Modern Water and Sediment Quality Criteria: Toxicological and Chemical Interactions

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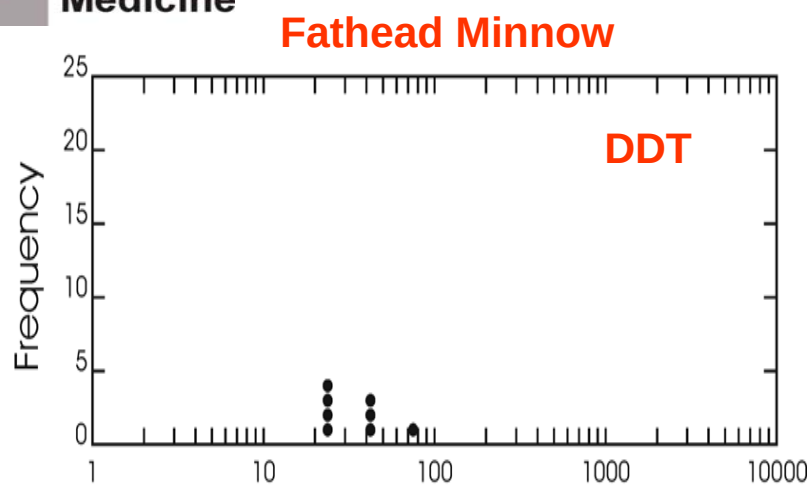
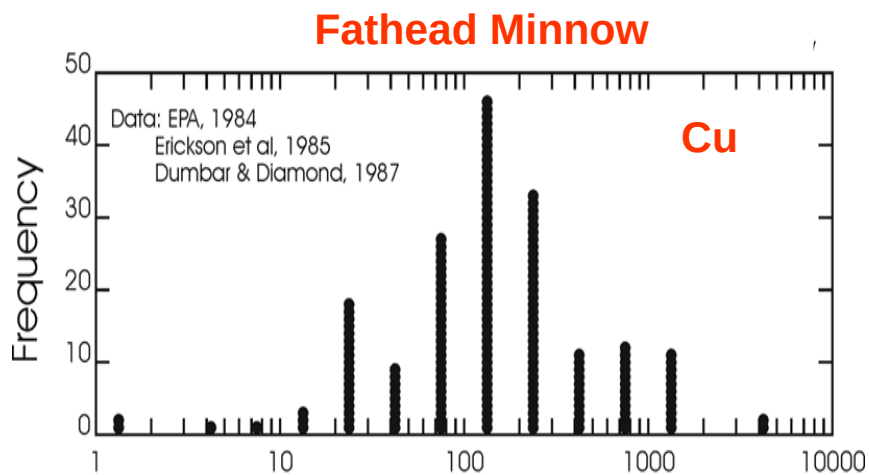
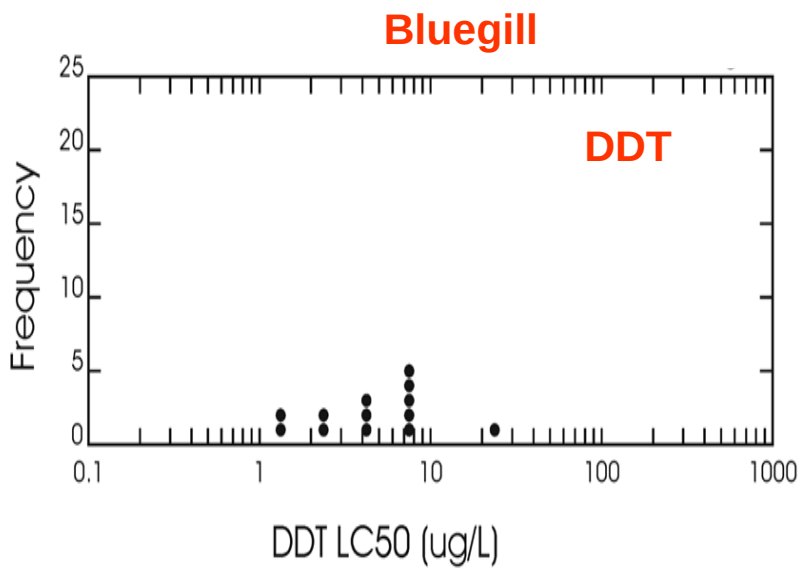
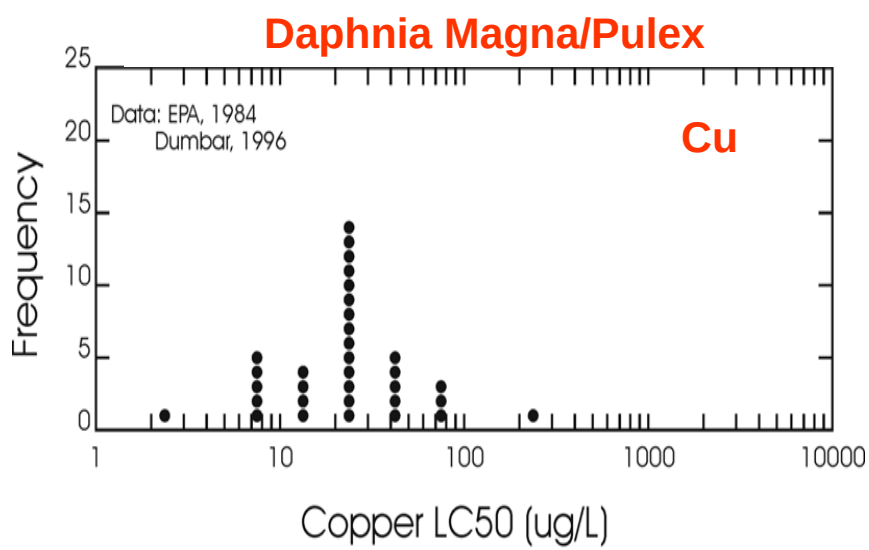
Variation in LC50
Same Organism and Chemical



