

Modern Water and Sediment Quality Criteria: Toxicological and Chemical Interactions

Dominic M. Di Toro

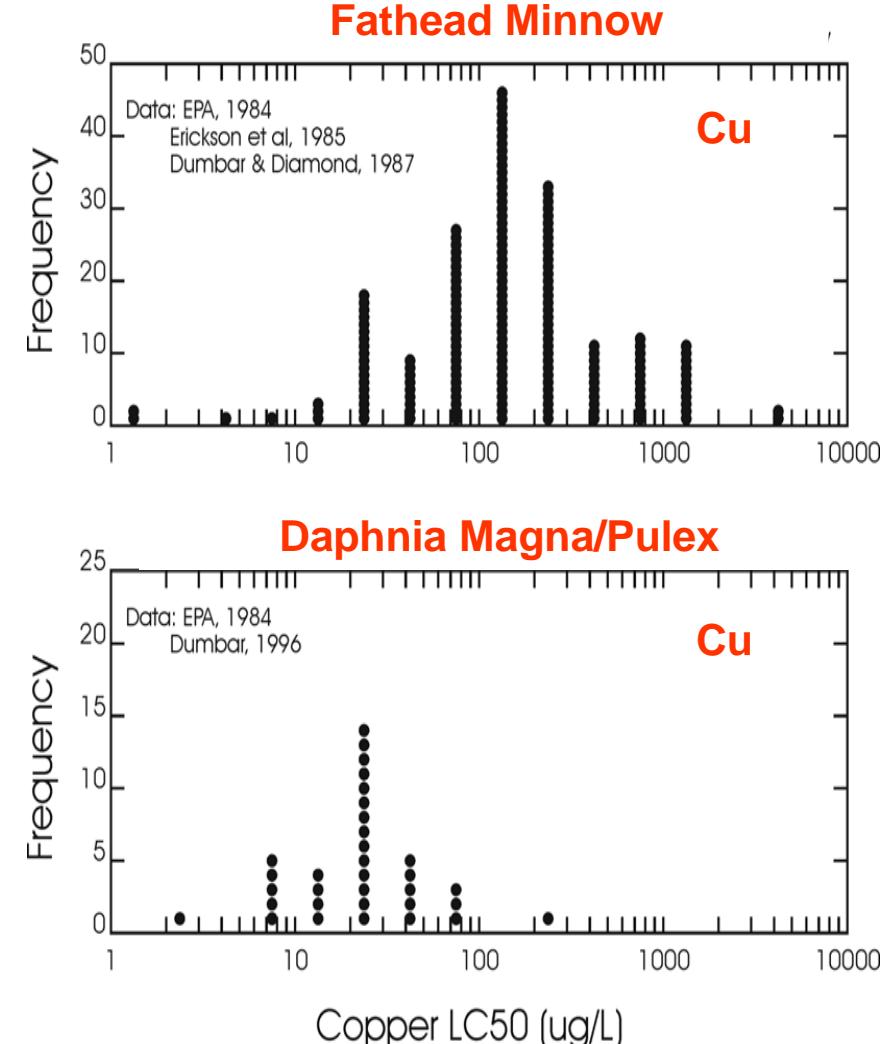
