

CURRICULUM VITAE

Terry W. Schultz

PERSONAL DATA:

Birthdate: February 26, 1946
Birthplace: Beloit, Wisconsin

EDUCATION:

High School:
Memorial High School, Beloit, WI, 1964

Undergraduate:
Austin Peay State University, 1968, B.S.

Graduate:
The University of Arkansas, 1972, M.S.
The University of Tennessee, 1975, Ph.D.

Postgraduate:
Biology Division, Oak Ridge National Laboratory, 1975-77

MILITARY SERVICE:

United States Army, 1969-70

UNIVERSITY APPOINTMENTS:

1977-1980 Assistant Professor, Biology Department, University of Texas- Pan American, Edinburg, TX
(Cell Biology, Anatomy and Physiology, Histology, Mammalian Physiology)

1982-1986 Assistant Professor, Department of Animal Science
College of Veterinary Medicine, The University of Tennessee, Knoxville, TN
(Embryology, Histology, Organology, Toxicology)

1986-1991 Associate Professor, Department of Animal Science
College of Veterinary Medicine, Knoxville, TN
(Embryology, Histology, Organology, Toxicology)

1991-2000 Professor, Department of Animal Science
College of Veterinary Medicine, The University of Tennessee, Knoxville, TN
(Veterinary Embryology and Microanatomy; Toxicology)

1995-2007 Professor, Department of Ecology and Evolutionary Biology, College of Arts
and Sciences, The University of Tennessee Knoxville, TN (Environmental
Toxicology)

2000-2007 Professor, Department of Comparative Medicine,
College of Veterinary Medicine, The University of Tennessee, Knoxville, TN
(Veterinary Embryology and Microanatomy; Toxicology)

2007-present Emeritus Professor, Department of Comparative Medicine,
College of Veterinary Medicine, The University of Tennessee, Knoxville, TN

OTHER RELEVANT APPOINTMENTS:

- 2007-2013 Science Advisor, Organization for Economic Cooperation and Development, Health and Environmental Safety Division, The QSAR Program.
- 2013-present Research Institute for Fragrance Materials, Expert Panel, Computational Toxicology.

PUBLICATIONS (JOURNALS):**Refereed journal articles**1969

1. Schmitz, E.H. and Schultz, T.W. 1969. Digestive anatomy of terrestrial isopoda: *Armadillidium vulgare* and *Armadillidium nasatum*. American Midland Naturalist 82: 163-181.

1973

2. Schultz, T.W. 1973. Digestive anatomy of *Lirceus fontinalis* Rafinesque (Crustacea: Isopoda). Transactions of the American Microscopical Society 92: 13-25.
3. Schultz, T.W. 1973. Functional morphology of the oral appendages and foregut of *Lirceus garmani* (Crustacea: Isopoda). Transactions of the American Microscopical Society 92: 349-364.

1976

4. Schultz, T.W. 1976. The ultrastructure of the hepatopancreatic caeca of *Grammarus minus* (Crustacea: Amphipoda). Journal Morphology 149: 383-400.
5. Schultz, T.W. and Kennedy, J.R. 1976. The fine structure of digestive system of *Daphnia pulex* (Crustacea: Cladocera). Tissue and Cell 8: 479-490.

1977

6. Schultz, T.W. and Kennedy, J.R. 1976. The Cytotoxic effects of the herbicide 3-amino-1,2,4-triazole on *Daphnia pulex* (Crustacea: Cladocera). Biology Bulletin 151: 370-385.
7. Schultz, T.W. and Jungreis, A.M. 1977. The goblet cavity matrix in the larval midgut of *Hyalophora cecropis*. Journal Insect Physiology 23: 29-32.
8. Schultz, T.W. and Kennedy, J.R. 1977. Analyses of the integument and muscle attachment in *Daphnia* (Crustacea: Cladocera). The Journal of Submicroscopical Cytology 9: 37-51.
9. Schultz, T.W. and Dumont, J.N. 1977. The cytotoxic effects of synthetic fuel products on *Tetrahymena pyriformis* I. Phenol. Journal Protozoology 24: 164-172.
10. Schultz, T.W. 1977. Structure of the ephippium of *Daphnia pulex* (Crustacea: Cladocera). Transactions of the American Microscopical Society 96: 413-421.
11. Schultz, T.W. and Jungreis, A.M. 1977. Origin of the short circuit decay profile and maintenance of the cation transport capacity of the larval lepidopteran midgut *in vitro* and *in vivo*. Tissue and Cell 9: 255-272.

1978

12. Schultz, T.W., Davis, S. and Dumont, J.N. 1978. Toxicity of coal conversion product water to the fathead minnow. Bulletin of Environmental Contamination and Toxicology 19: 237-243.
13. Schultz, T.W., Kyte, L.M. and Dumont, J.N. 1978. Structure-toxicity correlations of organic contaminants in aqueous coal conversion effluents. Archives of Environmental Contamination and Toxicology 7: 457-463.
14. Schultz, T.W., Perry, S.T. and Dumont, J.N. 1978. Reduced toxicity of an aqueous coal conversion effluent following waste disposal treatment. Bulletin of Environmental Contamination and Toxicology 20: 633-639.
15. Schultz, T.W., Dumont, J.N. and Kyte, L.M. 1978. Cytotoxicity of synthetic fuel products on *Tetrahymena pyriformis*. II. Shale oil retort water. Journal Protozoology 25: 502-509.
16. Schultz, T.W. and Dumont, J.N. 1978. Cytotoxicity of untreated coal liquefaction process water (and a comparison with gasification process water). The Journal of Environmental Science and Health A13: 641-651.

1979

17. Dumont, J.N., Schultz, T.W. and Jones, R. 1979. Toxicity and teratogenicity of aromatic amines to *Xenopus laevis*. Bulletin of Environmental Contamination and Toxicology 22: 159-166.

Refereed journal articles (continued)1979

18. Schultz, T.W. and Allison, T.C. 1979. The toxicity and toxic interaction of aniline and pyridine. *Bulletin of Environmental Contamination and Toxicology* 23: 714-719.

1980

19. Schultz, T.W., Freeman, S.R. and Dumont, J.N. 1980. Uptake, depuration and distribution of selenium in *Daphnia* and its effects on survival and ultrastructure. *Archives of Environmental Contamination and Toxicology* 9: 23-40.
20. Dumont, J.N. and Schultz, T.W. 1980. Effects of coal-gasification sour water of *Xenopus laevis* embryos. *The Journal of Environmental Science and Health A15*: 127-138.
21. Schultz, T.W., Cajina-Quezada, M. and Dumont, J.N. 1980. Structure toxicity relationships of selected nitrogenous heterocyclic compounds. *Archives of Environmental Contamination and Toxicology* 9: 591-598.

1981

22. Schultz, T.W., Lozano, G. and Cajina-Quezada, M. 1981. Histochemical analysis of the goblet cell matrix in the larval midgut of *Manduca sexta*. *Transactions of the American Microscopical Society* 100: 204-209.
23. Davis, K.R., Schultz, T.W. and Dumont, J.N. 1981. Toxic and teratogenic effects of selected aromatic amines on embryos of the amphibian *Xenopus laevis*. *Archives of Environmental Contamination and Toxicology* 10: 371-391.
24. Schultz, T.W., Richter, C.S. and Dumont, J.N. 1981. Cytotoxicity of acridine, a synfuel component, to *Tetrahymena*. *Environmental Pollution* 26: 215-226.
25. Davis, P.H., Schultz, T.W. and Spies, R.B. 1981. Toxicity of Santa Barbara, California, USA seep oil to starfish (*Patiria miniata*) embryos. 2. The growth assay. *Marine Environmental Research* 5: 287-294.

1982

26. Schultz, T.W. 1982. Acute cytotoxicity of fossil energy-related comparative research materials. *The Journal of Environmental Science and Health A17*: 153-617.
27. Schultz, T.W. and Cajina-Quezada, M. 1982. Structure toxicity relationships of selected nitrogenous heterocyclic compounds II. Dinitrogen molecules. *Archives of Environmental Contamination and Toxicology* 11: 353-361.
28. Schultz, T.W., Dumont, J.N., Clark, B.R. and Buchanan, M.V. 1982. Embryotoxic and teratogenic effects of aqueous extracts of a coal-gasification electrostatic precipitation tar. *Teratogenesis Carcinogenesis Mutagenesis* 2: 1-11.
29. Schultz, T.W., Kier, L.B. and Hall, L.H. 1982. Structure toxicity relationships of selected nitrogenous heterocyclic compounds III. Relations using molecular connectivity. *Bulletin of Environmental Contamination and Toxicology* 28: 373-378.
30. Schultz, T.W., Dumont, J.N., Rao, T.K., Guerin, M.R., Ma, C.Y. and Epler, J.L. 1982. Evaluation of hydrotreatment as a means of reducing biological activity of synfuel related materials. *Environmental Research* 29: 389-398.

1983

31. Schultz, T.W., Dumont, J.N., Sankey, F.D. and Schmoyer, R.L. 1983. Structure activity relationships of selected naphthalene derivatives. *Ecotoxicology and Environmental Safety* 7: 191-203.
32. Schultz, T.W., Dumont, J.N. and Buchanan, M.W. 1983. Toxic and teratogenic effects of chemical class fractions of a coal-gasification electrostatic precipitator tar. *Toxicology* 29: 87-99.

1984

33. Schultz, T.W. and Dumont, J.N. 1984. Teratogenicity and embryotoxicity of monosodium methanearsonate herbicide. *Transactions of the American Microscopical Society* 103: 263-274.

Refereed journal articles (continued)1984

34. Walker, R.D., Schultz, T.W., Hopkins, F.M. and Bryant, J.J. 1984. Growth phase dependent phagocytosis of *Pasteurella hemolytica* by bovine pulmonary macrophages. American Journal of Veterinary Research 45: 1230-1234.
35. Schultz, T.W. and Dumont, J.N. 1984. The mitigation of acute toxicity of coal-derived liquids by hydrotreatment. Journal of Environmental Science and Health A19: 405-415.

1985

36. Schultz, T.W. and Moulton, M.P. 1985. Structure-toxicity relationships of selected naphthalene derivatives. II. Principal components analysis. Bulletin of Environmental Contamination and Toxicology 34: 1-9.
37. Schultz, T.W. and Moulton, B.A. 1985. Structure-activity relationships for nitrogen-containing aromatics. Environmental Toxicology and Chemistry 4: 353-359.
38. Schultz, T.W. and Riggin, G.W. 1985. Predictive correlations for the toxicity of alkyl and halogen substituted phenols. Toxicology Letter 25: 47-54.
39. Schultz, T.W. and Applehans, F.M. 1985. Correlations for the acute toxicity of multiple nitrogen substituted aromatic molecules. Ecotoxicology and Environmental Safety 10: 75-85.
40. Schultz, T.W. and Moulton, B.A. 1985. Structure-activity relationships of selected pyridines I. Substituent constant analysis. Ecotoxicology and Environmental Safety 10: 97-111.
41. Walker, R.D., Hopkins, F.M., Schultz, T.W., McCracken, M.D. and Moore, R.N. 1985. Changes in leukocyte population in bovine pulmonary lavage fluids following inhalation exposure to *Pasteurella haemolytica*. American Journal of Veterinary Research 46: 2429-2433.
42. Schultz, T.W., Dumont, J.N. and Epler, R.G. 1985. The embryotoxic and osteolathrogenic effects of semicarbazide. Toxicology 36: 185-198.