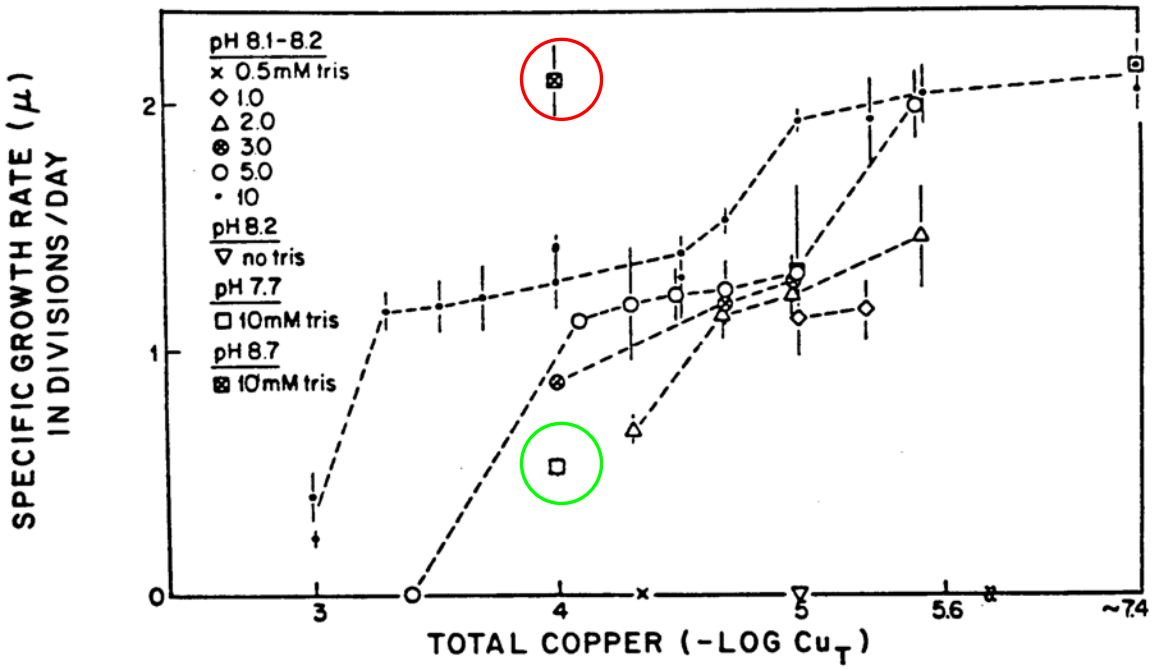


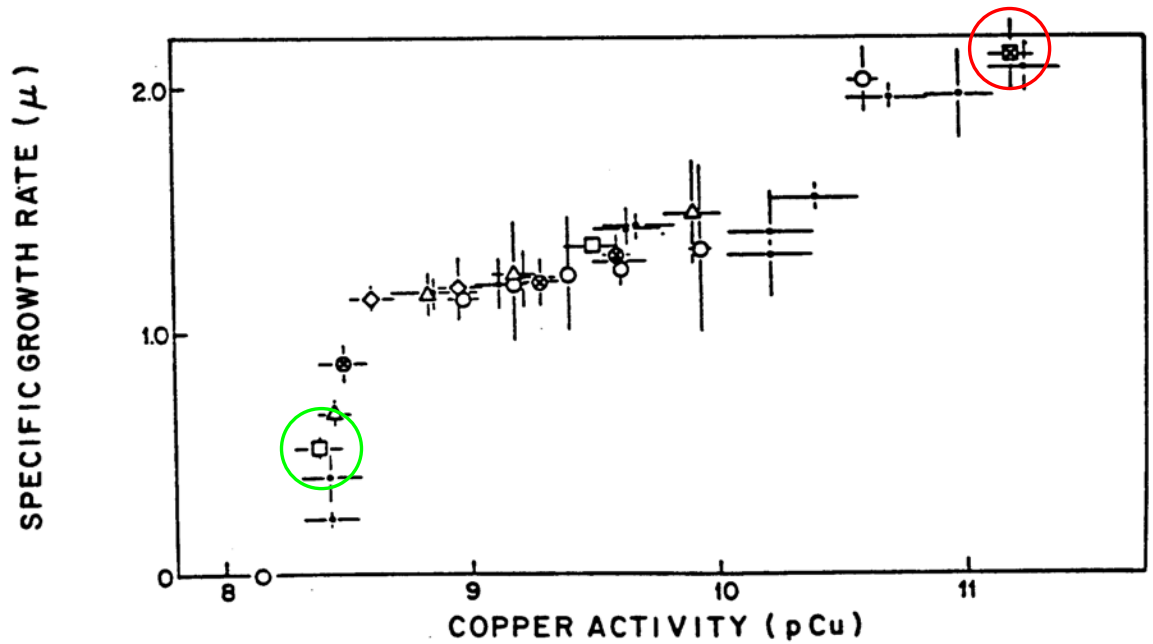




Free Ion Activity Model

FIAM

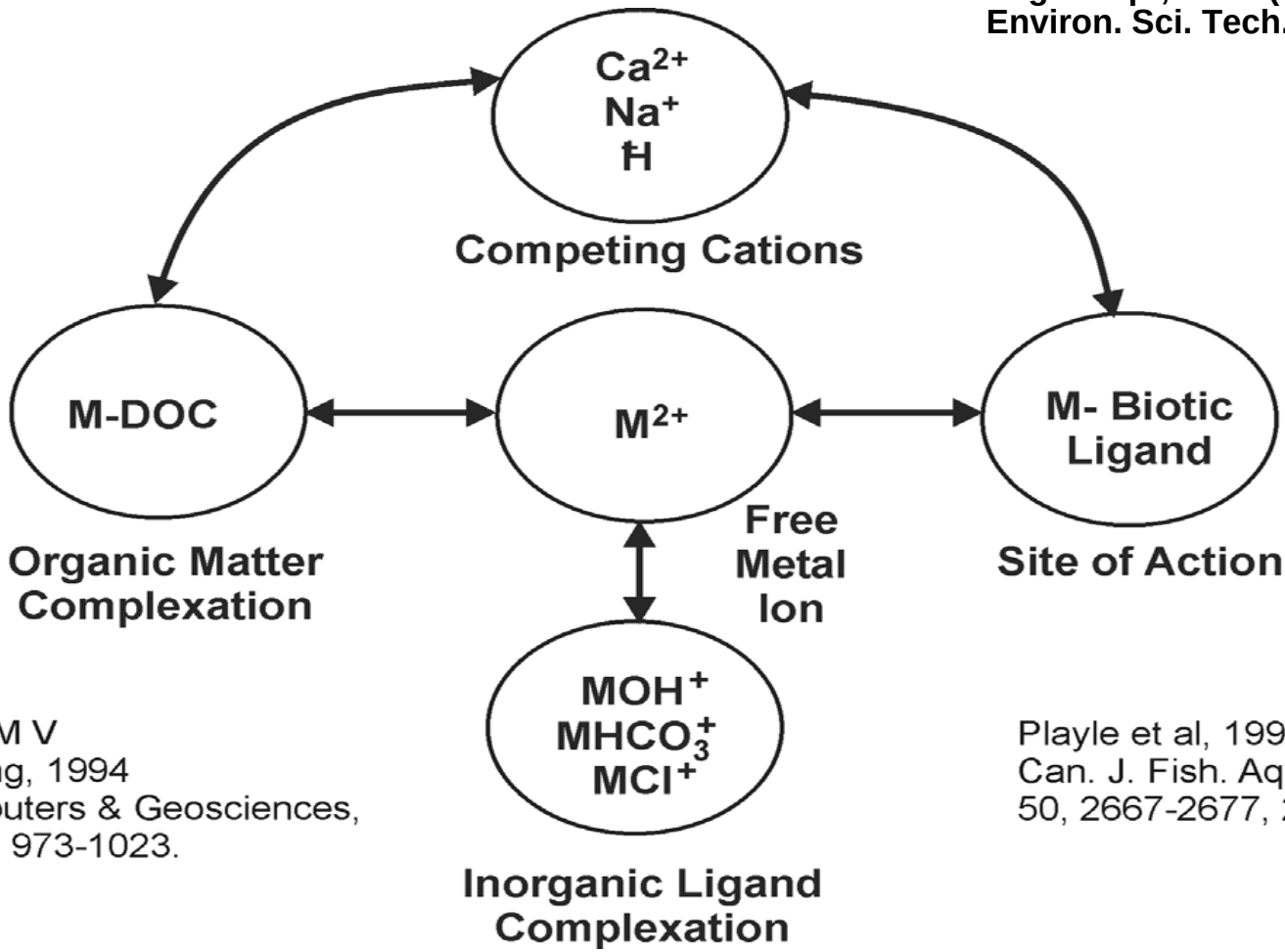




Sunda, W., & Guillard, R. R. L. (1976). J. Mar. Res., 34, 511-529.

