dill, D. C. 1983. A study to assess the influence of age on the response of Fathead Minnows in static acute toxicity tests. Bull. Environ. Contam. Toxicol. 31(2): 139-147.

-TM/CU for this chemical.

NIL: McCarty, Lynn S. 1987. Relationship between toxicity and bioconcentration for some organic chemicals. I. Examination of the relationship. QSAR Environ. Toxicol., Proc. Int. Workshop, 2nd : 207-20.

-QSAR / SDO.

#013104: McGowan, John C. and Mellors, Alan. 1986. Molecular volumes and the toxicities of chemicals to fish. Bull. Environ. Contam. Toxicol. 36(6): 881-7.

-REJECT (secondary data, only)

#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. Toxicology and Applied Pharmacology 77: 1-10.
-NUE.

NIL: Mikaelian, I., Y. de Lafontaine, J. C. Harshbarger, L. L. Lee, and D. 6) Martineau. 2002. Health of Lake Whitefish (*Coregonus chupeaformis*) with elevated tissue levels of environmental contaminants. Environ Toxicol Chem 21(3): 532-41.

-NUE: AMDO.

NIL: Nalecz-Jawecki, G. and Sawicki, J. 2002. A comparison of sensitivity of Spirotox biotest with standard toxicity tests. Arch Environ Contam Toxicol 42(4): 389-95.

-NUE: TONS, SDO.

NIL: Neely, W. B. 1984. An analysis of aquatic toxicity data: water solubility and acute LC50 fish data. Chemosphere 13(7): 813-820.

-MOD, SDO.

NIL: Netzeva, T. I., Aptula, A. O., Benfenati, E., Cronin, M. T., Gini, G., Lessigiarska, I., Maran, U., Vracko, M., and Schüürmann, G. 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.

-QSAR / SDO.

NIL: Niculescu, S. P., Atkinson, A., Hammond, G., and Lewis, M. 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.

-QSAR / MOD / SD.

NIL: Nouwen, Johan, Lindgren, Fredrik, Hansen, Bjorn, and Karcher, Walter. 1996. Fast screening of large databases using clustering and PCA based on structure fragments. J. Chemom. 10(5 & 6): 385-398.

-QSAR / SD.

NIL: Oberg, T. 2004. A QSAR for baseline toxicity: validation, domain of application, and prediction. Chem Res Toxicol 17(12): 1630-7.

-QSAR / MOD / SD.

NIL: Pagano, G., Cipollaro, M., Corsale, G., Esposito, A., Giordano, G. G., Ragucci, E., and Trieff, N. M. 1988. Comparative toxicities of benzene, chlorobenzene, and dichlorobenzenes to sea urchin embryos and sperm. Bull. Environ. Contam. Toxicol. 40(4): 481-488.

-SW.

#015771: Ramos, Enaut Urrestarazu, Vaes, Wouter H. J., Verhaar, Henk J. M., and Hermens, Joop L. M. 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, Gary D. and Samfield, Max. 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.

-WET.

#015324: Ribo, J. M. and Kaiser, K. L. E. 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.

-NUE, SD.

NIL: Ribo, Juan M. 1997. Interlaboratory comparison studies of the luminescent bacteria toxicity bioassay. Environmental Toxicology and Water Quality 12(4): 283-294.

-NUE: TONS, SD.

NIL: Roex, Erwin W. M., Van Gestel, Cornelis A. M., Van Wezel, Annemarie P., and Van Straalen, Nico M. 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.

-MOD, SDO.

NIL: 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.

-TONNA, QSAR, SDO.

NIL: 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*. Arch. Environ. Contam. Toxicol. 34(3): 248-252.

-TONNA, QSAR, SDO.

NIL: Schultz, T. W. and J. R. Seward. 2000. Dimyristoyl phosphatidylcholine/water partitioning-dependent modeling of narcotic toxicity to *Tetrahymena Pyriformis*. Quantitative structure-activity relationships including molecular modelling and applications of computer graphics in pharmacology, Chemistry, and Biology : QSAR 19(4): 339-345.

-QSAR / SD, TONS.

NIL: 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 Meeting Date 1996, 343-362. Editor(s): Chen, Fei; Schueuermann, Gerrit. Publisher: SETAC Press, Pensacola, Fla..

-TONS, QSAR / SDO.

NIL: Sixt, Stefan, Altschuh, Joachim, and Brueggemann, Rainer. 1995. Quantitative structure-toxicity relationships for 80 chlorinated compounds using quantum chemical descriptors. Chemosphere 30(12): 2397-414.

-QSAR / SDO.

#007901: Stephan, C. E. 1978. In-depth studies on health and environmental impacts of selected water pollutants. Contract No.68-01-4646, U.S.EPA :9 p.

-NUE; SW; also listed as ref #15446).

