

Rule 57 Aquatic Values Data Sheet

9/18/2006

Chemical or product name: 4-Nitrophenol

Developed by: Christopher Hull FAV*: 1,900 ug/l

(Tier: II)

Manufacturer (WTAs): ----

Approved by: D. Bush AMV*: 940 ug/l

(Tier: II)

C.A.S #: 100-02-7

Approval date: 6/30/08 FCV*: 200 ug/l

(Tier: II)

CAS, ACQUIRE: 7/17-18/06

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 pH (s.u.)	LC50/EC50 ug/L	SMAV ug/L	GMAV ug/L	Rank	Reference
Channel Catfish (<i>Ictalurus punctatus</i>)	LC50	96	FT,M	44.9	6.9-7.7	15,000	15,000	15,000	1	1
Water Flea (<i>Daphnia magna</i>)	LC50	48	S,U	173.0	7.4-9.4	22,000	22,000	22,000	2	2
Sheepshead Minnow (<i>Cyprinodon variegatus</i>)	LC50	96	FT,M	-----	-----	32,000	29,394	29,394	ACR only	3
	LC50	96	FT,M	-----	-----	27,000				4
Fathead Minnow (<i>Pimephales promelas</i>)	LC50	96	FT,M	47.8	7.66	58,600	44,338	44,338	3	5
	LC50	96	FT,M	43.2	7.32	41,000				1,5
	LC50	96	FT,M	45.1	7.56	37,300				5
	LC50	96	FT,M	43.3-48.5	-----	59,000				6
	LC50	96	FT,M	43.3-48.5	-----	62,000				6
	LC50	96	FT,M	45	7.8	30,400				7
	LC50	96	FT,M	45	7.8	33,800				7

CHRONIC DATA

Species	Test type (ELS, etc.)	Duration (days)	Study Conditions (FT,M etc.)	Hardness mg/L	Test pH (s.u.)	MATC ug/L	SMCV ug/L	GMCV ug/L	Rank	Reference
Water Flea ¹	LC	21	FT,M	128.4	8.1-8.9	6,299	6,299	6,299	1	8
(<i>Daphnia magna</i>)	LC	21	SR,M	128.4	7.7-8.8	7,340 ²				8
Sheepshead Minnow ³	ELS	28	FT,M	-----	-----	13,115	13,115	13,115	2	3
(<i>Cyprinodon variegatus</i>)										

*Value rounded to 2 significant figures.

¹ For MATC and ACR calculations, see Table 1.

² Value not used to calculate SMCV, because a value derived from a FT,M test is preferred over values from other test types (Rule 57(2)(i)(i)(C)).

³ For MATC and ACR calculations, see Table 2.

Table 1. MATC & ACR calculations for *Daphnia magna* tested with 4-Nitrophenol (Ref. # 8), 9/06.

Acute = 48-hr. $EC_{50} = 25,800 \text{ mg/L}$ (unsubstantiated).

Chronic =

- FT, M test = 21-day $NOEC$ (reprodu.) = $4,350 \text{ mg/L}$;
 $LOEC = 9,120 \text{ mg/L}$; $MATC = \bar{X}_g = 6,299 \text{ mg/L}$.

- SR, M test = 21-day $NOEC$ (reprodu.) = $5,150 \text{ mg/L}$; $LOEC = 10,460 \text{ mg/L}$;
 $MATC = \bar{X}_g = 7,340 \text{ mg/L}$.

ACR = No valid acute value, so no ACR possible.

Table 2. MATC & ACR calculations for Sheepshead Minnow tested with 4-Nitrophenol (Ref. # 3).

Acute = 96-hr. LC_{50} (FT, M) = $32,000 \text{ mg/L}$.

Chronic = 28-day $NOEC$ (growth, hatchability) = $10,300 \text{ mg/L}$;
 $LOEC = 16,700 \text{ mg/L}$; $MATC = \bar{X}_g = 13,115.258 \text{ mg/L}$.