1986

43. Moulton, M.P. and Schultz, T.W. 1986. Structure-activity relationships of selected pyridines. II. Principal components analysis. Chemosphere 15: 59-67.
44. Moulton, M.P. and Schultz, T.W. 1986. Comparisons of several structure-activity relationships for chlorophenols. Aquatic Toxicology 8: 129-137.
45. Riggin, G.W. and Schultz, T.W. 1986. Teratogenic effects of benzoyl hydrazine on the frog embryo. Transactions of the American Microscopical Society 105: 197-210.
46. 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. Ecotoxicology and Environmental Safety 12: 146-153.

1987

47. Schultz, T.W., Applehans, F.M. and Riggin, G.W. 1987. Structure-activity relationships of selected pyridines. III. Log K_{OW} analysis. Ecotoxicology and Environmental Safety 13: 76-83.
48. Schultz, T.W. and Cajina-Quezada, M. 1987. Structure-activity relationships for mono alkylated or halogenated phenol. Toxicology Letter 37: 121-130.
49. Schultz, T.W. 1987. Relative toxicity of para-substituted phenols: Log K_{OW} and pK_a -dependent structure-activity relationships. Bulletin of Environmental Contamination and Toxicology 38: 994-999.
50. Schultz, T.W. 1987. The use of the ionization constant (pK_a) in selecting models of toxicity of phenols. Ecotoxicology and Environmental Safety 14: 178-183.

1988

51. Schultz, T.W., Ranney, T.S., Riggin, G.W. and Cajina-Quezada, M. 1988. Structure-activity relationships for osteolathyrism: I. Effects of altering the semicarbazide structure. Transactions of the American Microscopical Society 107: 113-126.

Refereed journal articles (continued)1988

52. Breider, M.A., Hopkins, F.M., Schultz, T.W. and Bowersock, T.L. 1988. Pulmonary lesions induced by *Pasteurella haemolytica* in neutrophil sufficient and neutrophil deficient calves. *Can. Journal of Veterinary Research* 52: 205-209.
53. Schultz, T.W., Jain, R., Cajina-Quezada, M. and Lin, D.T. 1988. Structure-toxicity relationships for selected benzyl alcohols and the polar narcosis mechanism of toxicity. *Ecotoxicology and Environmental Safety* 16: 57-64.
54. Schultz, T.W. and Ranney, T.S. 1988. Structure-activity relationships for osteolathyrism: II. Effects of alkyl-substituted acid hydrazides. *Toxicology* 53: 147-159.

1989

55. Schultz, T.W., Wesley, S.K. and Baker, L.L. 1989. Structure-activity relationships for di and tri alkyl and/or halogen substituted phenols. *Bulletin of Environmental Contamination and Toxicology* 42: 192-198.
56. Schultz, T.W., Dawson, D.A. and Lin, D.T. 1989. Comparative toxicity of selected nitrogen-containing aromatic compounds in the *Tetrahymena pyriformis* and *Pimephales promelas* test systems. *Chemosphere* 18: 2283-2291.
57. Schultz, T.W., Cajina-Quezada, M. and Wesley, S.K. 1989. Structure-toxicity relationships for mono alkyl- or halogen-substituted anilines. *Bulletin of Environmental Contamination and Toxicology* 43: 564-569.

1990

58. Dawson, D.A., Schultz, T.W., Baker, L.L. and Mannar, A. 1990. Structure-activity for osteolathyrism: III. Substituted thiosemicarbazides. *Journal of Applied Toxicology* 10: 59-64.
59. Schultz, T.W., Arnold, L.M., Wilke, T.S. and Moulton, M.P. 1990. Relationships of quantitative structure-activity for normal aliphatic alcohols. *Ecotoxicology and Environmental Safety* 19: 243-253.
60. Schultz, T.W., Wyatt, N.L. and Lin, D.T. 1990. Structure-toxicity relationships for nonpolar narcotics: A comparison of data from the *Tetrahymena*, *Photobacterium* and *Pimephales* systems. *Bulletin of Environmental Contamination and Toxicology* 44: 67-72.
61. Cajina-Quezada, M. and Schultz, T.W. 1990. Structure-toxicity relationships for selected weak acid respiratory uncouplers. *Aquatic Toxicology* 17: 239-252.
62. Arnold, L.M., Lin, D.T. and Schultz, T.W. 1990. Structure-activity relationships for methyl and/or chloro substituted anilines and the polar narcosis mechanism of toxicity. *Chemosphere* 21: 183-191.

1991

63. Dawson, D.A., Schultz, T.W. and Baker, L.L. 1991. Structure-activity relationships for osteolathyrism: IV. Para-substituted benzoic acid-hydrazides and alkyl carbazates. *Environmental Toxicology and Chemistry* 10: 455-461.
64. Jaworska, J.S. and Schultz, T.W. 1991. Comparative toxicity and structure-activity in *Chlorella* and *Tetrahymena*: 1. Monosubstituted phenols. *Bulletin of Environmental Contamination and Toxicology* 47: 57-62.
65. Schultz, T.W., Lin, D.T. and Arnold, L.M. 1991. QSARs for monosubstituted anilines eliciting the polar narcosis mechanism of action. *Science Total Environment* 109/110: 569-580.
66. Schultz, T.W., Wilke, T.S., Bryant, S.E. and Hosein, L.M. 1991. QSARs for selected aliphatic and aromatic amines. *Science Total Environment* 109/110: 581-587.
67. Al-Tikriti, M., Henry, R.W., Eiler, H., Schultz, T.W., Breider, M.A. and Cullen, W.C. 1991. Fine structural aspects of postnatal development of feline lung. *Anatomia, Histologia Embryologia* 20: 311-319.

Refereed journal articles (continued)1992

68. Schultz, T.W., Wesley, S.W. and Lin, D.T. 1992. QSARs for monosubstituted phenols and the polar narcosis mechanism of toxicity. *Quality Assurance: Good Practice, Regulation, and Law* 1: 132-143.
69. Kot, M., Sayler, G.S. and Schultz, T.W. 1992. Complex dynamics in a model microbial system. *Bulletin Mathematical Biology* 54: 619-648.
70. Dawson, D.A., Schultz, T.W. and Schroeder, E.C. 1992. Laboratory care and breeding of the African clawed frog. *Laboratory Animal* 21(4): 31-36.

1993

71. Jaworska, J.S. and Schultz, T.W. 1993. Quantitative relationships of structure-activity and volume fraction for selected nonpolar and polar narcotic chemicals. *SAR and QSAR in Environmental Research* 1: 3-19.
72. Schultz, T.W. and Tichy, M. 1993. Structure-toxicity relationships for unsaturated alcohols to *Tetrahymena pyriformis*: C5 and C6 analogs and primary propargylic alcohols. *Bulletin of Environmental Contamination and Toxicology* 51: 681-688.
73. Carter, C.D., Schultz, T.W. and McDonald, T.P. 1993. Thrombopoietin from human embryonic kidney cells stimulates an increase in megakaryocyte size of sublethally irradiated mice. *Radiation Research* 135: 32-39.
74. Schultz, T.W., Lin, D.T. and Culberson, R.W. 1993. Predicted toxicities of selected aryl alkanols. *Journal of Applied Toxicology* 13: 429-434.
75. Culberson, R.W., Schultz, T.W. and McDonald, T.P. 1993. Effects of thrombopoietin on platelet counts and splenic megakaryocyte size and number in sublethally irradiated mice. *Transactions of American Microscopical Society* 112: 306-315.

1994

76. Schultz, T.W., Bryant, S.E. and Lin, D.T. 1994. Structure-toxicity relationships for *Tetrahymena*: Aliphatic aldehydes. *Bulletin of Environmental Contamination and Toxicology* 52: 279-285.
77. Bryant, S.E. and Schultz, T.W. 1994. Toxicological assessment of biotransformation products of pentachlorophenol: *Tetrahymena* growth impairment. *Archives Environmental Contamination Toxicology* 26: 299-303.
78. Schultz, T.W., Kissel, T.S. and Tichy, M. 1994. Structure-toxicity relationships for unsaturated alcohols to *Tetrahymena pyriformis*: 3-alkyn-1-ol and 2-alken-1-ols. *Bulletin of Environmental Contamination and Toxicology* 53: 179-185.
79. Jaworska, J.S. and Schultz, T.W. 1994. Mechanism-based comparisons of acute toxicity elicited by industrial organic chemicals in procaryotic and eucaryotic systems. *Ecotoxicology and Environmental Safety* 29: 200-213.

1995

80. Schultz, T.W. and Dawson, D.A. 1995. Developmental hazard assessment with FETAX: Aerobic metabolites of bacterial transformation of naphthalene. *Bulletin of Environmental Contamination and Toxicology* 54: 662-667.
81. Jaworska, J.S., Hunter, R.S. and Schultz, T.W. 1995. Quantitative structure-toxicity relationships and volume fraction analyses for selected esters. *Archives Environmental Contamination Toxicology* 29: 86-93.
82. Swann, J.M., Carver, T.A. and Schultz, T.W. 1995. Mechanism-based structure-toxicity relationships for *Chlorella Vulgaris*. *Toxicology Modeling* 1: 111-121.
83. Cronin, M.T.D., Bryant, S.E., Dearden, J.C. and Schultz, T.W. 1995. Quantitative Structure-activity study of the toxicity of benzonitriles to the ciliate *Tetrahymena pyriformis*. *SAR and QSAR in Environmental Research* 3: 1-13.
84. Schultz, T.W., Sinks, G.D. and Hunter, R.S. 1995. Structure-toxicity relationships for alkanones and alkenones. *SAR and QSAR in Environmental Research* 3: 27-36.

Refereed journal articles (continued)1995

85. Kucera, S.P., Swann, J.M., Kennedy, J.R. and Schultz, T.W. 1995. The effects of benomyl and its breakdown products carbendazim and butyl isocyanate on the structure and function of tracheal ciliated cells. *Journal of Environmental Science and Health. Part B--Pesticides, Food Contaminants, and Agricultural Wastes* 30: 779-799.
86. Dearden, J.C., Cronin, M.T.D., Lin, D.T. and Schultz, T.W. 1995. QSAR study of the toxicity of nitrobenzenes to *Tetrahymena pyriformis*. *Quantitative Structure-Activity Relationships* 14: 427-432.
87. Jones, S.L. and Schultz, T.W. 1995. Quantitative structure-activity relationships for estimating the no observable effects concentration (NOEC) in fathead minnows (*Pimephales promelas*). *Quality Assurance: Good Practice, Regulation, and Law* 4: 187-203.