Biotic Ligand Model

Pagenkopf, G. K. (1983).
Environ. Sci. Tech., 17, 342

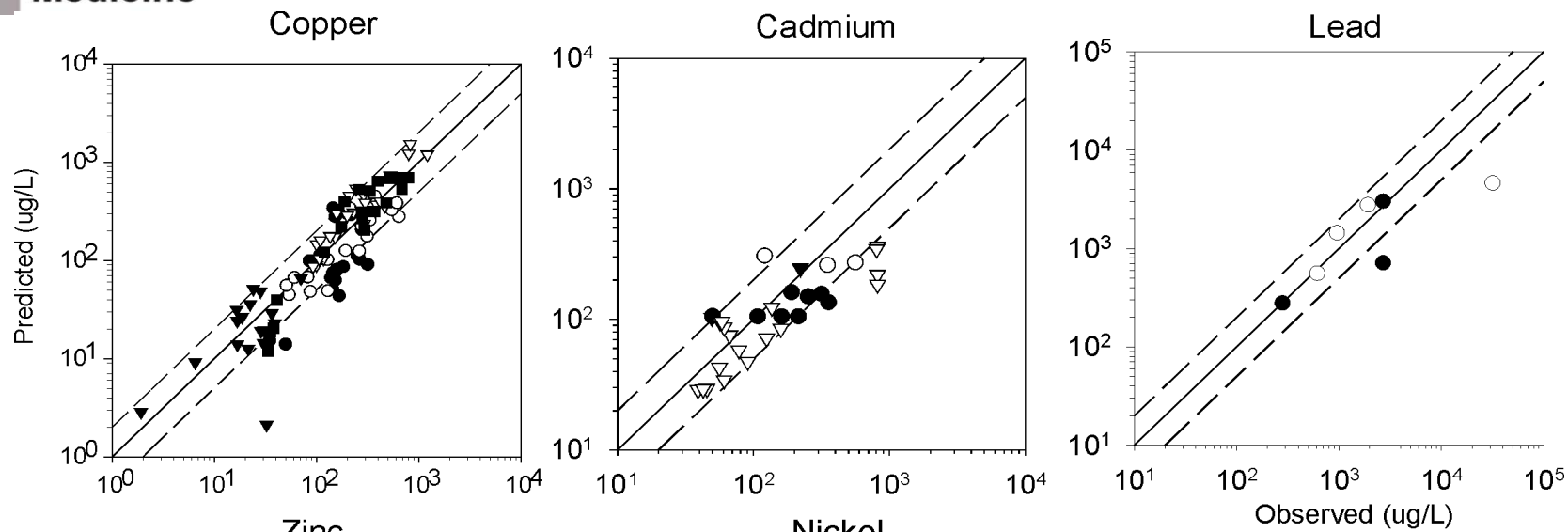


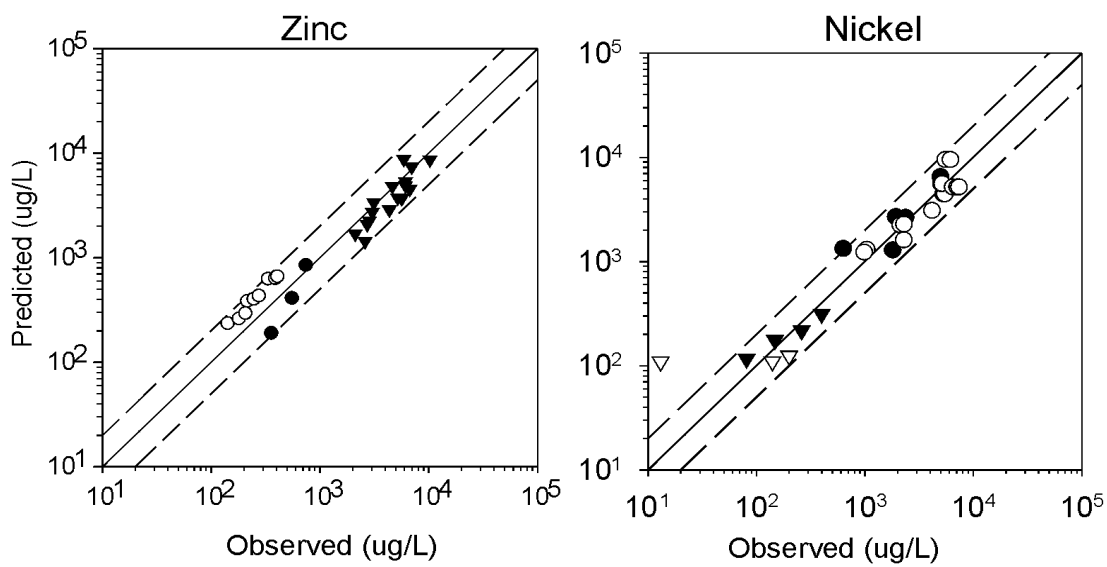
WHAM V
Tipping, 1994
Computers & Geosciences,
20(6), 973-1023.

Playle et al, 1993
Can. J. Fish. Aquat. Sci.,
50, 2667-2677, 2678-2687.

Di Toro, D. M., Allen, H. E., Bergman, H. L., Meyer, J. S., Paqiun, P. R., & Santore, R. C. (2001).
Environ. Tox. Chem., 20(10), 2383

Daphnia Magna BLM LC50 Concentrations



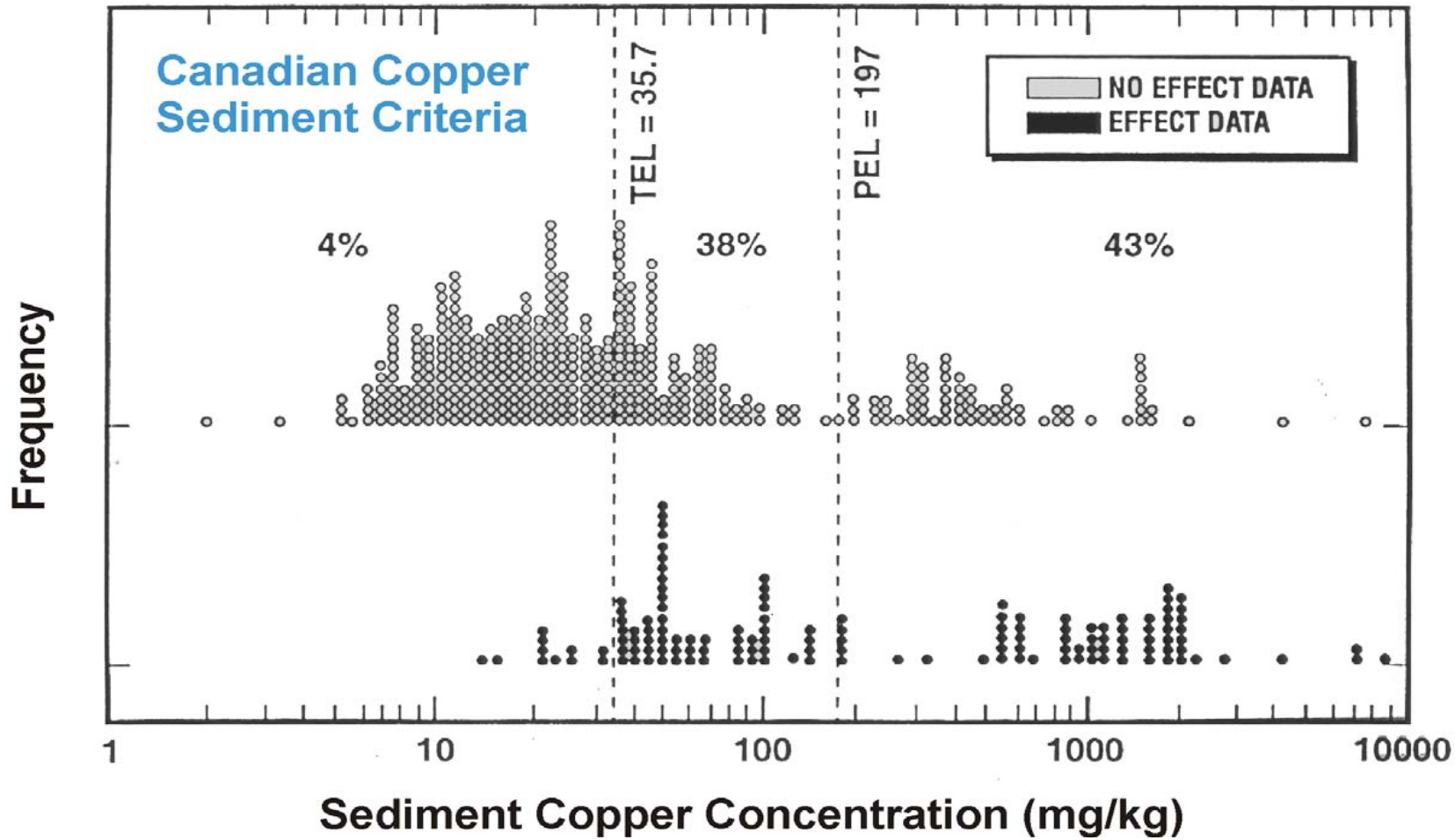


Di Toro, D. M., McGrath, J. M., Hansen, D. J., Berry, W. J., Paquin, P. R., Mathew, R., Wu, K. B., & Santore, R. C.

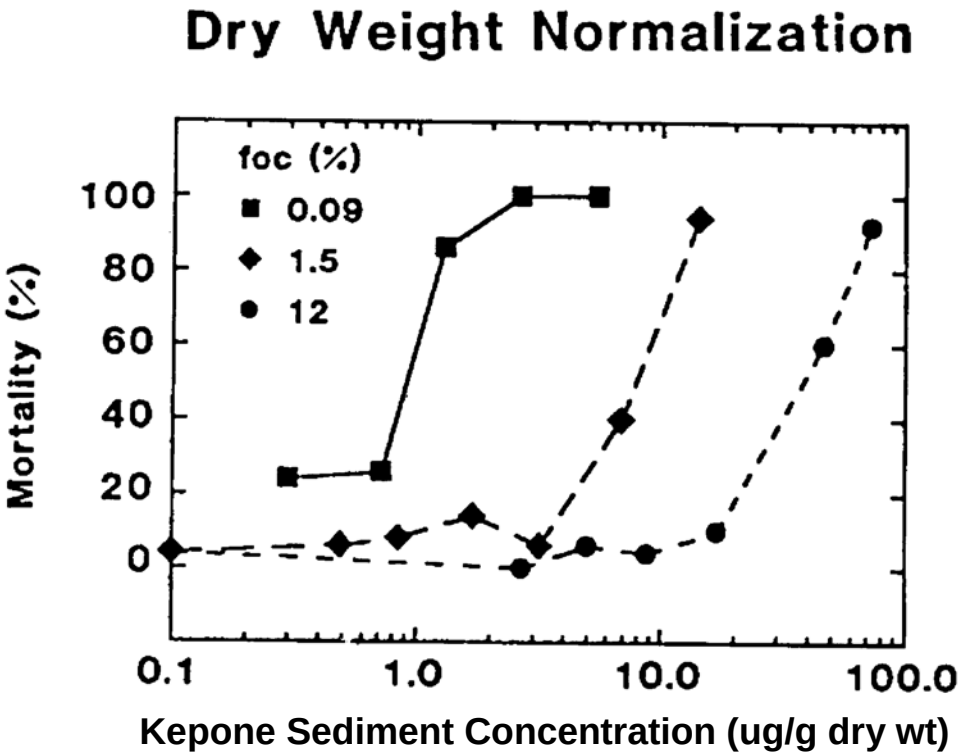
Predicting Sediment Metal Toxicity Using a Sediment Biotic Ligand Model: Methodology and Initial Application.