ACR = $\frac{96\text{-hr. } LC_{50} \text{ (Ref. \#3)}}{28\text{-day } MATC \text{ (Ref. \#3)}} = \frac{32,000 \text{ mg/L}}{13,115.258 \text{ mg/L}} = \underline{2.4399063}.$

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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

Chemical Name: 4-Nitrophenol
 C.A.S. #: 100-02-7

AQUATIC MAXIMUM VALUE CALCULATIONS, 9/06

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
$$FAV = \frac{\text{lowest AMAV}}{\text{Acute Factor}} = \frac{15,000 \text{ ug/l}}{8} = 1,875 \text{ ug/l}$$

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:
$$AMV = \frac{FAV}{2} = \frac{1,875 \text{ ug/l}}{2} = 937.5 \text{ ug/l}$$

4-NITROPHENOL =

Christfull

FINAL CHRONIC VALUE CALCULATIONS, 9/06

A. Minimum 8 species requirement is **not** met (Tier II). Minimum requirements met = 1 (GMCV route);
Minimum requirements missing for Tier I = 0 (ACR route);
Minimum requirements missing for Tier I = GMCV route = 8; ACR route = 2.

1. Acute to chronic ratio

a. Number ACRs meeting minimum data requirements = 1 (Table 2)

b. Acute to chronic ratio = $\bar{X}_g(\text{SUM ACR}, 18, 18) = \bar{X}_g(2.4399063, 18, 18)$

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

$$\text{FCV} = \frac{\text{FAV}}{\text{ACR}} = \frac{1,875 \text{ mg/L}}{9.2464009} =$$

$$= \frac{202.7816 \text{ mg/L}}{9.2464009}$$

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 =

4-NITROPHENOL REFERENCES, 9/06

References Used:

1. #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.
2. #007906: LeBlanc, Gerald A. 1980. Acute toxicity of Priority Pollutants to water flea (*Daphnia magna*). Bull. Environ. Contam. Toxicol. 24(5): 684-91.
3. #007902: Ward, G. S., Parrish, P. R., and Rigby, R. A. 1981. Early life stage toxicity tests with a saltwater fish: effects of eight chemicals on survival growth, and development of Sheepshead Minnows (*Cyprinodon variegatus*). J Toxicol Environ Health 8(1-2): 225-40.
4. #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.
5. #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*), Volume 2. Ctr.for Lake Superior Environ.Stud., Univ.of Wisconsin-Superior, Superior, WI :326 p.
6. #009059: Phipps, Gary L., Holcombe, Gary W., and Fiantdt, James T. 1981. Acute toxicity of phenol and substituted phenols to the Fathead Minnow. Bull. Environ. Contam. Toxicol. 26(5): 585-93.
7. #015404: Broderius, Steven J., Kahl, Michael D., and Hoglund, Marilyn D. 1995. Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environ. Toxicol. Chem. 14(9): 1591-605.
8. #018358: Francis, Paul C., Grothe, Douglas W., and Scheuring, John C. 1986. Chronic toxicity of 4-nitrophenol to *Daphnia magna* Straus under static-renewal and flow-through conditions. Bulletin of Environmental Contamination and Toxicology 36(5): 730-7.

References Reviewed, but Not Used:

- #006622: Alexander, Howard C., Bodner, Kenneth M., and Mayes, Monte A. 1983. Evaluation of the OECD Fish Prolonged Toxicity Study at Least 14 Days. Chemosphere 12(3): 415-23.
-SDO
- #SH 11 .A335 no.207: Applegate, V. C., J. H. Howell, A. E. Hall, and M. A. Smith. 1957. Toxicity of 4,346 chemicals to larval lampreys and fishes. Fish Wildl. Serv., U.S.D.I., Washington, D.C. Spec. Sci. Rep.-Fish. No. 207, p. 157p.
-NUE
- #V2852: Barahona, M. V. and S. Sanchez-Fortun. 1996. Comparative sensitivity of three age classes of *Artemia salina* larvae to several phenolic compounds. Bull. Environ. Contam. Toxicol. 56(2): 271-278.
-SW
- #V1096: Bearden, A. P. and Schultz, T. W. 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, 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
- #V2850: Brecken-Folse, J. A., Mayer, F. L., Pedigo, L. E., and Marking, L. L. 1994. Acute toxicity of 4-nitrophenol, 2,4-dinitrophenol, terbufos and trichlorfon to Grass Shrimp (*Palaemonetes* spp.) and Sheepshead Minnows (*Cyprinodon variegatus*) as affected by salinity and temperature. Environ. Toxicol. Chem. 13(1): 67-77.
-SW
- #015362: Bresch, H. 1982. Investigation of the long-term action of xenobiotics on fish with special regard to reproduction. Ecotoxicology and Environmental Safety 6: 102-112.
-TONNA
- #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 harmful biological effect of water pollutants in protozoa. II. Bacteriovorous ciliates (Bestimmung der Biologischen Schädigung Wassergefährdender Stoffe Gegen Protozoen. II. Bakterienfressende. Z. Wasser-Abwasser-Forsch. 13(1): 26-31.