1996

88. Schultz, T.W., Bryant, S.E. and Kissel, T.S. 1996. Toxicological assessment in *Tetrahymena* of intermediates in aerobic microbial transformation of toluene and p-xylene. *Bulletin of Environmental Contamination and Toxicology* 56: 129-134.
89. Piršelová, K., Baláz, Š. and Schultz, T.W. 1996. Model-based QSAR for ionizable compounds: toxicity of phenols against *Tetrahymena pyriformis*. *Archives of Environmental Contamination and Toxicology* 30: 170-177.
90. Swann, J.M., Schultz, T.W. and Kennedy, J.R. 1996. The effects of the organophosphorous insecticides Dursban and Lorsban on the ciliated epithelium of the frog palate *in vitro*. *Archives of Environmental Contamination and Toxicology* 30: 188-194.
91. Schultz, T.W. and Comeaux, J.L. 1996. Structure-toxicity relationships for aliphatic isothiocyanates to *Tetrahymena pyriformis*. *Bulletin of Environmental Contamination and Toxicology* 56: 638-642.
92. Baláz, Š., Piršelová, K., Schultz, T.W. and Hermens, J. 1996. Kinetics of subcellular distribution of multiple ionizable compounds: A mathematical description and its use in QSAR. *Journal of Theoretical Biology* 178: 7-16.
93. Jaworska, J.S., Hallam, T.G. and Schultz, T.W. 1996. A community model of ciliate *Tetrahymena* and bacteria *E. coli*: Part I. Individual-based models of *Tetrahymena* and *E. coli* populations. *Journal Mathematical Biology* 58: 247-264.
94. Jaworska, J.S., Hallam, T.G. and Schultz, T.W. 1996. A community model of ciliate *Tetrahymena* and bacteria *E. coli*: Part II. Interactions in a batch system. *Journal Mathematical Biology* 58: 265-284.
95. Schultz, T.W., Bearden, A.P. and Jaworska, J.S. 1996. A novel approach for estimating toxicity of phenols. *SAR and QSAR Environmental Research* 5: 99-112.
96. Jaworska, J.S., Hallam, T.G. and Schultz, T.W. 1996. Chronic effects of nonpolar narcotics on a model microbial community. *Environmental Toxicology and Chemistry* 15: 1049-1056.
97. Cronin, M.T.D. and Schultz, T.W. 1996. Structure-toxicity relationships for phenols to *Tetrahymena pyriformis*. *Chemosphere* 32: 1453-1468.
98. Mekenyan, O.G., Schultz, T.W., Veith, G.D. and Kamenska, V. 1996. "Dynamic" QSAR for semicarbazide-induced mortality in frog embryos. *Journal of Applied Toxicology* 16: 355-363.
99. Dawson, D.A., Schultz, T.W. and Hunter, R.S. 1996. Developmental toxicity of carboxylic acids to *Xenopus* embryos: A quantitative structure-activity relationship and computer-automated structure evaluation. *Carcinogenesis Mutagenesis and Teratogenesis* 16: 109-124.

1997

100. Schultz, T.W. and Cronin, M.D.T. 1997. QSARs for weak acid respiratory uncouplers to *Vibrio fischeri*. *Environmental Toxicology and Chemistry* 16: 357-360.
101. Swanson, M., Davis, G.A., Kincaid, L.E., Schultz, T.W., Bartmess, J., Jones, S. and George, E.L. 1997. A screening method for ranking and scoring chemicals by potential human health and environmental impacts. *Environmental Toxicology and Chemistry* 16: 372-383.

Refereed journal articles (continued)1997

102. Damborsky, J. and Schultz, T.W. 1997. Comparison of the QSAR models for toxicity and biodegradability of anilines and phenols. *Chemosphere* 34: 429-446.
103. Bearden, A.P. and Schultz, T.W. 1997. Relationships of structure-activity for *Tetrahymena* and comparative toxicity with *Pimephales*: A mechanism of action approach. *Environmental Toxicology and Chemistry* 16: 1311-1317.
104. Sink, G.D., Schultz, T.W. and Hunter, R.S. 1997. UVb-induced toxicity of PAHs: Effects of substituents and heteroatom substitution. *Bulletin of Environmental Contamination and Toxicology* 59: 1-8.
105. Schultz, T.W., Sinks, G.D. and Cronin, M.T.D. 1997. Quinone-induced aquatic toxicity to *Tetrahymena*: Structure-activity relationships. *Aquatic Toxicology* 39: 267-278.
106. Bearden, A.P., Gregory, B.W. and Schultz, T.W. 1997. Population growth kinetics of *Tetrahymena pyriformis* exposed to selected nonpolar narcotics. *Archives of Environmental Contamination and Toxicology* 33: 401-406.
107. Larsen, J., Schultz, T.W., Rasmussen, L., Hoofman, R. and Pauli, W. 1997. Progress in an ecotoxicological standard protocol with protozoa: Results from a pilot ring test with *Tetrahymena pyriformis*. *Chemosphere* 35: 1023-1041.
108. Bearden, A.P., Gregory, B.W. and Schultz, T.W. 1997. Growth kinetics of pre-exposed and naïve populations of *Tetrahymena pyriformis* to 2-decanone and acetone. *Ecotoxicology and Environmental Safety* 37: 245-250.
109. Cronin, M.T.D. and Schultz, T.W. 1997. Validation of *Vibrio fischeri* acute toxicity data: Mechanism of action-based QSARs for non-polar narcotics and polar narcotic phenols. *The Science of the Total Environment* 207: 75-88.
110. Schultz, T.W. 1997. TETRATOX: *Tetrahymena pyriformis* population growth impairment endpoint-A surrogate for fish lethality. *Toxicology Methods* 7: 289-309.

1998

111. Cronin, M.T.D. and Schultz, T.W. 1998. Structure-toxicity relationships for three mechanisms of action of toxicity to *Vibrio fischeri*. *Ecotoxicology and Environmental Safety* 39: 65-69.
112. Schultz, T.W., Kraut, D.H., Sayler, G.S. and Layton, A.C. 1998. Estrogenicity of selected biphenyls evaluated using a recombinant assay. *Environmental Toxicology and Chemistry* 17: 1727-1729.
113. Cronin, M.T.D., Gregory, B.W. and Schultz, T.W. 1998. Quantitative structure-activity analyses of nitrobenzene toxicity to *Tetrahymena pyriformis*. *Chemical Research in Toxicology* 11: 902-908.
114. Schultz, T.W. and Bearden, A.P. 1998. Structure-toxicity relationships for selected naphthoquinones to *Tetrahymena pyriformis*. *Bulletin of Environmental Contamination and Toxicology* 61: 405-410.
116. Bearden, A.P. and Schultz, T.W. 1998. Comparison of *Tetrahymena* and *Pimephales* toxicity based on mechanism of action. *SAR QSAR in Environmental Research* 9: 127-153.
115. Sinks, G.D., Carver, T.A. and Schultz, T.W. 1998. Structure-toxicity relationships for aminoalcohols: A comparison with alkanols and alkanamines. *SAR QSAR in Environmental Research* 9: 217-228.

1999

117. Kaiser, K.L.E., Dearden, J.C., Klein, W. and Schultz, T.W. 1999. A note of caution to users of ECOSAR. *Water Quality Research Journal Canada* 34: 179-182.
118. Swann, J.M., Kennedy, J.R. and Schultz, T.W. 1999. Evaluation of two *in vitro* ciliated epithelial systems, dog trachea and frog palate, for potential as screens for sensory irritation. *In Vitro and Molecular Toxicology* 12: 17-32.
119. Schultz, T.W. and DeWeese, A.D. 1999. Structure-toxicity relationships for selected lactones to *Tetrahymena pyriformis*. *Bulletin of Environmental Contamination and Toxicology* 62: 463-468.
120. Akers, K.S., Sinks, G.D. and Schultz, T.W. 1999. Structure-toxicity relationships for selected halogenated aliphatic chemicals. *Environmental Toxicology and Pharmacology* 7: 33-39.

Refereed journal articles (continued)1999

121. Schultz, T.W. and Cronin, M.T.D. 1999. Response-surface analyses for toxicity to *Tetrahymena pyriformis*: Reactive carbonyl-containing aliphatic chemicals. *Journal of Chemical Information and Computer Sciences* 39: 304-309.
122. Muccini, M., Layton, A.C., Sayler, G.S. and Schultz, T.W. 1999. Aquatic toxicities of halogenated benzoic acids to *Tetrahymena pyriformis*. *Bulletin of Environmental Contamination and Toxicology* 62: 616-622.
123. Bearden, A.P., Sinks, G.D. and Schultz, T.W. 1999. Acclimation to sublethal exposure to a model nonpolar narcotic: Population growth kinetics and membrane lipid alterations in *Tetrahymena pyriformis*. *Aquatic Toxicology* 46: 11-21.
124. Layton, A.C., Gregory, B.W., Schultz, T.W. and Sayler, G.S. 1999. Validation of genetically engineered bioluminescent surfactant resistant bacteria as toxicity assessment tools. *Ecotoxicology and Environmental Safety* 43: 222-228.
125. Bearden, A.P., Sinks, G.D., Vaes, W.H.J., Ramos, E.U., Hermens, J.L.M. and Schultz, T.W. 1999. Bioavailability, biodegradation, and acclimation of *Tetrahymena pyriformis* to 1-octanol. *Ecotoxicology Environmental Safety* 44: 86-91.
126. Schultz, T.W. 1999. Structure-toxicity relationships for benzenes evaluated with *Tetrahymena pyriformis*. *Chemical Research in Toxicology* 12: 1262-1267.
127. Seward, J.R. and Schultz, T.W. 1999. QSAR analyses of the toxicity of aliphatic carboxylic acids and salts to *Tetrahymena pyriformis*. *SAR QSAR in Environmental Research* 10: 557-567.

2000

128. Schultz, T.W., Sinks, G.D. and Seward, J.R. 2000. Estrogenicity of benzophenones evaluated with a recombinant yeast assay: Validation of a rules-based system of prediction. *Environmental Toxicology and Chemistry* 19: 301-304.
129. Leblond, J.D., Applegate, B.M., Menn, F.-M., Schultz, T.W. and Sayler, G.S. 2000. Structure-toxicity assessment of metabolites of the aerobic bacterial transformation of substituted naphthalenes. *Environmental Toxicology and Chemistry* 19: 1235-1246.
130. Schultz, T.W. and Seward, J.R. 2000. Health-effects related structure-toxicity relationships: a paradigm for the millennium. *The Science of the Total Environment* 249: 73-84.
131. Cronin, M.T.D., Bower, G.S., Sinks, G.D. and Schultz, T.W. 2000. Structure-toxicity relationships for aliphatic compounds encompassing a variety of mechanisms of toxic action to *Vibrio fischeri*. *SAR QSAR in Environmental Research* 11: 301-312.
132. Seward, J.R., Sinks, G.D. and Schultz, T.W. 2000. Population growth kinetics of *Tetrahymena pyriformis* exposed to select pyridines. *European Journal of Protistology* 36: 139-149.
133. Dimitov, S.D., Mekenyan, O.G. and Schultz, T.W. 2000. Interspecies modeling of narcotic toxicity in aquatic animals. *Bulletin of Environmental Contamination and Toxicology* 65: 399-406.
134. Niculescu, S.P., Kaiser, K.L.E. and Schultz, T.W. 2000. Modeling the toxicity of chemicals to *Tetrahymena pyriformis* using molecular fragment descriptors and probabilistic neural networks. *Archives of Environmental Contamination and Toxicology* 39: 289-298.
135. Layton, A.C., Gregory, B.W., Seward, J.R., Schultz, T.W. and Sayler, G.S. 2000. Mineralization of steroidal hormones in municipal sewage treatment systems in Tennessee USA. *Environmental Science and Technology* 34: 3925-3931.
136. Schultz, T.W., Sinks, G.D. and Cronin, M.T.D. 2000. Effects of substituent size and dimensionality on potency of phenolic xenoestrogens. *Environmental Toxicology and Chemistry* 19: 2637-2642.
137. Schultz, T.W. and Seward, J.R. 2000. Dimyristoyl phosphatidylcholine /water partitioning-dependent modeling of narcotic toxicity to *Tetrahymena pyriformis*. *Quantitative Structure-Activity Relationships* 19: 339-344.