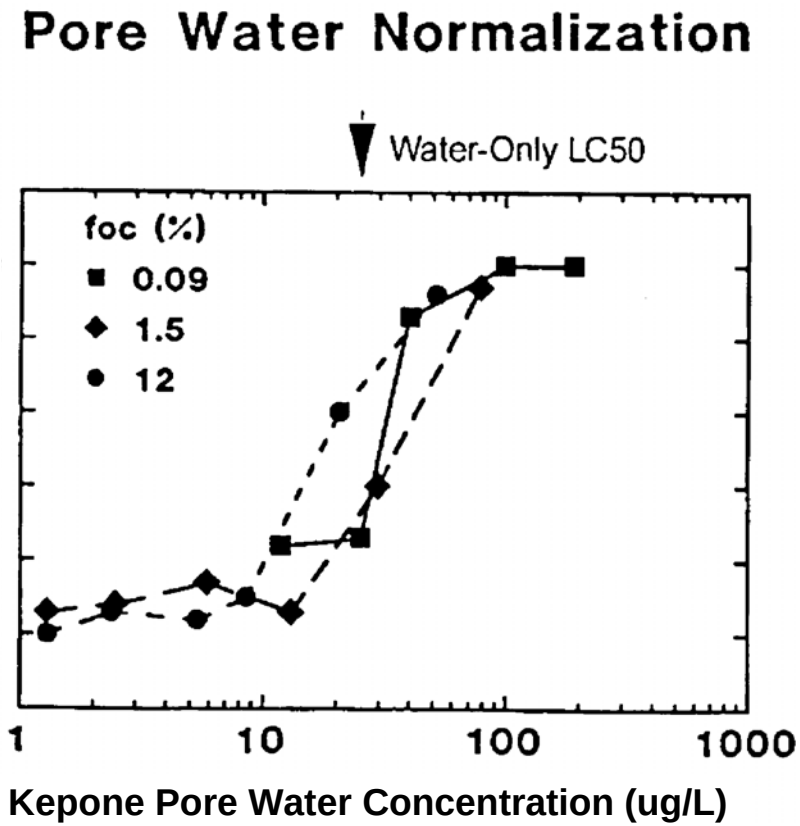
Environ Tox. Chem., (2005).

Bioavailability - Sediment



Pore water Concentration Predicts Sediment Toxicity

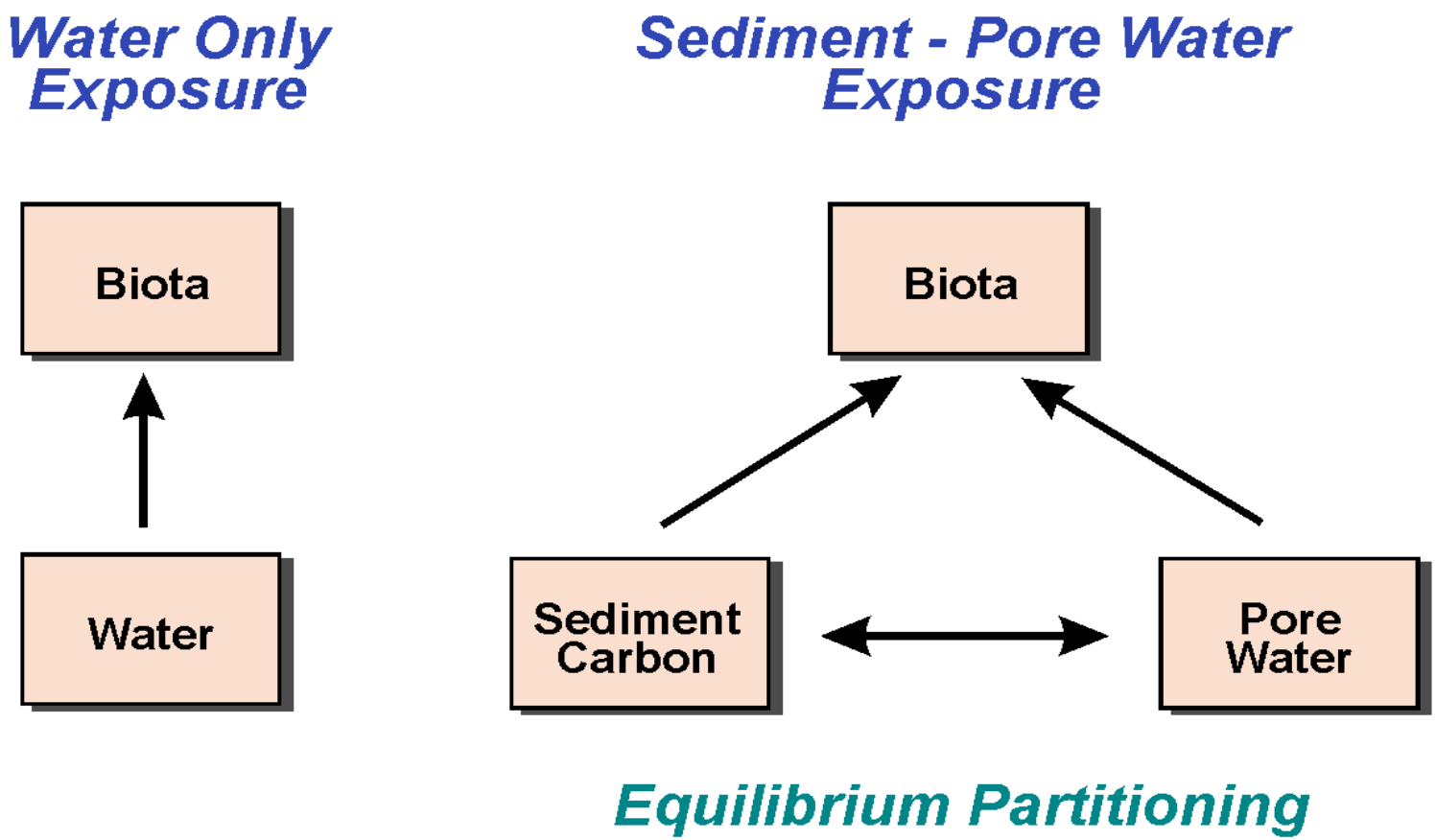




Adams, W. J., Kimerle, R. A., & Mosher, R. G. (1985). In R. D. Cardwell, R. Purdy, & R. C. Bahner (Eds.), Aquatic Toxicology and Hazard Assessment: Seventh Symposium. STP 854 (pp. 429-453). Am. Soc. for Testing and Materials.

Di Toro, D. M., C. S. Zarba, D J. Hansen, W J Berry, R C. Swartz, C E. Cowan, S P. Pavlou H E. Allen, N A Thomas, P R Paquin. (1991). Environ. Toxicol. Chem. 11(12): 1541-1583.