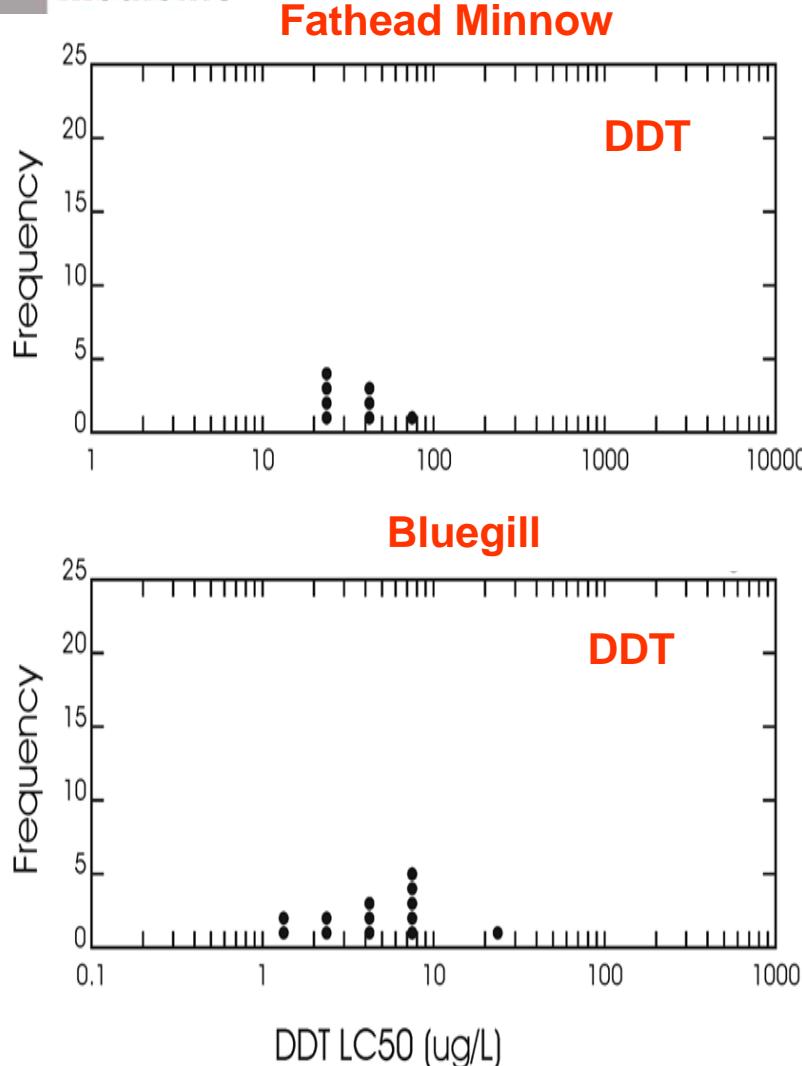
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University of Delaware
Newark, DE