Refereed journal articles (continued)2001

138. Seward, J.R., Cronin, M.T.D. and Schultz, T.W. 2001. Structure-toxicity analyses of *Tetrahymena pyriformis* exposed to pyridine – An examination into extension of surface-response domains. SAR QSAR in Environmental Research 11: 489-512.
139. Leblond, J.D., Schultz, T.W. and Sayler, G.S. 2001. Observations on the preferential biodegradation of selected components of polyaromatic hydrocarbon mixtures. Chemosphere 42: 333-343.
140. DeWeese, A.D. and Schultz, T.W. 2001. Structure-activity relationships for aquatic toxicity to *Tetrahymena*: Halogen-substituted aliphatic esters. Environmental Toxicology 16: 54-60.
141. Seward, J.R., Sinks, G.D. and Schultz, T.W. 2001. Reproducibility of toxicity across mode of toxic action the *Tetrahymena* population growth impairment assay. Aquatic Toxicology 53: 33-47.
142. Sinks, G.D. and Schultz, T.W. 2001. Correlations of *Tetrahymena* and *Pimephales* toxicity: Evaluation of 100 additional compounds. Environmental Toxicology and Chemistry 20: 917-921.
143. Cronin, M.T.D. and Schultz, T.W. 2001. Development of quantitative structure-activity relationships for the toxicity of aromatic compounds to *Tetrahymena pyriformis*: Comparative assessment of methodologies. Chemical Research in Toxicology 14: 1284-1295.
144. Cronin, M.T.D., Manga, N., Seward, J.R., Sinks, G.D. and Schultz, T.W. 2001. Parameterization of electrophilicity for the prediction of the toxicity of aromatic compounds. Chemical Research in Toxicology 14: 1498-1505.
145. Schultz, T.W., Sinks, G.D. and Miller, L.A. 2001. Population growth impairment of sulfur-containing compounds to *Tetrahymena pyriformis*. Environmental Toxicology 16: 543-549.

2002

146. Ren, S. and Schultz, T.W. 2002. Identifying the mechanism of aquatic toxicity of selected compounds by hydrophobicity and electrophilic descriptors. Toxicology Letters 129: 151-160.
147. Kaiser, K.L.E., Niculescu, S.P., and Schultz, T.W. 2002. Probabilistic neural network modeling of the toxicity of chemicals to *Tetrahymena pyriformis* with molecular fragment descriptors. SAR and QSAR in Environmental Research 13: 57-67.
148. Schultz, T.W. 2002. Estrogenicity of biphenylols: Activity in the yeast gene activation assay. Bulletin of Environmental Contamination and Toxicology 68: 332-338.
149. Schultz, T.W., Sinks, G.D. and Cronin, M.T.D. 2002. Structure-activity relationships for gene activation oestrogenicity: Evaluation of a diverse set of aromatic compounds. Environmental Toxicology 17: 14-23.
150. Seward, J.R., Hamblen, E.L. and Schultz, T.W. 2002. Regression comparison of *Tetrahymena pyriformis* and *Poecilia reticulata* toxicity. Chemosphere 47: 93-101.
151. Schultz, T.W. and Sinks, G.D. 2002. Xenooestrogenic gene expression: Structural feature of active polycyclic aromatic hydrocarbons. Environmental Toxicology and Chemistry 21: 783-786.
152. Seward, J.R., Cronin, M.T.D. and Schultz, T. W. 2002. Effect of precision of molecular orbital descriptors on the modeling of toxicity of selected pyridines. SAR QSAR in Environmental Research 13: 325-340.
153. Layton, A.C., Sanserverino, J., Gregory, B.W., Ester, J.P., Sayler, G.S. and Schultz, T.W. 2002. *In vitro* estrogen receptor binding of PCBs: Measured activity and detection of hydroxylated metabolites in a recombinant yeast assay. Toxicology and Applied Pharmacology 180: 157-163.
154. Aptula, A.O., Netzeva, T.I., Valkova, I.V., Cronin, M.T.D., Schultz, T.W., Kühne, R. and Schüürmann, G. 2002. Multivariate discrimination between modes of toxic action of phenols. Quantitative Structure-Activity Relationships 21: 12-22.
155. Schultz, T.W., Sinks, G.D. and Bearden-Lowit, A.P. 2002. Population growth kinetics and membrane lipid alterations in *Tetrahymena pyriformis* upon expose to pentachlorophenol. Cell Biology and Toxicology 18: 271-278.

Refereed journal articles (continued)2002

156. Cronin, M.T.D., Aptula, A.O., Dearden, J.C., Duffy, J.C., Netzeva, T.I., Patel, H., Rowe, P.H., Schultz, T.W., Worth, A.P., Voutzoulidia, K. and Schüürmann, G. 2002. Structure-based classification of antibacterial activity. *Journal of Chemical Information and Computer Science* 42: 869-878.
157. Patel, H., Schultz, T.W. and Cronin, M.T.D. 2002. Physico-chemical interpretation and prediction of the dimyristoyl phosphatidyl choline-water partition coefficient. *Journal of Molecular Structure-THEOCHEM* 593: 9-18.
158. Cronin, M.T.D., Aptula, A.O., Duffy, J.C., Netzeva, T.I., Rowe, P.H., Valkova, I.V., Schultz, T.W. 2002. Comparative assessment of methods to develop QSARs for the prediction of the toxicity of phenols to *Tetrahymena pyriformis*. *Chemosphere* 49: 1201-1221.
159. Schultz, T.W., Cronin, M.T.D., Netzeva, T.I. and Aptula, A.O. 2002. Structure-toxicity relationships for aliphatic chemicals evaluated with *Tetrahymena pyriformis*. *Chemical Research in Toxicology* 15: 1602-1609.

2003

160. Schultz T.W., Netzeva, T.I., and Cronin, M.T.D. 2003. The use of diversity versus representivity in the training and validation of quantitative structure-activity relationships. *SAR QSAR in Environmental Research* 14: 59-81.
161. Schultz, T.W. and Cronin, M.T.D. 2003. Essential and desirable characteristics of ecotoxicity QSARs. *Environmental Toxicology and Chemistry* 22: 599-607.
162. Schultz, T.W. and Dawson, D.A. 2003. Housing and husbandry of *Xenopus*. *Laboratory Animal* 32: 34-39.
163. Schultz, T.W., Cronin, M.T.D., Walker, J.D. and Aptula, A.O. 2003. Quantitative structure-activity relationships in (QSARs) in toxicology: A historical perspective. *Journal of Molecular Structure-THEOCHEM* 622: 1-22.
164. Schultz, T.W., Cronin, M.T.D. and Netzeva, T.I. 2003. The present status of QSAR in toxicology. *Journal of Molecular Structure-THEOCHEM* 622: 23-38.
165. Cronin, M.T.D. and Schultz, T.W. 2003. Pitfalls in quantitative structure-activity relationships (QSARs) for predicting toxicity. *Journal of Molecular Structure-THEOCHEM* 622: 39-52.
166. Dimitrov, S.D., Mekenyan, O.G., Sinks, G.D. and Schultz, T.W. 2003. Global modeling of narcotic chemicals: Ciliate and fish toxicity. *Journal of Molecular Structure-THEOCHEM* 622: 63-70.
167. Cottrell, M.B. and Schultz, T.W. 2003. Structure-toxicity relationships for methyl esters of cyanoacetic acids to *Tetrahymena pyriformis*. *Bulletin of Environmental Contamination and Toxicology* 70: 549-556.
168. Ren, S., Frymier, P.D. and Schultz, T.W. 2003. An exploratory study of using multivariate techniques to determine mechanism of toxic action. *Ecotoxicology Environmental Safety* 55: 86-97.
169. Toropov, A.A. and Schultz, T.W. 2003. Prediction of benzene aquatic toxicity: Use of optimization of correlation weights of local graph invariants. *Journal of Chemical Information and Computer Science* 43: 560-567.
170. Schultz, T.W. and Tucker, V.A. 2003. Structure-toxicity relationships for the effects of N- and N, N'-alkyl thioureas to *Tetrahymena pyriformis*. *Bulletin of Environmental Contamination and Toxicology* 70: 1251-158.
171. Hamblen, E.L., Cronin, M.T.D. and Schultz, T.W. 2003. Estrogenicity and acute toxicity of selected anilines using a recombinant yeast assay. *Chemosphere* 52: 1173-1181.
172. Walker, J.D., Comber, M.H.I., Schultz, T. W., Jaworska, J.S. and Dearden, J.C. 2003. Guidelines for developing and using quantitative structure activity relationships. *Environmental Toxicology and Chemistry* 22: 1653-1665.

Refereed journal articles (continued)2003

173. Bradbury, S.P., Russom, C.L., Ankley, G.T., Schultz, T.W. and Walker, J.D. 2003. Overview of data and conceptual approaches for derivation of QSARs for ecotoxicological effects of organic chemicals. *Environmental Toxicology and Chemistry* 22: 1789-1798.
174. Netzeva, T.I., Schultz, T.W., Aptula, A.O. and Cronin, M.T.D. 2003. PLS modelling of the acute toxicity of aliphatic compounds to *Tetrahymena pyriformis*. *SAR QSAR in Environmental Research* 14: 265-283.
175. Netzeva, T.I., Aptula, A.O., Chaudary, S.H., Duffy, J.C., Schultz, T.W., Schüürmann, G., Cronin, M.T.D. 2003. Structure-activity relationships for the toxicity of substituted poly-hydroxylated benzenes to *Tetrahymena pyriformis*: Influence of free radical formation. *QSAR and Combinatorial Sciences* 22: 575-582.
176. Saliner, A.G., Amat, L., Cabo-Dorca, R., Schultz, T.W. and Cronin, M.T.D. 2003. Molecular quantum similarity analysis of estrogenic activity. *Journal of Chemical Information and Computer Science* 43: 1166-1176.
177. Schultz, T.W. and Burgan, J.T. 2003. pH-stress and toxicity of nitrophenols to *Tetrahymena pyriformis*. *Bulletin of Environmental Contamination and Toxicology* 71: 1069-1076.

2004

178. Dimitrov, S., Koleva, Y., Schultz, T.W., Walker, J.D. and Mekenyan, O. 2004. Interspecies QSAR model for aldehydes: Aquatic toxicity. *Environmental Toxicology and Chemistry* 23: 463-470.
179. Schultz, T.W., Seward-Nagel, J., Foster, K.A. and Tucker, V.A. 2004. Structure-activity relationships for aliphatic alcohols and aquatic toxicity to *Tetrahymena*. *Environmental Toxicology* 19: 1-10.
180. Schultz, T.W. and Yarbrough, J.W. 2004. Trends in structure-toxicity for carbonyl-containing α,β -unsaturated compounds. *SAR QSAR in Environmental Research* 15: 139-146.
181. Ren, S., Schultz, T.W. and Frymier, P.D. 2004. Evaluation of the Shk1 activated sludge bacterial luminescence inhibition assay: Narcotic chemicals. *Bulletin of Environmental Contamination and Toxicology* 72: 1187-1194.
182. Schultz, T.W., Netzeva, T.I. and Cronin, M.T.D. 2004. Ecotoxicity QSARs: A method for assigning quality and confidence. *SAR QSAR in Environmental Research* 15: 385-397.