Equilibrium Partitioning Model of Sediment Toxicity

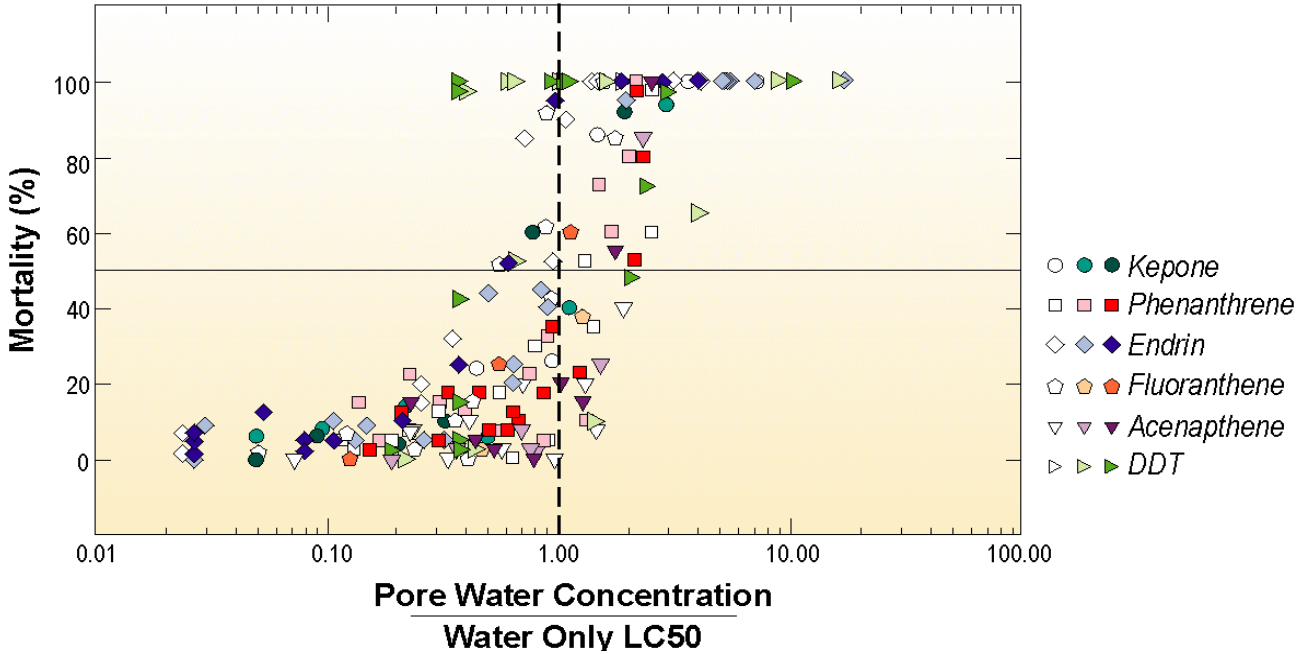


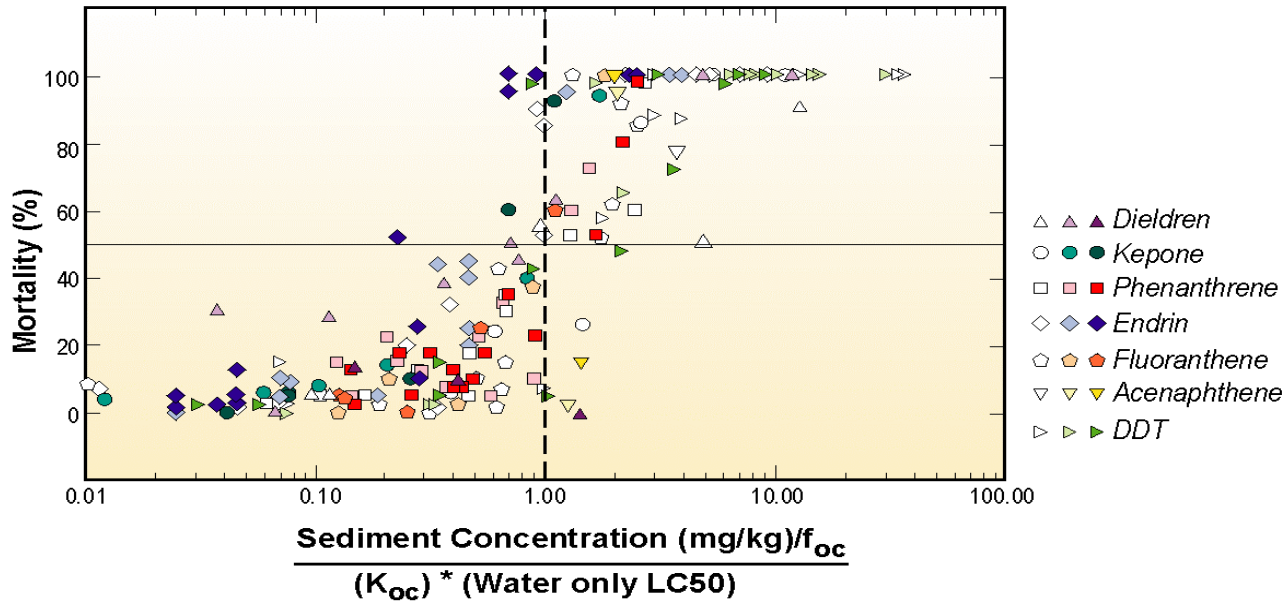
Di Toro, D. M., C. S. Zarba, D J. Hansen, W J Berry, R C. Swartz, C E. Cowan, S P. Pavlou H E. Allen, N A Thomas, P R Paquin. (1991). Environ. Toxicol. Chem. 11(12): 1541-1583.

Sediment Toxicity Prediction

Pore Water

Organic Carbon Normalized





USEPA (2000). Draft Technical Basis for the derivation of Equilibrium Partitioning sediment guidelines (ESG) for the protect of benthic organisms: Nonionic organics No. EPA-822-R-00-001)

SEM – AVS Model of Metal Bioavailability

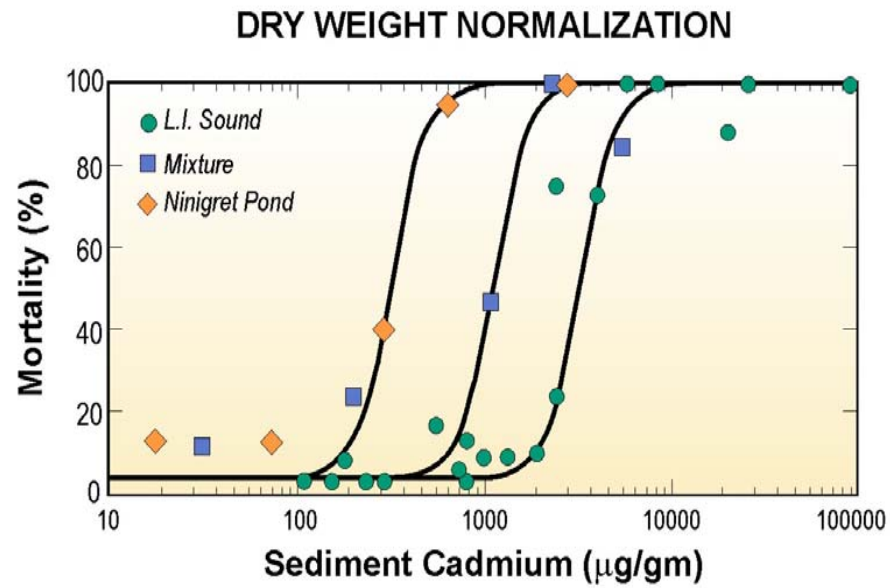
Metals are precipitated by reacting with iron monosulfide (AVS)

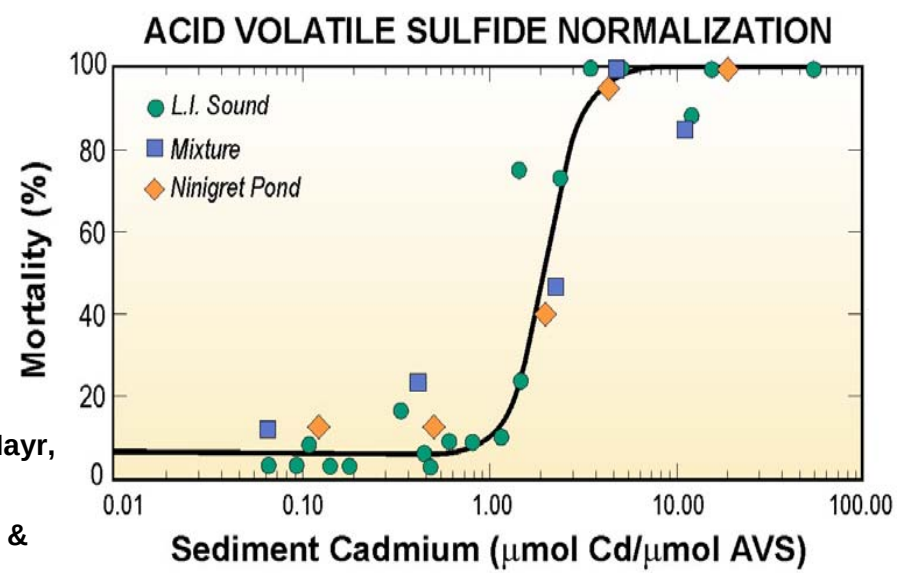
$$M^{2+} + FeS \longrightarrow Fe^{2+} + MS$$

Sediment metal (SEM) is quantified using same extraction as for AVS (1N HCl)