-NUE; TONS.

#005672: Bringmann, G. and Kuhn, R. 1977. The effects of water pollutants on *Daphnia magna* (Befunde der Schädigung Wassergefährdender Stoffe Gegen *Daphnia magna*). Z. Wasser-Abwasser-Forsch. 10(5): 161-166(ENG TRANSL)(OECDG Data File).

-TDI.

#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, Gottfried and Kuhn, R. 1977. Results of the damaging effect of water pollutants on *Daphnia magna*. Z. Wasser Abwasser Forsch. 10(5): 161-6.

-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.

-TDI; TM/CU.

#018325 : Broderius, S. J., Kahl, M. D., Elonen, G. E., Hammermeister, D. E., and Hoglund, M. D. 2005. A comparison of the lethal and sublethal toxicity of organic chemical mixtures to the Fathead Minnow (*Pimephales Promelas*). Environmental toxicology and chemistry 24(12): 3117-27.

-SDO

#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; IITM/C.

#002653: Cairns, J., Calhoun, W. F., McGinniss, M. J., and Straka, W. 1976. Aquatic organisms response to severe stress following acutely sublethal toxicant exposure. Water Resour. Bull. 12(6): 1233-1243.

-IITM/C.

#009241: Call, D. J., Brooke, L. T., and Lu, P. Y. 1980. Uptake, elimination, and metabolism of three phenols by Fathead Minnows. Arch. Environ. Contam. Toxicol. 9(6): 699-714.

-BCF/UDO.

#RA 1199 .E5 77-066: Carlson, R. M. and Caple, R. 1977. Chemical/biological implications of using chlorine and ozone for disinfection. Epa-600/3-77-066, U.S.Epa, Duluth, Mn:88 P.(U.S.Ntis Pb-270694) .

-SDO.

#V1119: Cash, G. G. and Clements, R. G. 1996. Comparison of structure-activity relationships derived from two methods for estimating octanol-water partition coefficients. SAR QSAR Environ. Res. 5(2): 113-124.

-QSAR / SDO.

#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.

-SD; IITM/C.

#V1123: 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 / SDO.

#V1170: Devillers, J. and Chambon, P. 1988. A methodological framework for the early detection of drinking water pollutants. Chemosphere 17(9): 1647-54.

-NUE; TDI.

#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.

#V1180: Devillers, J. , Meunier, T., and Chambon, P. 1985. Advantage of the dosage-action-time relation in ecotoxicology for the test of the various chemical species of toxics. Tech.Sci.Munic 80(7-8): 329-334 .

-NUE; TDI.

#V1236: 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.
 -NUE; QSAR / SDO.

#015619: Ensenbach, U. and Nagel, R. 1991. Toxicokinetics of xenobiotics in Zebrafish - comparison between tap and river water. Comp. Biochem. Physiol. C 100(2-Jan): 49-53.
 -NUE: BCF, UDO.

#V1645: EPA. Office of Pesticide Programs. Environmental Fate and Effects Division. 2000. In: Pesticide Ecotoxicity Database (Formerly: Environmental Effects Database (EEDB)) .
 -SDO; used for reference, only.

#V1237: 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; SDO.

#V1253: 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.

#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. 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.

#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.
 -REJECT (IITM/C; TM/CU).

#005855: Gersdorff, W. A. 1939. Effect of the introduction of the nitro group into the phenol molecule on toxicity to Goldfish. J. Cell. Comp. Physiol. 14: 61-71.
 -NUE.

#V2847: Grosch, D. S. 1973. Reproduction tests: the toxicity for *Artemia* of derivatives from non-persistent pesticides. Biol. Bull. 145(2): 340-351.
 -SW.