2005

183. Gagliardi, S.R. and Schultz, T.W. 2005. Regression comparisons of aquatic toxicity of benzene derivatives: *Tetrahymena pyriformis* and *Rana japonica*. *Bulletin of Environmental Contamination and Toxicology* 74: 256-262.
184. Schultz, T.W., Netzeva, T.I., Roberts, D.W. and Cronin, M.T.D. 2005. Structure-toxicity relationships for carbonyl-containing α,β -unsaturated aliphatic chemicals evaluated with *Tetrahymena pyriformis*. *Chemical Research in Toxicology* 18: 330-341.
185. Netzeva, T.I., Worth, A.P., Aldenberg, T. Benigni, R. Cronin, M.T.D., Gramatica, P., Jaworska, J.S., Klopman, G. Marchant, C.A., Myatt, G., Nikolova-Jeliazkova, N., Patlewicz, G.Y., Perkins, R. Roberts, D.W., Schultz, T.W., Stanton, D.T., van de Sandt, J.J.M., Tong, W. Veith, G.D. and Yang, C. 2005. Current status of methods for defining the applicability domain of (quantitative) structure-activity relationships: The report and recommendations of ECVAM workshop 52. *Alternatives to Laboratory Animals* 33: 155-173.
186. Aptula, A.O., Jeliazkova, N.G., Schultz, T.W. and Cronin, M.T.D. 2005. The better predictive model: High q^2 for the training set or low root mean square error of prediction for the test set? *QSAR and Combinatorial Sciences* 24: 385-396.
187. Sanseverino, J., Gupta, R.K., Layton, A.C., Patterson, S.S., Ripp, S., Saidak, L., Simpson, M.L., Schultz, T.W. and Sayler, G.S. 2005. *Saccharomyces cerevisiae* BLYES expressing bacterial bioluminescence for rapid, sensitive detection of estrogenic compounds. *Applied and Environmental Microbiology* 71: 4455-4460.

Refereed journal articles (continued)2005

188. Aptula, A.O., Roberts, D.W., Cronin, M.T.D. and Schultz, T.W. 2005. Chemistry-toxicity relationships for the effects of di- and tri-hydroxybenzenes to *Tetrahymena pyriformis*. *Chemical Research in Toxicology* 18: 844-854.
189. Hansen, L., Machela, M., Fischer, L. James, M. Henning, J.B., Glauert, H., Narbonne, J.-F., van Bree, L., Schultz, T.W., Grevatt, P. Suk, W., Holoubek, I., Robertson, L. 2005. Research needs identified at the Second PCB Workshop in Brno, Czech Republic, May 7–11, 2002. *Toxicological & Environmental Chemistry* 87: 261–265.
190. Schultz, T.W., Yarbrough, J.W. and Johnson, E.L. 2005. Structure-activity relationships for glutathione reactivity of carbonyl-containing compounds. *SAR QSAR in Environmental Research* 16: 313-322.
191. Schultz, T.W., Yarbrough, J.W. and Woldemeskel, M. 2005. Toxicity to *Tetrahymena* and abiotic thiol reactivity of aromatic isothiocyanates. *Cell Biology and Toxicology* 21: 181-189.
192. Netzeva, T.I., and Schultz, T.W. 2005. QSARs for the aquatic toxicity of aromatic aldehydes from *Tetrahymena* data. *Chemosphere* 61: 1632-1643.

2006

193. Aptula, A.O., Roberts, D.W., Patlewicz, G. and Schultz, T.W. 2006. Non-enzymatic glutathione reactivity and in vitro toxicity: A non-animal approach to skin sensitization. *Toxicology in Vitro* 20: 239-247.
194. Wan, B., Fleming, J.T., Schultz, T.W. and Sayler, G.S. 2006. In vitro immune toxicity of depleted uranium: Effects on murine macrophages, CD4+ T-cells and gene expression profiles. *Environmental Health Perspectives* 114: 85-91.
195. Schultz, T.W., Yarbrough, J.W. and Koss, S.K. 2006. Identification of reactive toxicants: Structure-activity relationships for amides. *Cell Biology and Toxicology* 22: 339-349.
196. Dawson, D.A., Pöch, G. and Schultz, T.W. 2006. Chemical mixture toxicity testing with *Vibrio fischeri*: Combined effects of binary mixtures of ten soft electrophiles. *Ecotoxicology Environmental Safety* 65: 171-180.
197. Schultz, T.W., Carlson, R.E., Cronin, M.T.D., Hermens, J.L.M., Johnson, R., O'Brien, P.J., Roberts, D.W., Siraki, A., Wallace, K.D. and Veith, G.D. 2006. A conceptual framework for predicting toxicity of reactive chemicals: Models for soft electrophilicity. *SAR QSAR in Environmental Research* 17: 413-428.
198. Wan, B. Sayler, G.S. and Schultz, T.W. 2006. Structure-activity relationships for flow cytometric data of smaller polycyclic aromatic hydrocarbons. *SAR QSAR in Environmental Research* 17: 597-605.

2007

199. Schultz, T.W., Yarbrough, J.W. and Pilkington, T. 2007. Aquatic toxicity and abiotic thiol reactivity of aliphatic isothiocyanates: Effects of alkyl-size and -shape. *Environmental Toxicology and Pharmacology* 23: 10–17.
200. Schultz, T.W., Ralston, K.E., Roberts, D.W., Veith, G.D. and Aptula, A.O. 2007. Structure-activity relationships for abiotic thiol reactivity and aquatic toxicity of halo-substituted carbonyl compounds. *SAR QSAR in Environmental Research* 18: 21-29.
201. Gagan, E.M., Hull, M. Schultz, T.W., Pöch, G. and Dawson, D.A. 2007. Time-dependence in mixture toxicity with soft-electrophiles: 1. Combined effects of selected S_N2 and S_NAr reactive agents with a non-polar narcotic. *Archives of Environmental Contamination and Toxicology* 52: 283-293.

Refereed journal articles (continued)2007

202. Schultz, T.W., Hewitt, M., Netzeva, T.I. and Cronin, M.T.D. 2007. Assessing applicability domains of toxicological QSARs: definition, confidence in predicted values, and the role of mechanisms of action. *QSAR and Combinatorial Sciences* 26: 238-254.
203. Yarbrough, J.W. and Schultz, T.W. 2007. Abiotic sulfhydryl reactivity: A predictor of aquatic toxicity for carbonyl-containing α,β -unsaturated compounds. *Chemical Research in Toxicology* 20: 558-562.
204. Kahn, I., Maran, U., Benfenati, E., Netzeva, T.I., Schultz, T.W. and Cronin M.T.D. 2007. Comparative quantitative structure-activity-activity relationships for toxicity to *Tetrahymena pyriformis* and *Pimephales promelas*. *Alternatives to Laboratory Animals* 35: 15-24.
205. Eldridge, M., Sanseverino, J., Layton, A., Easter, J., Schultz, T.W. and Sayler, G.S. 2007. *S. cerevisiae* BLYAS: A new bioluminescent bioreporter for the detection of androgenic compounds. *Applied and Environmental Microbiology* 73: 6012-6018.
206. Schultz, T.W., Yarbrough, J.W., Hunter, R.S. and Aptula, A.O. 2007. Verification of the structural alerts for Michael acceptors. *Chemical Research in Toxicology* 20: 1359-1363.

2008

207. Dawson, D.A., Allen, J.L., Schultz, T.W. and Pösch, G. 2008 Time-dependence in mixture toxicity with soft-electrophiles: 2. Effects of relative reactivity level on time-dependent toxicity and combined effects for selected Michael acceptors. *Journal Toxicology and Environmental Health Part A*. 43:43-52.
208. Enoch, S.J., Cronin, M.T.D., Schultz, T.W. and Madden, J.C. 2008. Quantitative and mechanistic read-across for predicting skin sensitization potential of alkenes acting via Michael addition. *Chemical Research in Toxicology* 21: 513-520.
209. Gerberick, G.F., Aleksic, M., Basketter, D.A., Casati, S., Karlberg, A.-T., Kern, P., Kimber, I., Lepoittevin, J.P., Natsch, A., Ovigne, J.M., Rovida, C., Sakaguchi, H. and Schultz, T.W. 2008. Chemical reactivity measurement and the predictive identification of skin sensitizers. *Alternatives to Laboratory Animals* 36: 215-242.
210. Wan, B., Yarbrough, J.W. Schultz, T.W. 2008. Structure-related clustering of gene expression fingerprints of THP-1 cells exposed to smaller polycyclic aromatic hydrocarbons. *SAR QSAR in Environmental Research* 19: 351-373.
211. Enoch, S., Cronin, M.T.D., Schultz, T.W. and Madden, J. 2008. An evaluation of global QSAR models for predicting the toxicity of phenols to *Tetrahymena pyriformis*. *Chemosphere* 71: 1225-1232.
212. Ellison, C.M., Cronin, M.T.D., Madden, J.C. and Schultz, T.W. 2008. Definition of the structural domain of the baseline non-polar narcosis model for *Tetrahymena pyriformis*. *SAR QSAR in Environmental Research* 19: 751-783.

2009

213. Sanseverino, J., Eldridge, M.E., Layton, A.C., Easter, J.P., Yarbrough, J.W., Schultz, T.W. and Sayler, G.S. 2009. Screening of potentially hormonally active chemicals using bioluminescent yeast bioreporters. *Toxicological Sciences* 107: 122-134.
214. Schultz, T.W., Rogers, K. and Aptula, A.O. 2009. Read-across to rank skin sensitization potential: Subcategories for the Michael acceptor domain. *Contact Dermatitis* 60: 21-31.
215. Van Leeuwen, K., Schultz, T.W., Henry, T., Diderich, R. and Veith, G.D. 2009. Using chemical categories to fill data gaps in hazard assessment. *SAR QSAR in Environmental Research* 20: 207-220.

2010

216. Roberts, D.W. Schultz, T.W., Wolf, E.M, and Aptula, A.O. 2010. Experimental reactivity parameters for toxicity modeling: Application to aquatic toxicity of Sn2 electrophiles to *Tetrahymena pyriformis*. *Chemical Research in Toxicology* 23:228-234.

Refereed journal articles (continued)

2010

217. Dawson, D.A., Jeyaratnam, J., Mooneyham, T., Pöch, G. and Schultz, T.W. 2010. Mixture toxicity of S_N2 reactive soft electrophiles: 1 – Evaluation of mixtures containing α -halogenated acetonitriles. Archives Environmental Contamination and Toxicology 59: 532-541.
218. Schultz, T.W., Sprafkin, C.L., and Aptula, A.O. 2010. Reactivity-based toxicity modeling of 5-membered heterocyclic compounds: Application to *Tetrahymena pyriformis*. SAR QSAR in Environmental Research 21:681-691.