AVS > SEM No toxicity possible

AVS < SEM Toxicity possible



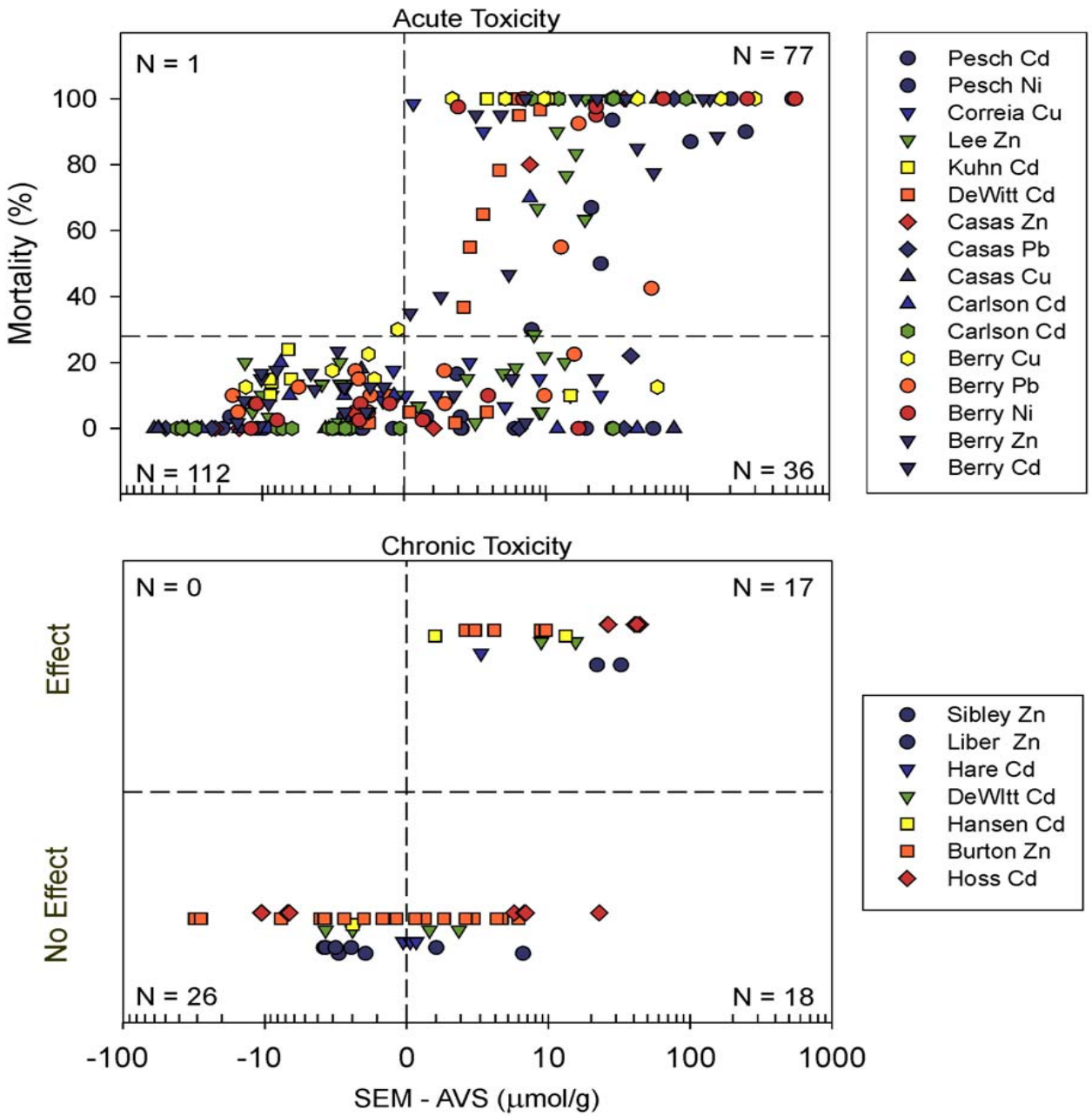


Di Toro, D. M., Mahony, J. D., Hansen, D. J., Scott, K. J., Hicks, M. B., Mayr, S. M., & Redmond, M. S. (1990). Environ. Toxicol. Chem., 9, 1487-1502.

Di Toro, D. M., Mahony, J. D., Hansen, D. J., Scott, K. J., Carlson, A. R., & Ankley, G. T. (1992). Environ. Sci. Tech., 26(1), 96-101.