NYU Department of Environmental Medicine

Superfund Basic Research Program
National Institute of Environmental Health Science
Bioavailability Workshop
Newark NJ
November 9-10



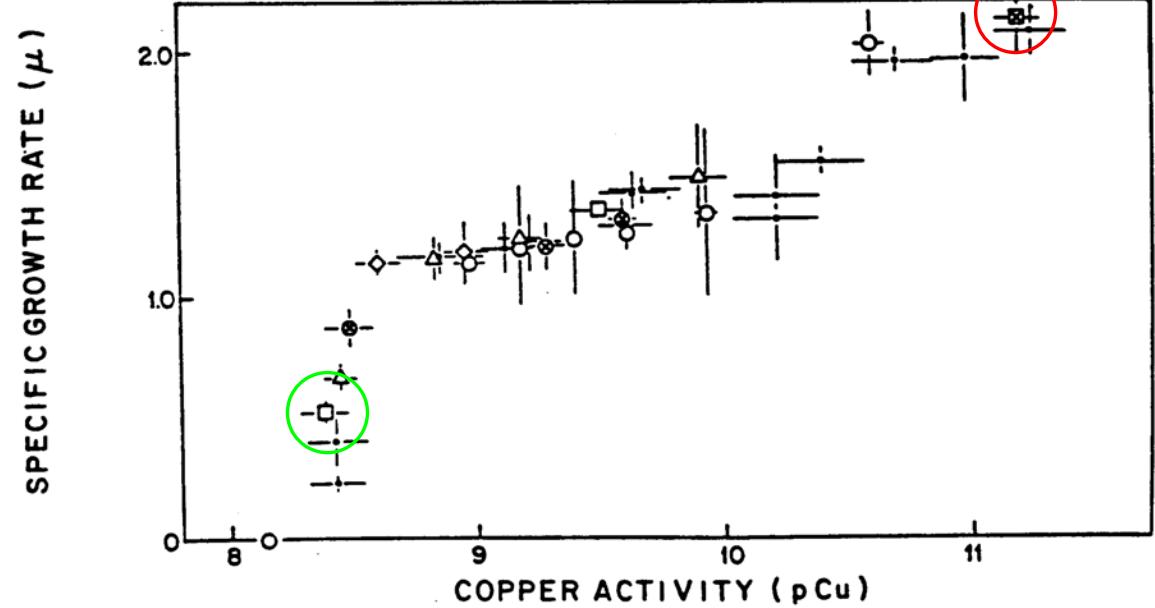
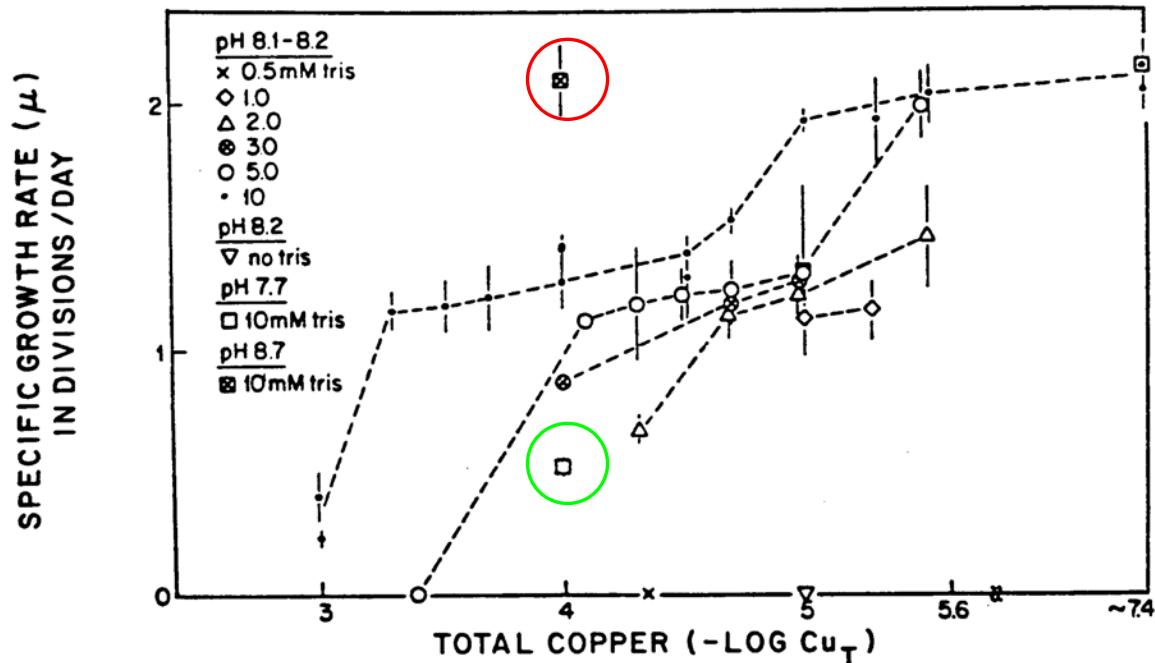
Variation in LC50 Same Organism and Chemical