2011

219. Bajot, F. Cronin, M.T.D. Roberts, D.W. and Schultz, T.W. 2011. Reactivity and aquatic toxicity of aromatic compounds transformable to quinone-type Michael acceptors. SAR QSAR in Environmental Research 22: 51-65.
220. Schwöbel, J.A.H., Koleva, Y.K., Bajot, F., Enoch, S.J., Hewitt, M., Madden, J.C., Roberts, D.W. Schultz, T.W., and Cronin, M.T.D. 2011. Measurement and estimation of electrophilic reactivity for predictive toxicology. Chemical Reviews 111: 2562–2596. [Supporting information and database available from: <http://pubs.acs.org/doi/suppl/10.1021/cr100098n>]
221. Dawson, D.A., Mooneyham, T., Jeyaratnam, J., Schultz, T.W. and Pöch, G. 2011. Mixture toxicity of S_N2 reactive soft electrophiles: 2 – Evaluation of mixtures containing halogenated ethyl α -halogenated acetates. Archives Environmental Contamination and Toxicology 61: 547-557.
222. Hewitt, M., Rowe, P., Cronin, M.T.D. and Schultz, T.W. 2011. Repeatability analysis of the *Tetrahymena pyriformis* population growth assay. SAR QSAR in Environmental Research 22: 621-637.
223. Enoch, S.J., Ellison, C.M., Schultz, T.W. and Cronin, M.T.D. 2011. A review of the electrophilic reaction chemistry involved in covalent protein binding relevant to toxicity. Critical Reviews in Toxicology 41: 783-802.

2012

224. Dawson, D.A., Genco, N., Bensinger, H., Guinn, D. Il'Giovine, Z., Schultz, T.W. and Pöch, G. 2012. Evaluation of an asymmetry parameter for curve-fitting in single-chemical and mixture toxicity assessment. Toxicology 292: 156-161.
225. Enoch, S.J., Schultz, T.W. and Cronin, M.T.D 2012. The definition of the applicability domain for the aromatic nucleophilic substitution electrophilic mechanism. SAR QSAR in Environmental Research 23: 649-663.
226. Kinsner-Ovaskainen,A., Maxwell, G., Kreysa,J., Barroso, J., Adriaens, E., Alépée, N., Berg, N., Bremer, S., Coecke,S., Comenges, J.Z., Corvi, R., Casati, S., Dal Negro,G., Marrec-Fairley, M., Griesinger, C., Halder, M., Heisler, E., Hirmann, D., Kleensang, A., Kopp-Schneider,A., Lapenna, S., Munn, S., Prieto, P., Schechtman, L., Schultz, T., Vidal,J.-M., Worth, A. and Zuang, V. 2012. Report of the EPAA–ECVAM Workshop on the Validation of Integrated Testing Strategies (ITS). Alternatives to Laboratory Animals 40: 175-181.

2013

227. Enoch, S.J., Cronin, M.T.D. and Schultz, T.W. 2013. The definition of the toxicologically relevant applicability domain for the S_NAr reaction for substituted pyridines and pyrimidines. SAR QSAR in Environmental Research. 24: 385-392.
228. Nelms, M.D., Cronin, M.T.D., Schultz, T.W. and Enoch, S.J. 2013. Experimental verification of and domain definition of structural alerts for protein binding: Epoxides, lactones, nitroso, nitros, aldehydes and ketones. SAR QSAR in Environmental Research. 24: 695- 709.
229. Rodriguez-Sanchez, N. Schultz, T.W. Cronin M.T.D. and Enoch, S.J. 2013. Experimental verification of structural alerts for the protein binding of cyclic compounds acting as Michael acceptors. SAR QSAR in Environmental Research. 24: 963-977.

2014

230. Dawson, D.A., Pöch, G. and Schultz, T.W. 2014. Mixture toxicity of SN2-reactive soft electrophiles: 3. Evaluation of ethyl α -halogenated acetates with α -halogenated acetonitriles. Archives Environmental Contamination and Toxicology 66: 248-258.
231. Willett, C. Rae, J.C., Goyak, K.O., Minsavage, G. Westmoreland, C., Andersen, M., Avigan, M., Duché, D., Hartung, T., Jaeschke, H., Kleensang, A., Landesmann, B. Toole, C., Rowan, A., Schultz, T., Seed, J., Senior, J., Shah, I., Subramanian, K., Vinken, M. and Watkins, P. 2014. Building shared experience to advance practical application of pathway-based toxicology: Liver toxicity mode-of-action. ALTEX 31: 500-519.
232. Schultz T.W. 2014. Gilman D. Veith (1944-2013). SAR QSAR in Environmental Research 25: 249-251.
233. Richarz, A.-N. Schultz, T.W. Cronin M.T.D. and Enoch, S.J. 2014. Experimental verification of structural alerts for the protein binding of sulfur-containing compounds. SAR QSAR in Environmental Research 25: 325-341.
234. Bradbury, S.P., Russom, C.L., Schmieder, P.K., Henry, T.R., Schultz, T.W. Diderich, R. and Auer, C.M. 2014. Advancing computational toxicology in a regulatory setting: A selected review of the accomplishments of Gilman D. Veith (1944 – 2013). Applied In Vitro Toxicology 1: 11-20.
235. Dawson, D.A. Allen, E.M.G. Allen, J. Baumann, H. Bensinger, H.M. Genco, N. Guinn, D. Hull, M.W. Il'Giovine, Z.J. Kaminski, C. Peyton, J. Schultz, T.W. and Pöch, G. 2014. Time-dependence in mixture toxicity prediction. Toxicology 326: 153-163.
236. Shen, J., Kromidas, L., Schultz, T. and Bhatia, S. 2014. An *in silico* skin absorption model for fragrance materials. Food and Chemical Toxicology 74: 164-176.

2015

237. Bhatia, S., Schultz, T. Roberts, D., Shen, J. Kromidas, L. and Api, A.-M. 2015. Comparison of Cramer class prediction between Toxtree, OECD QSAR Toolbox and expert judgment—Strategies for refinement. Regulatory Toxicology and Pharmacology 71: 52-62.
238. Api, A.M., Belsito, D., Bruze, M., Cadby, P., Calow, P., Dagli, M.L., Dekant, W., Ellis, G., Fryer, A.D. Fukayama, M., Griem, P., Hickey, C., Kromidas, L., Lalko, J.F., Liebler, D.C., Miyachi, Y., Politano, V.T., Renskers, K., Ritacco, G., Salvito, D., Schultz, T.W., Sipes, I.G., Smith, B., Vitale, D. and Wilcox, D.K. 2015. Criteria for the Research Institute for Fragrance Materials, Inc. (RIFM) safety evaluation process for fragrance ingredients. Food and Chemical Toxicology doi: 10.1016/j.fct.2014.11.014
239. Api, A.-M., Belsito, D., Bhatia, S. Bruze, M. Calow, P. Dagli, M., Dekant, W. Fryer, A. Kromidas, L., Lalko, J. Lapczynski, A. Liebler, D., Miyachi, Y. Politano, V. Ritacco, G., Salvito, D. Shen, J., Schultz, T., Sipes, G. Wall, B. and Wilcox, D. 2015. RIFM FRAGRANCE INGREDIENT SAFETY ASSESSMENT, Allyl (cyclohexyloxy)acetate, CAS Registry Number 68901-15-5. Food and Chemical Toxicology
240. Api, A.-M., Belsito, D, Bhatia, S., Bruze, M., Calow, P., Dagli, M.L., Dekant, W., Fryer, A.D., Kromidas, L., Cava, S.L.A., Lalko, J.F., Lapczynski, A., Liebler, D.C., Miyachi, Y., Politano, V.T., Ritacco, G., Salvito, D, Shen, J., Schultz, T.W., Sipes, I.G., Wall, B. and Wilcox, D.K. 2015. RIFM fragrance ingredient safety assessment, Linalool, CAS registry number 78-70-6. Food and Chemical Toxicology <http://dx.doi.org/10.1016/j.fct.2015.01.005>
241. Api, A.-M., Belsito, D, Bhatia, S., Bruze, M., Calow, P., Dagli, M.L., Dekant, W., Fryer, A.D., Kromidas, L., Cava, S.L.A., Lalko, J.F., Lapczynski, A., Liebler, D.C., Miyachi, Y., Politano, V.T., Ritacco, G., Salvito, D, Shen, J., Schultz, T.W., Sipes, I.G., Wall, B. and Wilcox, D.K.. 2015. RIFM fragrance ingredient safety assessment, methyl dihydrojasmonate, CAS registry number 24851-98-7. Food and Chemical Toxicology <http://dx.doi.org/10.1016/j.fct.2015.01.006>

Refereed journal articles (continued)2015

242. Api, A.-M., Belsito, D, Bhatia, S., Bruze, M., Calow, P., Dagli, M.L., Dekant, W., Fryer, A.D., Kromidas, L., Cava, S.L.A., Lalko, J.F., Lapczynski, A., Liebler, D.C., Miyachi, Y., Politano, V.T., Ritacco, G., Salvito, D, Shen, J., Schultz, T.W., Sipes, I.G., Wall, B. and Wilcox, D.K. 2015. RIFM fragrance ingredient safety assessment, 2,6-Dimethyl-5-heptenal, CAS Registry Number 106-72-9 Food and Chemical Toxicology <http://dx.doi.org/10.1016/j.fct.2015.01.007>
243. Api, A.-M., Belsito, D, Bhatia, S., Bruze, M., Calow, P., Dagli, M.L., Dekant, W., Fryer, A.D., Kromidas, L., Cava, S.L.A., Lalko, J.F., Lapczynski, A., Liebler, D.C., Miyachi, Y., Politano, V.T., Ritacco, G., Salvito, D, Shen, J., Schultz, T.W., Sipes, I.G., Wall, B. and Wilcox, D.K. 2015. RIFM fragrance ingredient safety assessment, α -amylcinnamaldehyde, CAS registry number 122-40-7 Food and Chemical Toxicology <http://dx.doi.org/10.1016/j.fct.2015.01.008>
244. Api, A.-M., Belsito, D, Bhatia, S., Bruze, M., Calow, P., Dagli, M.L., Dekant, W., Fryer, A.D., Kromidas, L., Cava, S.L.A., Lalko, J.F., Lapczynski, A., Liebler, D.C., Miyachi, Y., Politano, V.T., Ritacco, G., Salvito, D, Shen, J., Schultz, T.W., Sipes, I.G., Wall, B. and Wilcox, D.K. 2015. RIFM fragrance ingredient safety assessment, Linalyl hexanoate, CAS Registry Number 7779-23-9. Food and Chemical Toxicology <http://dx.doi.org/10.1016/j.fct.2015.01.009>
245. Api, A.-M., Belsito, D, Bhatia, S., Bruze, M., Calow, P., Dagli, M.L., Dekant, W., Fryer, A.D., Kromidas, L., Cava, S.L.A., Lalko, J.F., Lapczynski, A., Liebler, D.C., Miyachi, Y., Politano, V.T., Ritacco, G., Salvito, D, Shen, J., Schultz, T.W., Sipes, I.G., Wall, B. and Wilcox, D.K.. 2015. RIFM fragrance ingredient safety assessment, Linalyl acetate, CAS Registry Number 115-95-7. Food and Chemical Toxicology <http://dx.doi.org/10.1016/j.fct.2015.01.010>
246. Petkov, P.I., Patlewicz, G., Schultz, T.W., Honma, M., Todorov, M., Kotov, S., Dimitrov, S.D. Donner, E.M. and Mekenyan, O.G. 2015. A feasibility study: Can information collected to classify for mutagenicity be informative in predicting carcinogenicity? Regulatory Toxicology and Pharmacology 72: 17-25.
247. Schultz, T.W., Amcoff, P. Berggren, E., Gautier, F. Klaric, M., Knight, D. J. Mahony, C. Schwarz, M., White, A. and Cronin, M.T.D. 2015. A strategy for structuring and reporting a read-across prediction of toxicity. Regulatory Toxicology and Pharmacology 72: 586-601.
248. Berggren, E., Amcoff, P., Benigni, R., Blackburn, K. Carney, E. Cronin, M., Deluyker, H., Gautier, F., Judson, R.S., Kass, G.E.N., Keller, D., Knight, D., Lilienblum, W., Mahony, C., Rusyn, I., Schultz, T., Schwarz, M., Schüürman, G., White, A., Burton, J., Lostia, A., Munn, S., and Worth, A. 2015. Chemical safety assessment using read-across: How can novel testing methods strengthen evidence base for decision-making. Environmental Health Perspectives 123:1232-1240.
249. Roberts, D.W., Aptula, A., Schultz, T.W., Shen, J., Api, A.M., Bhatia, S. and Kromidas, L. 2015. A practical guidance for Cramer class determination. Regulatory Toxicology and Pharmacology 73: 971-984.