SEM – AVS

Model Validation



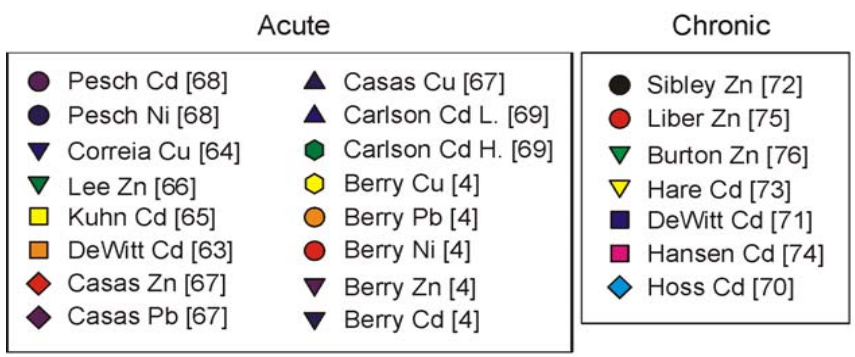
Predicting Sediment Metal Toxicity

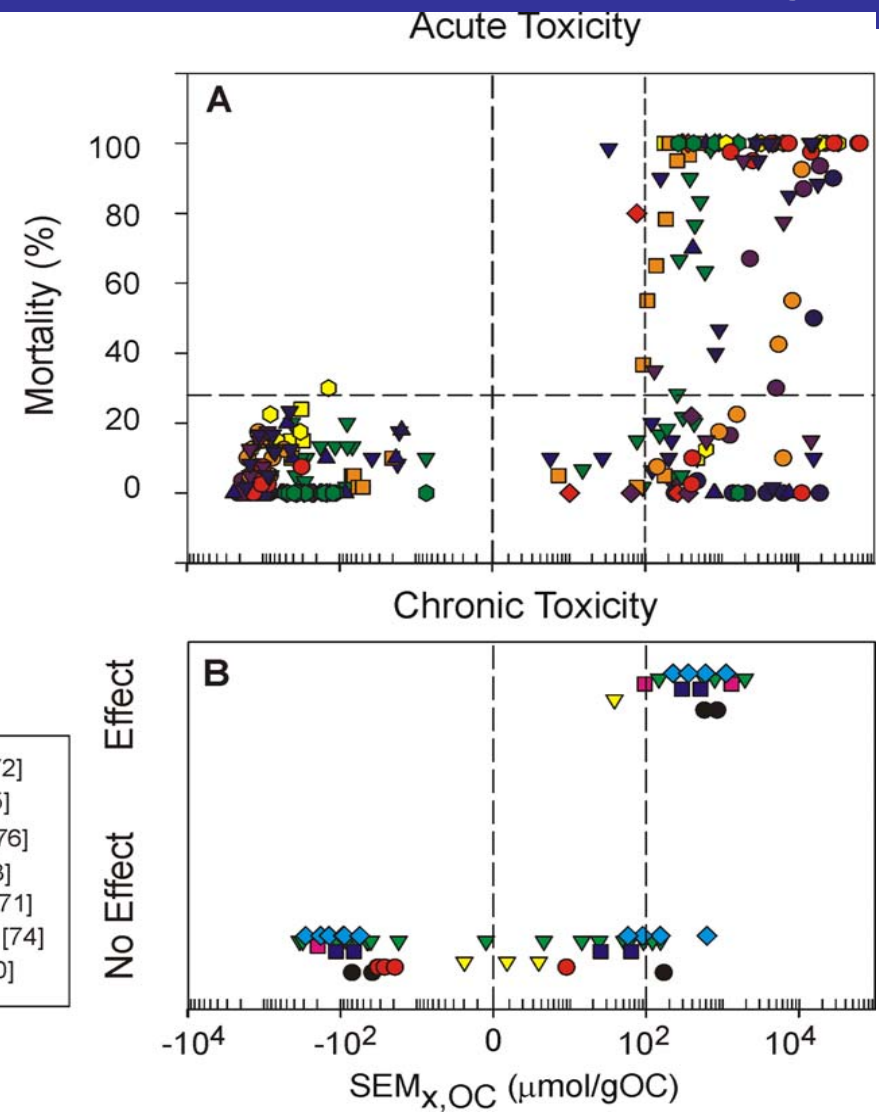
Organic Carbon Normalized Excess SEM

$SEM_{x,oc} = (SEM - AVS)/f_{oc}$

Observed Toxicity Boundary

$SEM_{x,oc} = 100\ \mu mol/gOC$





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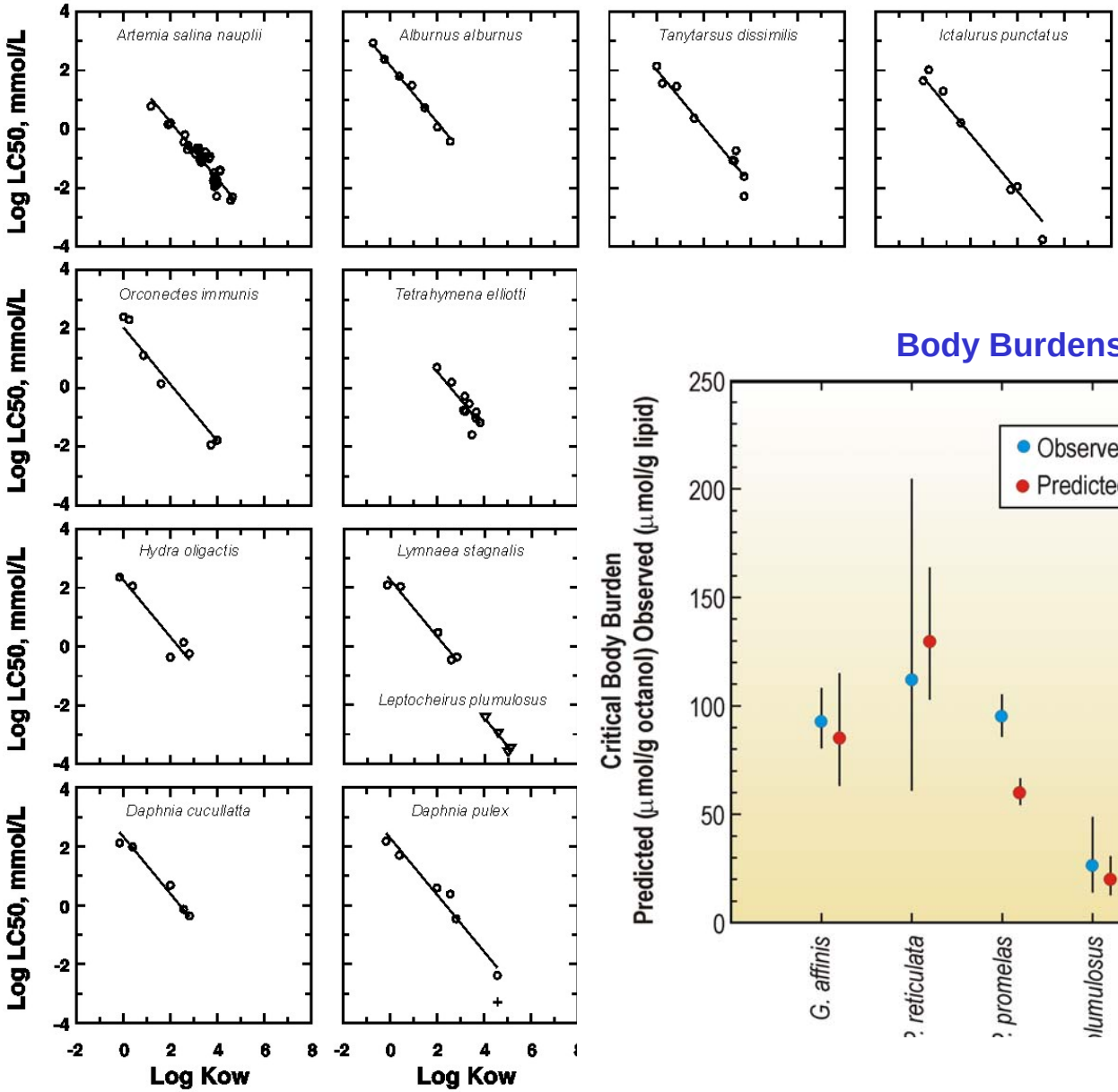
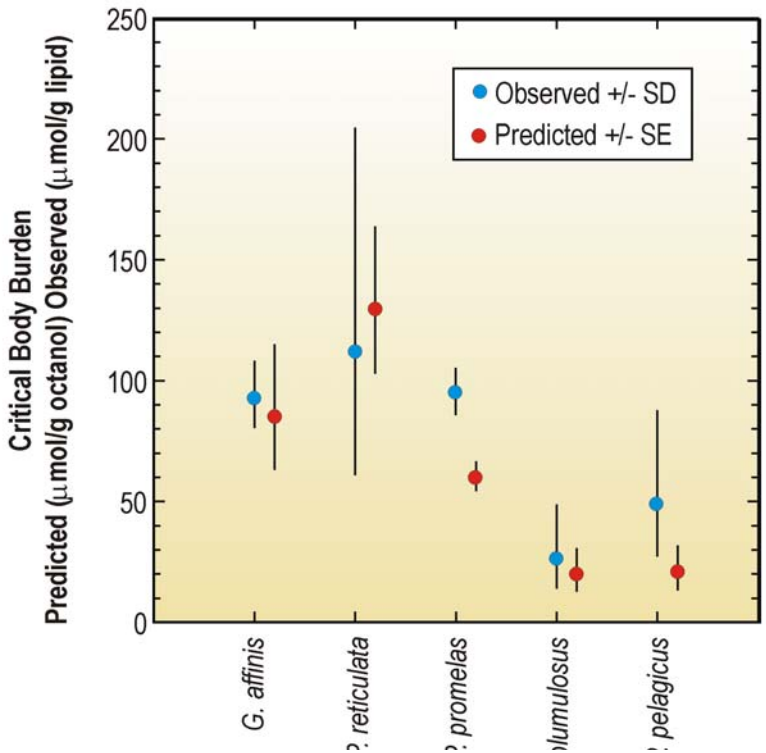
Narcosis Target Lipid Model

LC50s for Various Species

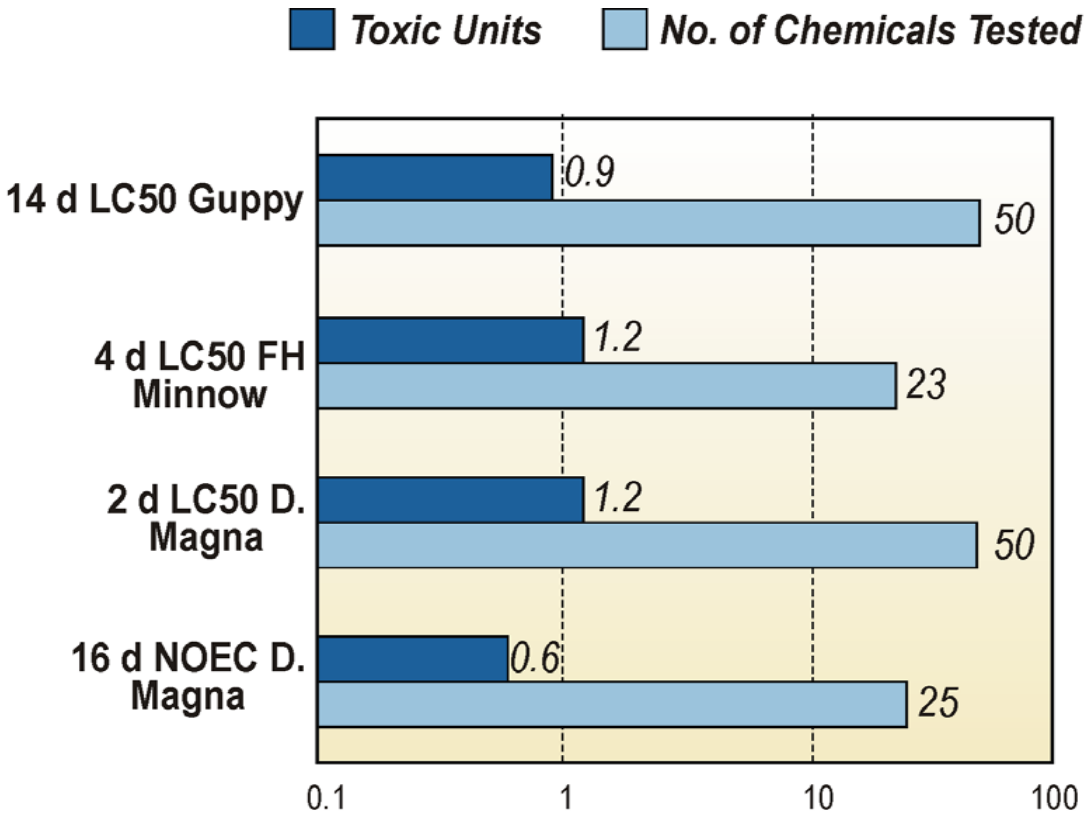


Body Burdens



Di Toro, D. M., McGrath, J. A., & Hansen, D. J. (2000).
Technical basis for narcotic chemicals and polycyclic aromatic hydrocarbon criteria. I. Water and tissue.
Environ.Toxicol.Chem., 19, 1951-1970.