Free Ion Activity Activity Model

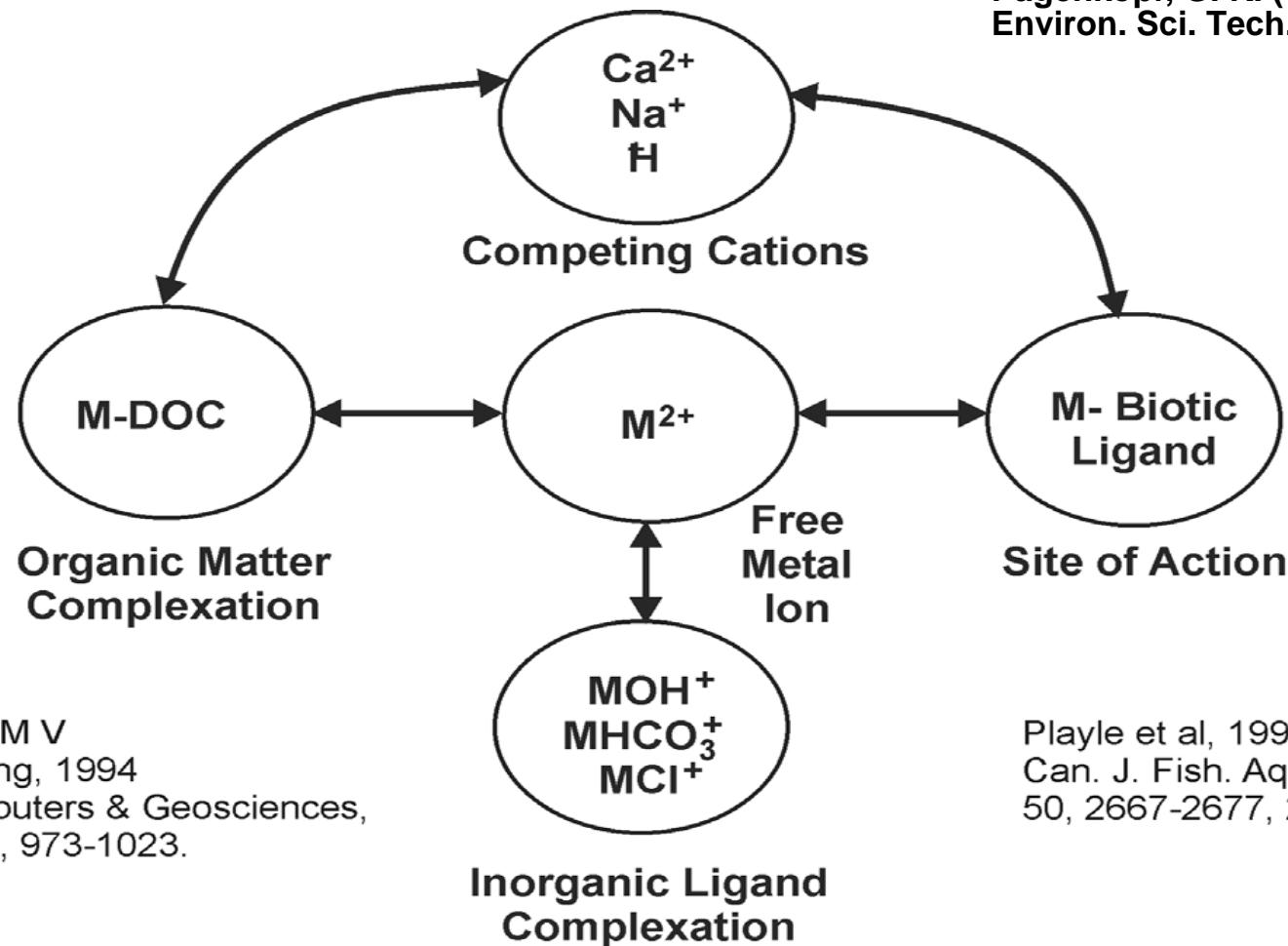
FIAM

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