2016

250. Toropovo, A.A., Schultz, T.W. and Toropova, A.P. 2016. Building up a QSAR model for toxicity towards *Tetrahymena pyriformis* by the Monte Carlo method: A case of benzene derivatives. Environmental Toxicology and Pharmacology 42: 135-145.
251. Petkov, P.I., Schultz, T.W., Donner, E.M., Honma, M., Morita, T., Hamada, S., Wakata, A., Mishima, M., Maniwa, J., Todorov, M., Kaloyanova, E., Kotov, S. and Mekenyan, O.G. 2016. Integrated approach to testing and assessment for predicting carcinogenesis. Environmental Toxicology and Pharmacology (in press)
252. Roberts, D.W., Api, A.M., Patlewicz, G.Y. and Schultz, T.W. 2016. Chemical applicability domain of the Local Lymph Node Assay (LLNA) for skin sensitisation potency. Part 1. Underlying physical organic chemistry principles and the extent to which they are represented in the LLNA validation dataset. Chemical Research in Toxicology (in press)

Refereed journal articles (continued)2016

253. Schultz, T.W. and Aptula, A.O. 2016. Kinetic-based reactivity for Michael acceptors: Structural activity relationships and its relationship to excess acute fish toxicity. *Bulletin of Environmental Contamination and Toxicology* (in press)
254. Ebbrell, D.J., Madden, J.C., Cronin, M.T., Schultz, T.W., and Enoch, S.J. 2016. Development of a Fragment-Based in Silico Profiler for Michael Addition Thiol Reactivity. *Chemical Research in Toxicology* (in press)

PUBLICATIONS (BOOKS):Refereed book chapters1978

1. Schultz, T.W., Dumont, J.N. and Kyte, L.M. 1978. Cytotoxicity of untreated coal-conversion gasifier condensate. In: Thorp, J.H. and Gibbons, J.W. (eds.) *Energy and Environmental Stress in Aquatic Systems*. DOE Symposium Series. (Conf-771114). NTIS. Springfield, VA. pp. 204-218.

1983

2. Schultz, T.W. 1983. Aquatic toxicology of nitrogen heterocyclic molecules: Quantitative structure activity relationships. In: Nriagu, J.O. (ed.) *Aquatic Toxicology*. John Wiley and Sons, NY. pp. 411-424.
3. Dumont, J.N., Schultz, T.W., Buchanan, M.V. and Kao, G.L. 1983. Frog embryo teratogenesis assay: *Xenopus* (FETAX) - A short-term assay applicable to complex environmental mixtures. In: Waters, M.D., Sandhu, S.S., Lewtas, J., Claxton, L., Chernoff, N. and Nesnow, S. (eds.) *Short-Term Bioassays in the Analysis of Complex Environmental Mixtures III*. pp. 393-405.

1984

4. Schultz, T.W., Kier, L.B. and Dumont, J.N. 1984. Structure-activity relationships: Their function in biological prediction. In: Cowser, K.E. (ed.) *Synthetic Fossil Fuel Technologies*. Butterworth Publishers, Stoneham, MA. pp. 373-386.
5. Schultz, T.W. and Moulton, B.A. 1984. Structure-activity correlations of selected azaarenes, aromatic amines and nitrobenzenes. In: Kaiser, K.L.E. (ed.) *QSAR in Environmental Toxicology*. D. Reidel Publishing Co., Dordrecht, Holland. pp. 337-357.

1987

6. Schultz, T.W., Riggan, G.W. and Wesley, S.K. 1987. Structure-activity relationships for para-substituted phenols. In: Kaiser, K.L.E. (ed.) *QSAR in Environmental Toxicology-II*. D. Reidel Publishing Co., Dordrecht, Holland. pp. 333-345.

1988

7. Schultz, T.W. 1988. The assessment of toxicity of substituted benzenes: A knowledge based system approach. In: Turner, J.E., England, M.W., Schultz, T.W. and Kwaak, N.J. (eds.) *QSAR 88 Proceedings of the 3rd International Workshop of Quantitative Structure-Activity (QSAR) in Environmental Toxicology*. (Conf-880520--DE88013180) NTIS, Springfield, VA. pp. 51-60.
8. Dawson, D.A., Lin, D.T. and Schultz, T.W. 1988. Comparative toxicity of selected anilines, pyridines and nitrobenzenes in the *Tetrahymena pyriformis* and *Pimephales promelas* test systems. In: Turner, J.E., England, M.W., Schultz, T.W. and Kwaak, N.J. (eds.) *QSAR 88 Proceedings of the 3rd International Workshop on Quantitative Structure-Activity Relationships (QSAR) in Environmental Toxicology*. (Conf-880520--DE88013180) NTIS, Springfield, VA. pp. 169-173.
9. Baker, L.L., Wesley, S.K. and Schultz, T.W. 1988. Quantitative structure activity relationships for alkylated and/or halogenated phenols eliciting the polar narcosis mechanism of toxic action. In: Turner, J.E., England, M.W., Schultz, T.W. and Kwaak, N.J. (eds.) *QSAR 88 Proceedings of the 3rd International Workshop on Quantitative Structure-Activity Relationships (QSAR) in Environmental Toxicology*. (Conf-880520--DE88013180) NTIS, Springfield, VA. pp. 165-169.

1989

10. Schultz, T.W., Cajina-Quezada, M., Chang, M., Lin, D.T. and Jain, R. 1989. Structure-toxicity relationships of para-position alkyl- and halogen-substituted monoaromatic compounds. In: G.W. Suter II and A.M. Lewis (eds.) *Aquatic Toxicology and Environmental Fate: Eleventh Volume, ASTM STP 1007*. American Society for Testing and Materials, Philadelphia, PA. pp. 410-423.
11. Schultz, T.W. 1989. Nonpolar Narcosis: A review of the mechanism of action for baseline toxicity. In: Cowgill, U.M. and Williams, L.R. (eds.) *Aquatic Toxicology and Environmental Fate: Twelfth Volume, ASTM STP 1027*. American Society for Testing and Materials, Philadelphia, PA. pp. 104-109.

PUBLICATIONS (BOOKS): (continued)Refereed book chapters1990

12. Dawson, D.A., Schultz, T.W., Baker, L.L. and Wilke, T.S. 1990. Comparative developmental toxicity of acetylenic alcohols on embryos and larvae of *Xenopus laevis*. In: Landus, W.G. and van der Schalie, W.H. (eds.) *Aquatic Toxicology and Risk Assessment: Thirteenth Volume, ASTM STP 1096*. American Society for Testing and Materials, Philadelphia, PA. pp. 267-277.
13. Schultz, T.W., Lin, D.T., Wilke, T.S. and Arnold, L.M. 1990. Quantitative structure-activity relationships for *Tetrahymena pyriformis* population growth endpoint: A mechanism of action approach. In: Karcher, W. and Devillers, J. (eds.) *Practical Application of Quantitative Structure-Activity Relationships (QSAR) in Environmental Chemistry and Toxicology*. Kluwer Academic Publishers, Dordrecht, The Netherlands. pp. 241-262.
14. Schultz, T.W. and Dawson, D.A. 1990. Structure-activity relationships for teratogenicity and developmental toxicity. In: Karcher, W. and Devillers, J. (eds.) *Practical Application of Quantitative Structure-Activity Relationships (QSAR) in Environmental Chemistry and Toxicology*. Kluwer Academic Publishers, Dordrecht, The Netherlands. pp. 389-409.

1993

15. Tichy, M. and Schultz, T.W. 1993. A note on excess toxicity of acetylenic alcohols to ciliate *Tetrahymena pyriformis*. In: Wermath, C.G. (ed.) *Trends in QSAR and Molecular Modeling 92: Proceedings of the 9th European Symposium on Structure-Activity Relationships: QSAR and Molecular Modeling*, September 7-11, 1992, Strasbourg, France. ESCOM Science Publishers, Leiden, The Netherlands. pp. 575-576.

1995

16. Schultz, T.W., Jaworska, J.S. and Hunter, R.S. 1995. Volume fraction analyses for selected mechanism of toxic action. In: Hughes, J.S., Biddinger, G.R. and Mones, E. (eds.) *Environmental Toxicology and Risk Assessment - Third Volume, ASTM STP 1218*. American Society for Testing and Materials, Philadelphia, PA. pp. 172-184.
17. Tichy, M. and Schultz, T.W. 1995. Excess toxicity of unsaturated aldehydes - Log P-dependent QSAR model. In: Sanz, F., Giraldo, J. and Manaut, F. (eds.) *QSAR and Molecular Modeling: Concepts, Computational Tools and Biological Applications*. Prous Science Publishers, Barcelona, Spain, pp. 125-127.

1997

18. Jaworska, J.S., Hunter, R.S., Gobble, J.R. and Schultz, T.W. 1997. Structure-activity relationships for diesters: Aquatic Toxicity to *Tetrahymena*. In: Fredenslund, F.C. and Schüürmann, G. (eds.) *Quantitative Structure-Activity Relationships in Environmental Sciences-VII*. SETAC Press, Pensacola, FL, USA, pp. 277-283.
19. Schüürmann, G., Flemming, B., Dearden, J.C., Cronin, M.D.T. and Schultz, T.W. 1997. CoMFA study of acute toxicity of nitrobenzenes to *Tetrahymena pyriformis*. In: Fredenslund, F.C. and Schüürmann, G. (eds.) *Quantitative Structure-Activity Relationships in Environmental Sciences-VII*. SETAC Press, Pensacola, FL, USA, pp. 315-327.
20. Schultz, T.W., Sinks, G.D. and Cronin, M.T.D. 1997. Structure-toxicity evaluation of phenols: A mechanism of action approach. In: Fredenslund, F.C. and Schüürmann, G. (eds.) *Quantitative Structure-Activity Relationships in Environmental Sciences-VII*. SETAC Press, Pensacola, FL, USA, pp. 329-342.

1998

21. Schultz, T.W., Sinks, G.D. and Bearden, A.P. 1998. QSARs in aquatic toxicology: A mechanism of action approach comparing toxic potency to *Pimephales promelas*, *Tetrahymena pyriformis*, and *Vibrio fischeri*. In: Devillers, J. (ed.) *Comparative QSAR*. Taylor and Francis, London, pp. 52-109.