#017257: Guilhermino, Lucia, Diamantino, Teresa, Carolina Silva, M., and Soares, A. M. V. M. 2000. Acute toxicity test with *Daphnia magna*: an alternative to mammals in the prescreening of chemical toxicity? Ecotoxicol. Environ. Saf. 46(3): 357-362.
 -IITM/C, or SDO.

#017636: Halbach, U., Siebert, M., Westermayer, M., and Wissel, C. 1983. Population ecology of rotifers as a bioassay tool for ecotoxicological tests in aquatic environments. Ecotoxicol. Environ. Saf. 7(5): 484-513.
 -IITM/C.

#013976: Hall, Lowell H. and Kier, Lemont B. 1984. A molecular connectivity study of phenols and their toxicity to fish. QSAR Des. Bioact. Compd. 53-9. Editor(s): Kuchar, M. Publisher: Prous, Barcelona, Spain..
 -MDO.

#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.

#V2213: Hemmer, M. J. , Middaugh, D. P., and Comparetta, V. 1992. Comparative acute sensitivity of larval Topsmelt, *Atherinops affinis*, and Inland Silverside, *Menidia beryllina*, to 11 chemicals. Environ. Toxicol. Chem. 11(3): 401-408.
 -NUE; TONNA; TM/CU.

#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; these data are later reported in #012010 and #013981.

#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.

#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 (*Oncorhynchus mykiss*). Can. Tech. Rep. Fish. Aquat. Sci. 1784: 55 p.

-TDI.

#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 (#00473).

#V1388: Holdway, D. A., Dixon, D. G., and Kaiser, K. L. 1991. The acute toxicity of pulse-dosed, para-substituted phenols to larval American flagfish (*Jordanella floridae*): a comparison with toxicity to photoluminescent bacteria and predicted toxicity using log Kow. Sci Total Environ 104(3): 229-37.

-NUE.

#013843: Howe, G. E., Marking, L. L., and Bills, T. D. 1994. Effects of water temperature and pH on toxicity of terbufos, trichlorfon, 4-nitrophenol, and 2,4-dinitrophenol to the amphipod *Gammarus pseudolimnaeus* and Rainbow Trout (*Oncorhynchus mykiss*). Environmental Toxicology and Chemistry 13: 51-66.

-NUE; IITM/C; TM/CU.

#013842: Howe, G. E., Marking, L. L., and Bills, T. D. 1994. Effects of water temperature on the toxicity of 4-nitrophenol and 2,4-dinitrophenol to developing Rainbow Trout (*Oncorhynchus mykiss*). Environmental Toxicology and Chemistry 13: 79-84.

-NUE.

#V2855: Huber, H. C., Ritter, U., Huber, W., and Mucke, W. 1994. Photometrische Bestimmung der Zytotoxizität von Chemikalien mit Mikrokulturen von *Tetrahymena pyriformis* und *Pseudomonas aeruginosa*. Umweltwissenschaften und Schadstoff-Forschung 6(5): 251-253.

-NUE; TONNA.

#016591: Hutchinson, T. H., Solbe, J., and Kloepper-Sams, P. J. 1998. Analysis of the ECETOC Aquatic Toxicity (EAT) database. III - Comparative toxicity of chemical substances to different life stages of aquatic organisms. Chemosphere 36(1): 129-142.

-SDO.

#V1348: Hutchinson, Thomas H., Scholz, Norbert, and Guhl, Walter. 1997. Analysis of the ECETOC aquatic toxicity (EAT) database. IV - Comparative toxicity of chemical substances to freshwater versus saltwater organisms. Chemosphere Volume Date 1998, 36(1): 143-153.

-SDO.

#V1416: 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.

#V1417: 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 document cited in CA127:132092]. Water Qual. Res. J. Can. 32(4): 855.

-NUE.

#V1418: 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; SDO

#018360: Kanabur, V. V. and Sangli, Asheera Banu. 2000. Acute toxicity of resorcinol and nitrophenol to a freshwater fish, *Gambusia affinis*, and their effects on oxygen uptake. Geobios 27(4): 188-190.

-IITM/C.

#V1422: 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.

#010495: Keen, R. and Baillod, C. R. 1985. Toxicity to *Daphnia* of the end products of wet oxidation of phenol and substituted phenols. Water Research 19(6): 767-772.