Biotic Ligand Model

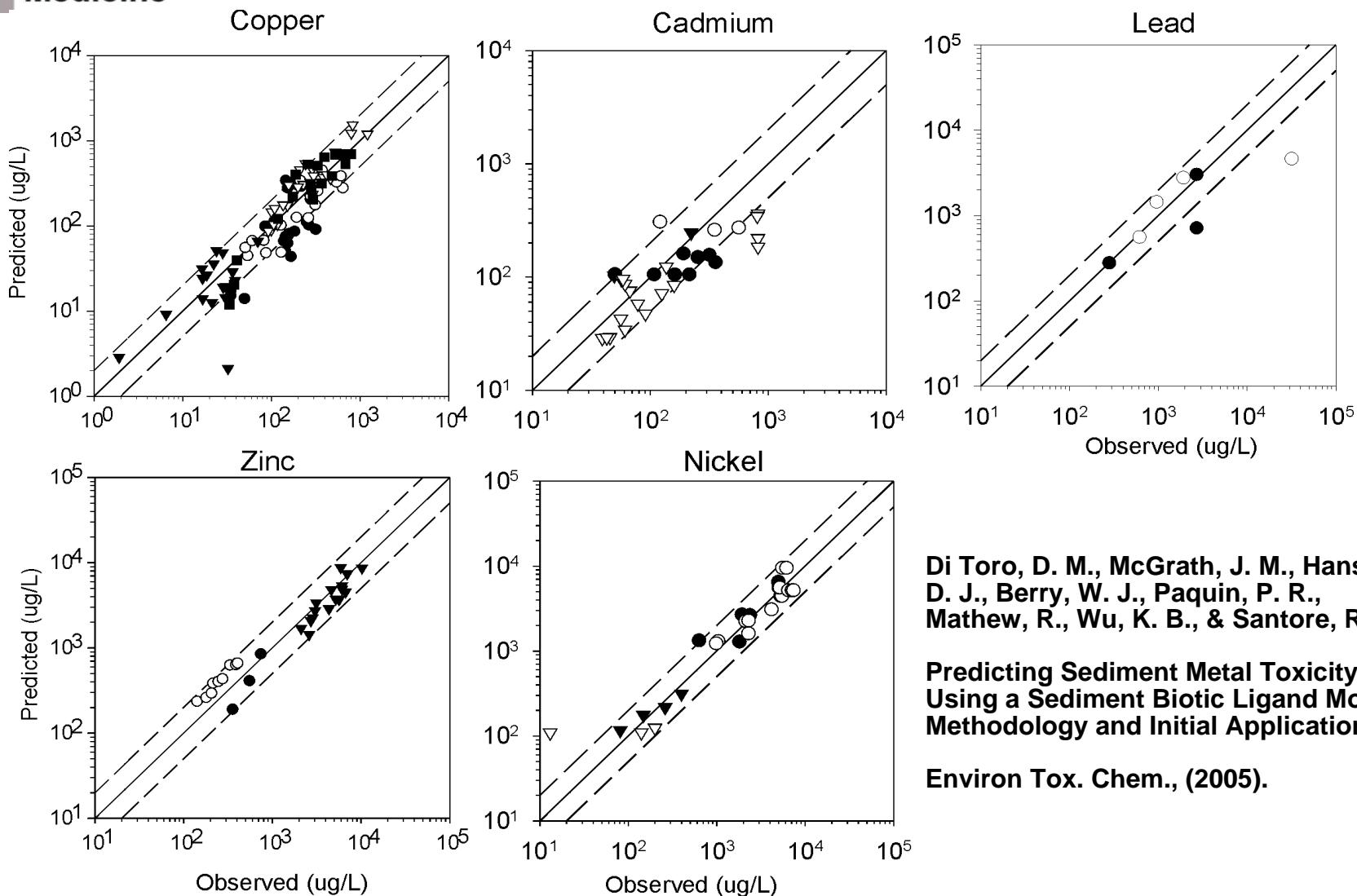
Pagenkopf, G. K. (1983).
Environ. Sci. Tech., 17, 342