PUBLICATIONS (BOOKS): (continued)Refereed book chapters1999

22. Sanseverino J., Menn, F-M., Gregory, B. , Sampsel, E., Shi, Z., Ghosh, M., Schultz, T.W. and Sayler, G.S. 1999. Bioavailability, estrogenicity, and toxicity of surfactant-PCB mixtures after biodegradation and photolysis. In: *Bioremediation of Nitroaromatic and Haloaromatic Compounds*. (B.C. Alleman and A. Leeson, eds.) pp. 155-160.
23. Bearden, A.P., Sinks, G.D. and Schultz, T.W. 1999. Population growth kinetics of *Tetrahymena pyriformis* exposed to selected electrophiles. In: Henshel, D.S., Black, M.C. and Harrass, M.C. (eds.) *Environmental Toxicology and Risk Assessment: Standardization of Biomarkers for Endocrine Disruption and Environmental Assessment: Eighth Volume, ASTM STP 1364*. American Society for Testing and Materials, West Conshohocken, PA. pp. 319-328.

2001

24. Cronin, M.T.D., Sinks, G.D. and Schultz, T.W. 2001. Modelling of toxicity to the ciliate *Tetrahymena pyriformis*: the Aliphatic Carbonyl domain. In: Rainbow, P.S., Hopkin, S.P. and Crane, M. (eds.) *Forecasting the Environmental Fate and Effects of Chemicals*. John Wiley & Sons, Ltd. Chichester, UK pp. 113-124.

2002

25. Schaeffer, D.O. and Schultz, T.W. 2002. Biology and Diseases of Amphibians. In: Fox, J.G., Anderson, L.C., Loew, F.M., and Quimby, F.W. (eds.) *Laboratory Animal Medicine*. 2nd Ed., Academic Press, San Diego, CA, USA, pp. 793-826.
26. Walker J.D. and Schultz T.W. 2002. Structure activity relationships for predicting ecological effects of chemicals. In: Hoffman, D.J, Rattner, B.A. Burton, G.A. Jr., and Cairns, J. Jr. (eds.) *Handbook of Ecotoxicology* 2nd Ed. CRC Press, Boca Raton, FL, USA, pp. 893-910.
27. Committee on Bioavailability of Contaminants in Soils and Sediments, Water Science and Technology Board, Division of Earth and Life Studies, National Research Council of the National Academies (committee member). 2002. *Bioavailability of Contaminants in Soils and Sediments Processes, Tools and Applications*. The National Academies Press, Washington, D.C. 420 p.

2003

28. Walker, J.D., Dearden, J.C., Schultz, T.W., Jaworska, J. and Comber, M.H.I. 2003. QSARs for new practitioners. In: Walker , J.D. (ed), *QSARs for Pollution Prevention, Toxicity Screening, Risk Assessment, and Web Application*. SETAC Press, Pensacola, FL, USA, pp. 3-18.
29. Netzeva, T.I., Aptula, A.O., Schultz, T.W. and Cronin, M.T.D. 2003. Modelling the acute eco-toxicity of aliphatic chemicals to *Tetrahymena pyriformis*. In: *Designing Drugs and Crop Protectants: Processes, Problems and Solutions*. Ford, M., Livingstone, D., Dearden, J., Van de Waterbeemd (Eds.). Thanet Press, Margate, pp. 12-14.

2004

30. Schultz, T.W. and Netzeva, T.I. 2004. Development and evaluation of QSARs for ecotoxic endpoints: The benzene response-surface model for *Tetrahymena* toxicity. In: Cronin M. and Livingstone D. (eds), *Modelling Environmental Fate and Toxicity*. CRC Press, Boca Raton, FL, USA, pp. 265-284.

2005

31. Sanseverino, J., Layton, A.C., Easter, J.P. Menn, F-M, Saidak, L., Garrett, V., Schultz, T.W. and Sayler, G.S. 2005. Application of a Bioluminescent Estrogen Yeast-Reporter System for Determining the Estrogenic Activity in Water and Sediment Samples at a Superfund Site. National Ground Water Association.

2010

32. Schultz, T.W. 2010. Adverse outcome pathways: A way of linking chemical structure to in vivo toxicological hazards. In: Cronin, M.T.D. and Madden, J.C. eds., *Issues in Toxicology No. 7 In Silico Toxicology: Principles and Applications*, The Royal Society of Chemistry pp. 346-371.

2011

33. Schultz, T.W., Diderich, B. and Enoch, S.J. 2011. The OECD Adverse Outcome Pathway Approach: A Case Study for Skin Sensitisation. In: Seidle, T. and Spielmann, H. (eds), *Alternative Testing Strategies Progress Report 2011 & AXLR8-2 Workshop Report on a 'Roadmap to Innovative Toxicity Testing*. pp. 288- 300.

2012

34. Schultz, T.W. and Diderich, B. 2012. The Assessment and Use of Adverse Outcome Pathways (AOPs) by Organisation for Economic Co-operation and Development (OECD). In: Seidle, T. and Spielmann, H. (eds), *Alternative Testing Strategies Progress Report 2012 & AXLR8-2 Workshop Report on a 'Roadmap to Innovative Toxicity Testing*. pp.244-250.

2013

35. Przybylak, K.R. and Schultz, T.W. 2013. Informing Chemical Categories through Development of Adverse Outcome Pathway. In: Cronin, M., Madden, J., Enoch, S. and Roberts, D. (eds), *Chemical Toxicity Prediction Category Formation and Read-Across*. The Royal Society of Chemistry pp. 44-71.

PAPERS PUBLISHED IN ABSTRACT FORM:

(Presentation and Posters Presented at Scientific Meetings) 261 - prior to 2014

2014

262. Richarz, A.-N. Schultz, T.W., Cronin M.T.D. and Enoch, S.J. 2014. Experimental verification of structural alerts for the protein binding. Presented at the Annual Meeting of the Society of Toxicology, Phoenix, AZ.
263. Bhatia, S., Shen, J., Kromidas, L., Schultz, T.W., Ford, R., Roberts, S.W. and Api, A.-M. 2014. Comparison of Cramer class prediction between Toxtree, OECD QSAR Toolbox and expert judgment –Strategies for refinement. Presented at the Annual Meeting of the Society of Toxicology, Phoenix, AZ.
264. Ruusmann V., Maran, U. and Schultz, T.W. 2014. Unsupervised classification of mechanisms of action for aquatic toxicity of benzenes. Presented at the “16th Workshop on QSAR in Environmental Sciences.” Milan, Italy.
265. Schultz, T.W. and Roberts, D.W. 2014. *In chemico* reactivity of unsaturated aliphatic alcohols. Presented at the 16th Workshop on QSAR in Environmental Sciences.” Milan, Italy.
266. Shen,J., Kromidas, L. Schultz, T.W. and Bhatia, S. 2014. An *in silico* skin absorption model for fragrance materials. Presented at the 16th Workshop on QSAR in Environmental Sciences.” Milan, Italy.
267. Petkov, P., Kotov, S., Todorov, M., Mekenyan, O., Honma, M., Patlewicz, G. and Schultz, T. 2014. Implementation of detoxification pathways in TIMES *in vivo* genotoxicity models. Presented at the 16th Workshop on QSAR in Environmental Sciences.” Milan, Italy.
268. Petkov, P., Kotov, S., Todorov, M., Mekenyan, O., Honma, M., Patlewicz, G. and Schultz, T. 2014. Modeling mutagenicity and carcinogenicity accounting for metabolic activation and detoxification of chemicals. Presented at the “Genetic Impurities Conference” Berlin, Germany.
269. Shen,J., Kromidas, L. Schultz, T.W. and Bhatia, S. 2014. Benchmark study: Structural similarity search methods for identifying read-across analogs. Presented at the “248th American Chemical Society (ACS) National Meeting.”, San Francisco, CA.

2015

270. Schultz, T.W., Mellor, C., Przybylak, K., Cassano, A., Steinmetz, F.P., Ebbrell, D., Cronin, M.T.D. and Richarz, A.-N. 2015. SEURAT-1 level3 read-across case study: Scoping of the category members for the scenario of chemical similarity involving metabolism – Unsaturated alcohols. Presented at the “2015 SEURAT Meeting.”, Barcelona, Spain.
271. Schultz, T., Mahony, C., Lostia, A., Richarz, A., Hardy, B., Elmar Heinzle, E., Benfenati, E. Hengstler, J. van Grunsven, L., Judson, R., Escher, S. Berggren, E. 2015. Using AOPs to support read-across predictions – ‘Testing the hypothesis in Seurat-1’ Presented at “Annual Meeting Society of Toxicology and Chemistry (SETAC) Europe”. Barcelona, Spain.

2016

272. Schultz, T.W. 2016. Results from Read-Across Case Studies: First Lessons Learned. Presented at GlobalChem 2016. Wahsington DC, USA.
273. Schultz, T.W., Mellor, C.L., Przybylak, K.R. Escher, S.E., Judson, R., Tsakovka, I., Richarz, A.-N. and Cronin, M.T.D. 2016. Read-Across for 90-Day Rat Oral Repeated-Dose Toxicity for Selected Perfluoroalkyl Acids: A Case Study. Presented at “European Chemical Agency Topical Scientific Workshop on New Approach Methodologies in Regulatory Science.” Helsinki, Finland.

PAPERS PUBLISHED IN ABSTRACT FORM: (continued)

2016

274. Przybylak, K.R., Schultz, T.W., Mellor, C.L., Richarz, A.-N., Hiemstra, S, Escher, Sylvia E., Leite, S.B., van Grunsven, L.A., van de Water, B. and Cronin, M.T.D. 2016. Read-across of 90-Day Oral Repeated-Dose Oral Toxicity for β -Olefinic Alcohols: A Case Study of Compounds with Similar Metabolism. Presented at “European Chemical Agency Topical Scientific Workshop on New Approach Methodologies in Regulatory Science.” Helsinki, Finland.
275. Richarz, A.-N., Cronin M.T.D. and Schultz, T.W., 2016. Essential Aspects of Read-Across for Repeated-Dose Toxicity Predictions. Presented at “European Chemical Agency Topical Scientific Workshop on New Approach Methodologies in Regulatory Science.” Helsinki, Finland.
276. Schultz, T.W., Bradbury, S.P. and Cronin, M.T.D. 2016. Read-Across for 90-Day Oral Repeated-Dose Toxicity for Primary Alkanols: The Importance of Toxicokinetic Similarity. Presented at “European Chemical Agency Topical Scientific Workshop on New Approach Methodologies in Regulatory Science.” Helsinki, Finland.
277. Richarz, A.-N., Berggren, E., Klaric, M., Mahony, C. and Schultz, T.W., 2016. SEURAT-1 Proof-of-Concept Read-Across Case Study for Repeated-Dose Toxicity. Presented at “European Chemical Agency Topical Scientific Workshop on New Approach Methodologies in Regulatory Science.” Helsinki, Finland.
278. Schultz, T.W., 2016. Kinetic-based Reactivity: SARs for Michael Acceptors. Presented at the 17th Workshop on QSAR in Environmental Sciences.” Miami Beach FL, USA.
279. Schultz, T.W., Mellor, C.L., Przybylak, K.R., Richarz, A.-N. and Cronin, M.T.D. 2016. Sources of Uncertainty in Read-Across: Results for Case Studies. Presented at the 17th Workshop on QSAR in Environmental Sciences.” Miami Beach FL, USA.
280. Petkov, P.I., Schultz, T.W., Donner, E.M., Honma, M., Morita, T., Hamada, S., Wakata, A., Mishima, M., Maniwa, J., Todorov, M., Kaloyanova, E., Kotov, S. and Mekenyan, O.G. 2016. Integrated Approach to Testing and Assessment for Predicting Carcinogenesis. Presented at the 17th Workshop on QSAR in Environmental Sciences.” Miami Beach FL, USA.