-TM/CU; IITM/C.

#003169: Kenaga, Eugene 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., Geyer, H., Freitag, D., and Rohleder, H. 1984. Sensitivity of schemes for ecotoxicological

hazard ranking of chemicals. Chemosphere 13(1): 203-211.

-SDO.

#V1475: Kobayashi, K., Oshima, Y., Hamada, S., and Taguchi, C. 1987. Induction of phenol-sulfate conjugating activity by exposure to phenols and duration of its induced activity in Short-Necked Clam. Bull. Jpn. Soc. Sci. Fish. -NUE; SW; TONNA.

#013449: Kopperman, Herbert L., Carlson, Robert M., and Caple, Ronald. 1974. Aqueous chlorination and ozonation studies. I. Structure-toxicity correlations of phenolic compounds to *Daphnia magna*. Chem.-Biol. Interact. 9(4): 245-51.

-REJECT (test organisms fed during test; test temperature inappropriate).

#V1432: Kuhn, R. 1988. Schadstoffwirkungen von Umweltchemikalien im Daphnien-Reproduktions-Test als Grundlage für die Bewertung der Umweltgefährlichkeit in Aquatischen Sys... Forschungsbericht .

-NUE.

#012430: Kuhn, R., Pattard, M., Pernak, K., and Winter, A. 1989. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to *Daphnia magna*. Water Res 23(4): 495-499.

-TM/CU.

#010310: Kuhn, R., Pattard, Monika, Pernak, Klaus Dieter, and Winter, Angela. 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.

#V1524: Lange, Monica, Gebauer, Wolfgang, Markl, Juergen, and Nagel, Roland. 1995. Comparison of testing acute toxicity in embryo of Zebrafish, *Brachydanio rerio* and RTG-2 cytotoxicity as possible alternative to the acute fish test. Chemosphere 30(11): 2087-102.

-NUE; TONNA.

#009664: LeBlanc, Gerald A. 1984. Interspecies relationships in acute toxicity of chemicals to aquatic organisms. Environ. Toxicol. Chem. 3(1): 47-60.

-REJECT (SW; IITM/C).

#018359: Lee, Y. G., Hwang, S. H., and Kim, S. D. 2006. Predicting the Toxicity of Substituted Phenols to Aquatic Species and Its Changes in the Stream and Effluent Waters. Archives of environmental contamination and toxicology 50(2): 213-9.

-IITM/C; TONNA; PD.

#V2846: Leland, H. V. 1968. Biochemical factors affecting toxicity of parathion and selected analogs to fishes. Ph.D. Thesis, University of Michigan, Ann Arbor, MI :123 p.

-NUE.

#V2843: Linton, T. K. 1992. Salinity and temperature effects on the chronic toxicity of 2,4-dinitrophenol and 4-nitrophenol to Sheepshead Minnows (*Cyprinodon variegatus*). M.S. Thesis, University of West Florida, Pensacola, FL :85 p.

-SW.

#V2849: Linton, T. K., Mayer, F. L., Simon, T. L., Malone, J. A., and Marking, L. L. 1994. Salinity and temperature effects on chronic toxicity of 2,4-dinitrophenol and 4-nitrophenol to Sheepshead Minnows (*Cyprinodon variegatus*). Environ. Toxicol. Chem. 13(1): 85-92.

-SW.

#V2809: Lipnick, Robert L., Bickings, Charlene K., Johnson, David E., and Eastmond, David A., 1985. Comparison of QSAR predictions with fish toxicity screening data for 110 phenols. ASTM Spec. Tech. Publ.

-QSAR / SDO.

#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 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.

-NUE; QSAR / SDO.

#V1542: McCarty, L. S., Hodson, P. V., Craig, G. R., and Kaiser, K. L. E. 1985. The use of quantitative structure-activity relationships to predict the acute and chronic toxicities of organic chemicals to fish. Environ. Toxicol. Chem. 4(5): 595-606.

-QSAR / SDO.

#005766: McLeese, D. W., Zitko, V., and Peterson, M. R. 1979. Structure-Lethality Relationships for Phenols, Anilines and Other Aromatic Compounds in Shrimp and Clams. Chemosphere 8(2): 53-57.

-NUE; QSAR/SDO.