Toxicity of Narcotic Mixtures is Additive

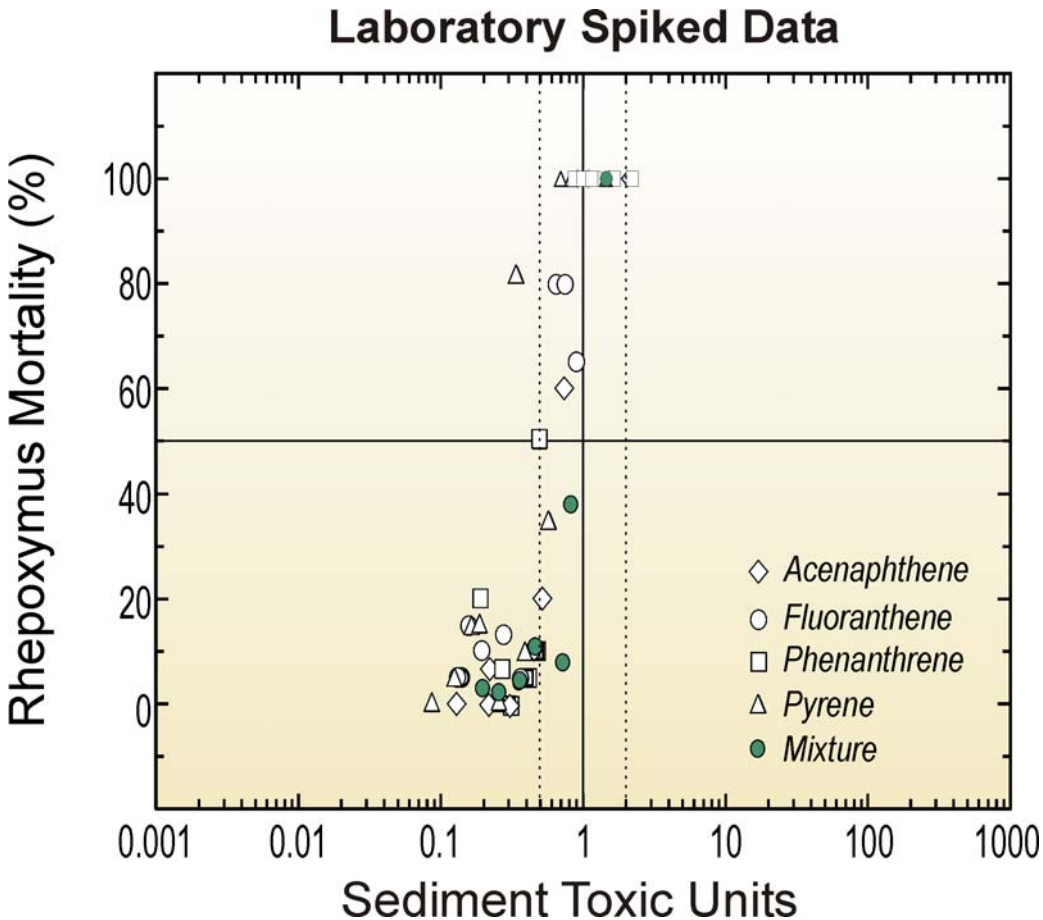


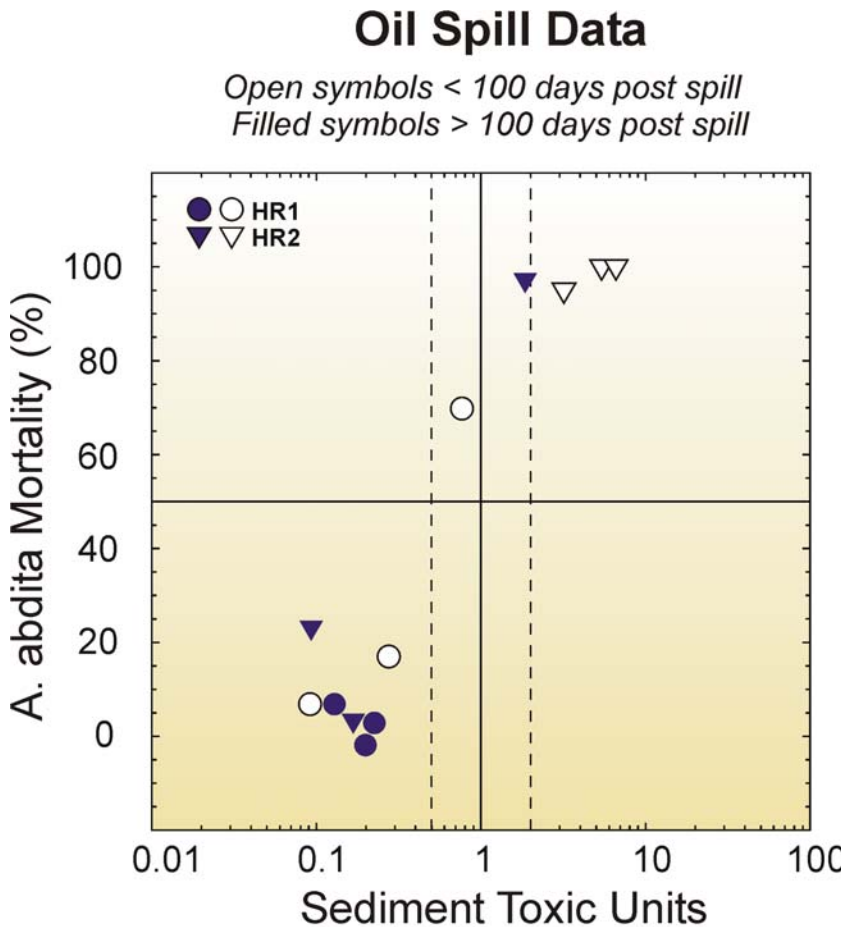
$$TU = \text{Measured Concentration} / \text{LC50 Concentration}$$

$$TU_{mixture} = \Sigma\, TU$$

Hermens, J. L. M. (1989). Quantitative structure-activity relationships of environmental pollutants. In O. Hutzinger (Eds.), Handbook of Environmental Chemistry. Vol. 2E. Reactions and Processes (pp. 111-162). Berlin: Springer Verlag.

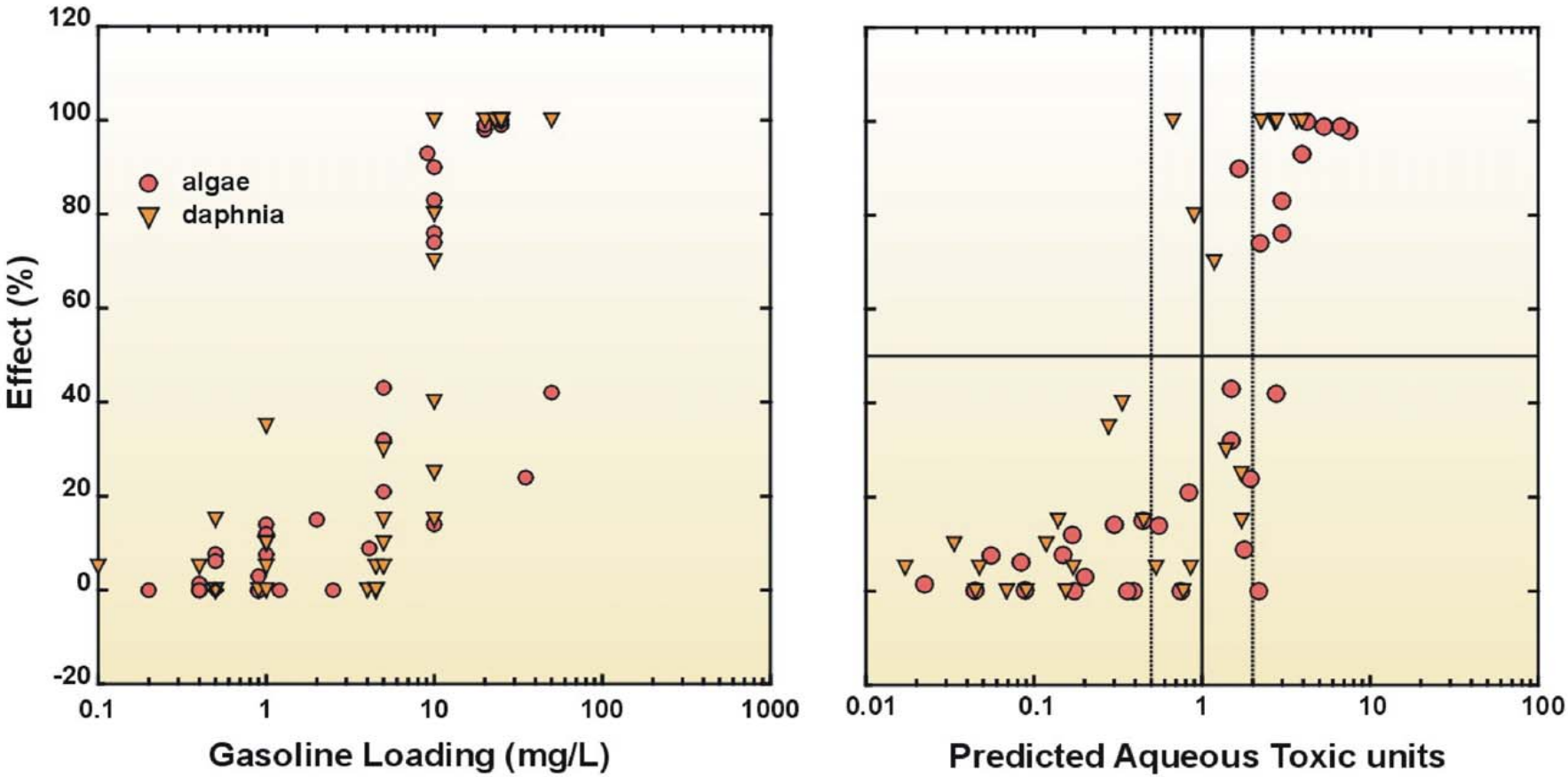
Predicted Sediment Toxicity for Single PAHs and PAH Mixtures Narcosis Target Lipid Model





(Ho et al., Marine Pollution Bulletin 1999)

Toxicity of Gasoline
Narcosis Target Lipid Model



McGrath, J., Parkerton, T., Hellweger, F., & Di Toro, D. (2005).
Validation of the narcosis target lipid model for petroleum products: Gasoline as a case study.
Environ. Toxicol. Chem., 24(9), 2382-2394.