ET&C v.16 n.9: Twerdok, Lorraine E., Burton, Dennis T., Gardner, Henry S., Shedd, Tommy R., and Wolfe, Marilyn J. 1997. The use of nontraditional assays in an integrated environmental assessment of contaminated ground water. Environ. Toxicol. Chem. 16(9): 1816-1820.

-NUE: GWDO.

NIL: 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.

-QSAR / SDO.

#014413: Van der Zandt, P. T. J., Heinis, F., and Kikkert, A. 1994. Effects of narcotic industrial pollutants on behaviour of midge larvae (*Chironomus riparius* (Meigen), Diptera): a quantitative structure-activity. Aquat Toxicol 28(4-Mar): 209-221.

-NUE.

#013648: Van Leeuwen, C. J., Adema, D. M. M., and Hermens, J. 1990. Quantitative structure-activity relationships for fish early life stage toxicity. Aquat. Toxicol. 16(4): 321-34.

-NUE.

NIL: van Wijk, D., Thompson, R. S., De Rooij, C., Garny, V., Lecloux, A., and Kanne, R. 2004. Monochlorobenzene marine risk assessment with special reference to the OSPARCOM region: North Sea. Environ Monit Assess 97(1-3): 69-86.

-SW, MOD, SD.

NIL: Veith, G. D. and Mekenyan, O. G. 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.

NIL: Verhaar, Henk J. M., Ramos, Enaut Urrestarazu, and Hermens, Joop L. M. 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.

-QSAR / SDO.

NIL: Verhaar, Henk J. M., Solbe, John, Speksnijder, John, Van Leeuwen, Cees J., and Hermens, Joop L. M. 2000. Classifying environmental pollutants: Part 3. External validation of the classification system. Chemosphere 40(8): 875-883.

-MOD, SD.

NIL: 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.

-QSAR / SDO.

NIL: Wang, Guilian and Bai, Naibin. 1997. Study on QSAR for general pollutants in organic industrial waste. Toxic Subst. Mech. 16(4): 315-326.

-QSAR / SDO.

NIL: Wang, Lianshen, Liu, Zhengtao, Zhou, Fengfan, Yu, Hongxia, and Gao, Hong. 1994. QSAR model parameters research on substituted aromatic compounds. Huanjing Kexue 15 (3): 7-10.

-QSAR / SDO.

#016611: Wei, Liping, Zhang, Wenhua, Han, Shuokui, Wang, Liansheng, and Zhao, Yuanhui. 1999. Acute/chronic ratios to estimate chronic toxicity from acute data. *Toxicol. Environ. Chem.* 69(3-4): 395-401.

-QSAR / SD; TDI.

NIL: Williams, D and Fulthorpe, Roberta. 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.

-AMDO.

NIL: Yin, H. and J. Lu. 1993. Toxic effect of two organic toxicants on *Penaeus chinensis*. *Mar.Sci./Haiyang Kexue* 1: 59-62.

-TONNA, SW.

NIL: Yin, Yiwei, Lin, Jia, and Zhu, Yongan. 1994. Acute toxicity of benzene, chlorobenzenes, phenol, and chlorophenols towards the fry of loach (*Paramisgurnus dabryanus* Sauvage) induced by artificial ovulation. *Jinan Daxue Xuebao, Ziran Kexue Yu Yixueban* 15(3): 106-109.

-TONNA, SW.

NIL: Zaroogian, G., Heltshe, J. F., and Johnson, M. 1985. Estimation of toxicity to marine species with structure-activity models developed to estimate toxicity to freshwater fish. *Aquat. Toxicol.* 6(4): 251-70.

-SW, QSAR.

#013103: Zhao, Yuanhui, Wang, Liansheng, Gao, Hong, and Zhang, Zheng. 1993. Quantitative structure-activity relationships-relationship between toxicity of organic chemicals to fish and to *Photobacterium phosphoreum*. *Chemosphere* 26(11): 1971-9.

-IITM/C; TDI; SD.

NIL: Zholdakova, Z. I. and Kokh, R. 1986. Molecular connectiveness and acute chemical toxicity. *Gig. Sanit.* (7): 18-19.

-NUE: MOD.

NIL: Zhou, Wen-fu. 2002. QSAR study for the SHOE1, - log LC50 and log Kow of halogeno benzene and phenol derivatives. *Youji Huaxue* 22(9): 658-662.

-QSAR / SDO.

*For key to abbreviations, see Appendix, attached.

APPENDIX: REFERENCE ABBREVIATIONS USED, 10/05

AMD = ambient monitoring data.
BCF = bioconcentration factor.
D = data (as a suffix to other abbreviations listed here).
DO = data only (as a suffix to other abbreviations listed here)..
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 data (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.
NUE = no useable endpoint.
O = only (as a suffix to other abbreviations listed here).
PD = phytotoxicity 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.
UP = uptake data.
WET = whole-effluent testing.