#V2842: Nagel, R. 1992. Toxicity of pesticides to aquatic vertebrates illustrated by the example of the fish. In: H.Becker and R.Heitefuss Determination of Herbicides in Aquatic Ecosystems . Germany: Johannes Gutenberg- Univ.Mainz, pp. 88-104.
-NUE.

#V1617: Neely, W. B. 1984. An analysis of aquatic toxicity data: water solubility and acute LC50 fish data. Chemosphere 13(7): 813-820.
-SDO.

#V1616: 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 .
-NUE; QSAR / SDO.

#V2861: Nishiuchi, Yasuharu. 1984. Toxicity of agrochemicals to freshwater organisms. 2. Dyes. Suisan Zoshoku 32(1): 61-4.
-NA; NR; probably TDI, based upon all previous experience with this researcher.

#V2801: Papa, E., Villa, F., and Gramatica, P. 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, Netzeva, T. I, and Worth, A. P. 2006. Validation of a QSAR model for acute toxicity. SAR and QSAR in Environmental Research 17(2): 147-171.
-QSAR / SDO.

#015890: Piontek, Marlena. 1999. Use of a planarian *Dugesia tigrina* Girard in the studies of acute toxicity of organic substances. Pol. Arch. Hydrobiol. 46(3-4): 331-338.
-TONNA.

#015353: Protic, Miroslava and Sabljic, Aleksandar. 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.

#V1704: Ramos, Enaut Urrestarazu, Vaal, Manon A., and Hermens, Joop L. M. 2002. Interspecies sensitivity in the aquatic toxicity of aromatic amines. Environmental Toxicology and Pharmacology 11(3-4): 149-158.
-SDO

#007715: Randall, T. L. and Knopp, P. V. 1980. Detoxification of specific organic substances by wet oxidation. J Water Pollut Control Fed 52(8): 2117-2130.
-IITM/C; or 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 .
-WETO.

#V1722: Roche, H. and Boge, G. 1996. Fish blood parameters as a potential tool for identification of stress caused by environmental factors and chemical intoxication. Mar. Environ. Res. 41(1): 27-43.
-NUE.

#V1690: 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.
-SDO.

#009688: Saarikoski, Juhani and Viluksela, Matti. 1982. Relation between physicochemical properties of phenols and their toxicity and accumulation in fish. Ecotoxicol. Environ. Saf. 6(6): 501-12.
-TM/CU; IITM/C; some are SDO from #009538.

#015372: Saito, Hotaka, Koyasu, Junko, Yoshida, Kikuo, Shigeoka, Tadayoshi, and Koike, Sakae. 1993. Cytotoxicity of 109 chemicals to goldfish GFS cells and relationships with 1-octanol/water partition coefficients. Chemosphere 26(5): 1015-28.
-NUE.

#V2854: Sangli, A. B. and Kanabur, V. V. 1998. Toxicity of resorcinol and nitrophenol to a freshwater fish *Lepidocephalus guntea*. Environ. Ecol. 16(3): 642-644.
-TONNA.

#V2863: Sangli, Asheera Banu and Kanabur, V. V. 2001. Influence of temperature on the acute toxicity of nitrophenol and resorcinol to a freshwater fish *Lepidocephalichthys guntea*. Environment and Ecology 19(1): 23-25.
-TONNA.

#V2845: Scholz, N. 1987. *Barentsia matsushimana*, a marine Entoproct suitable for bioassays. Bull. Environ.

Contam. Toxicol. 38(4): 634-640.

-SW; TONNA.

#016606: Schueuermann, Gerrit, Segner, Helmut, and Jung, Klaus. 1997. Multivariate mode-of-action analysis of acute toxicity of phenols. Aquat. Toxicol. 38(4): 277-296.

-NUE, TONNA, or SDO.

#005178: Schultz, T. W., Holcombe, G. W., and Phipps, G. L. 1986. Relationships of Quantitative Structure-Activity to comparative toxicity of selected phenols in the *Pimephales promelas* and *Tetrahymena pyriformis* test systems. Ecotoxicol Environ Saf 12(2): 146-53.

-SDO, reporting data from #009059 and # QL 638 .C94 A27.

#016596: Steinberg, Christian E. W., Sturm, Armin, Kelbel, Jutta, Lee, Sung Kyu, Hertkorn, Norbert, Freitag, Dieter, and Kettrup, Antonius A. 1992. Changes of acute toxicity of organic chemicals to *Daphnia magna* in the presence of dissolved humic material (DHM). Acta Hydrochim. Hydrobiol. 20(6): 326-32.

-NUE.

#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; IITM/C; SDO (SW mysid acute data without accompanying chronic data. Also listed as ref #015446).

#V2840: Svobodova, Z. and Vykusova, B. 1988. Comparing the sensitivity of Rainbow Trout and *Rasbora heteromorpha* to various toxic substances (Porovnani Citlivosti Pstruha Duhoveho a Razbory Klinoskvrne k Ruznym Cizorodym Latkam). Bul. Vyzk. Ustav Ryb. Hydrobiol. Vodnany (CZE) (ENG ABS) 24(2): 14-19.

-NUE; TONNA.

#V2853: Svobodova, Z., Vykusova, B., and Machova, J. 1994. The effects of pollutants on selected haematological and biochemical parameters in fish. In: R. Muller and R. Lloyd (Eds.), Sublethal and Chronic Effects of Pollutants on Freshwater Fish, Chapter 4, Fishing News Books, London :39-52 .

-NUE.

#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.

#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, Yasuhide and Ito, Yoshio. 1984. Toxicity of organic nitrogen compounds to fish. Syncopic effect of aniline derivatives on fish. Seitai Kagaku 7(1): 17-26.

-TONNA.

#017592: Villar, D., Gonzalez, M., Gualda, M. J., and Schaeffer, D. J. 1994. Effects of organophosphorus insecticides on *Dugesia tigrina*: cholinesterase activity and head regeneration. Bull. Environ. Contam. Toxicol. 52(2): 319-324.

-TM/CU; IITM/C.

#V2844: Villar, D., Li, M. H., and Schaeffer, D. J. 1993. Toxicity of organophosphorus pesticides to *Dugesia dorotocephala*. Bull. Environ. Contam. Toxicol. 51: 80-87.

NUE: TDI.

#V1953: von der Ohe, P. C., Kühne, R., Ebert, R. U., Altenburger, R., Liess, M., and Schüürmann, G. 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.

#V2848: Vykusova, B. and Svobodova, Z. 1990 . Acute toxicity of standards to fish (Akutni Toxicita Standardu pro Ryby). Bul. Vyzk. Ustav Ryb. Hydrobiol. Vodnany (CZE) 26(3): 15-20.

-TDI.

#V1927: Wang, X., Dong, Y., Xu, S., Wang, L., and Han, S. 2000. Quantitative Structure-Activity Relationships for the toxicity to the tadpole *Rana japonica* of selected phenols. Bull. Environ. Contam. Toxicol. 64(6): 859-865.

-TONNA; QSAR / SDO.

#V2856: Wang, Y-F and Lu, Y-X. 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.

#V2851: Williamson, K. C., Shofer, S. L., and Tjeerdema, R. S. 1995. Toxicokinetics and biotransformation of p-nitrophenol in the Black Turban Snail (*Tegula funebris*). Aquat. Toxicol. 33(2): 113-123.

-NUE; SW.

- #018068: Yen, J. H., Lin, K. H., and Wang, Y. S. 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.
- #V1910: Zarogian, 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.
-QSAR / SDO; SW.
- #014780: Zhao, Yuan-Hui, Yuan, Xing, Ji, Guo-Dong, Sheng, Lian-Xi, and Wang, Lian-Sheng. 1997. Quantitative Structure-Activity Relationships of nitroaromatic compounds to four aquatic organisms. *Chemosphere* 34(8): 1837-1844.
-QSAR / SDO.
- #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.
-TDI; SDO; IITM/C.
- #V2841: Zieris, F. J., Feind, D., and Huber, W. 1988. Long-term effects of 4-nitrophenol in an outdoor synthetic aquatic ecosystem. *Arch. Environ. Contam. Toxicol.* 17(2): 165-175.
-NUE: TDI.

*For abbreviations used, see Appendix.

APPENDIX: REFERENCE ABBREVIATIONS USED, 7/06

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)..
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.
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.
UD or UP = uptake data.
WET = whole-effluent testing.