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

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

Daphnia Magna BLM LC50 Concentrations

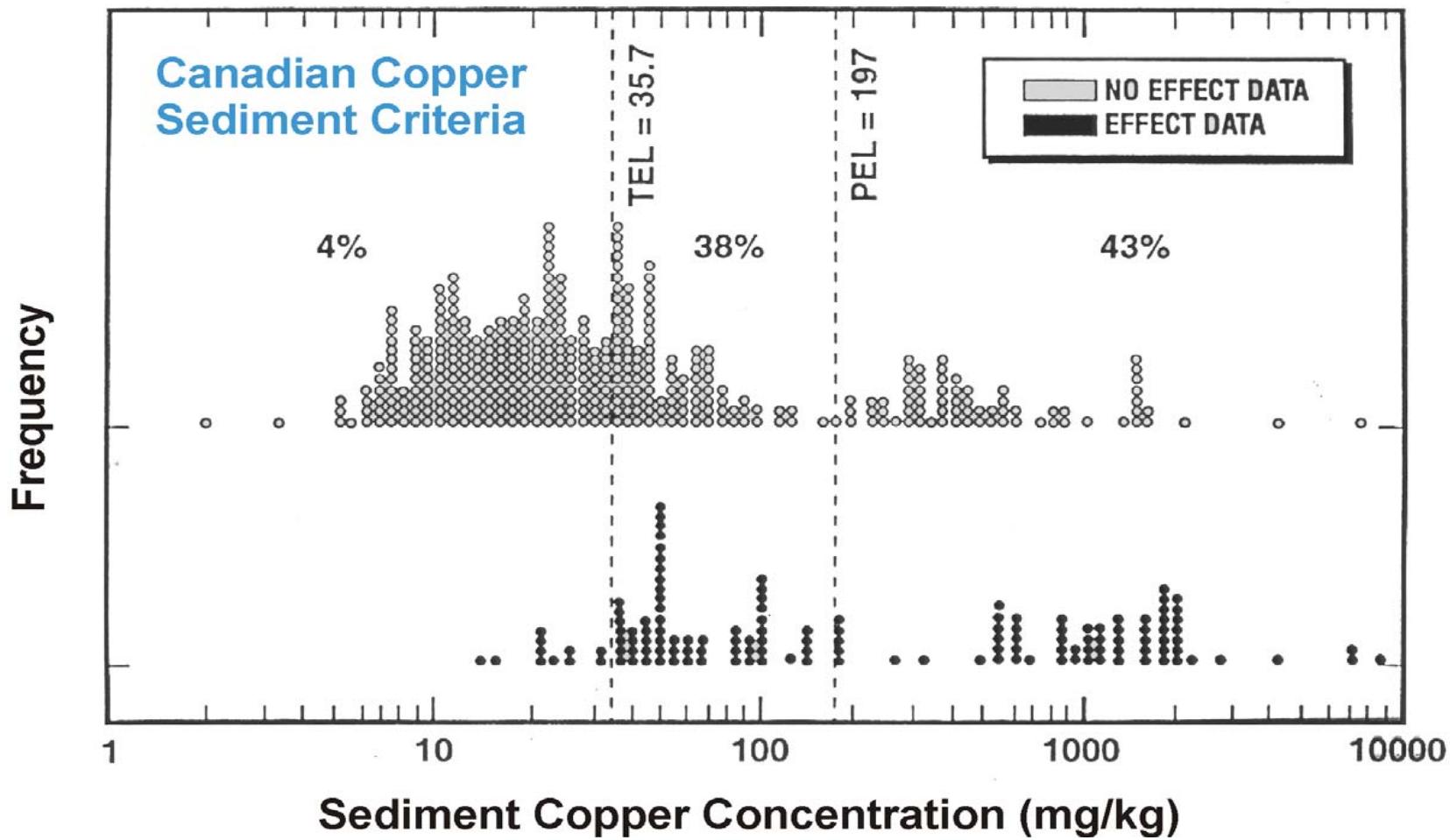


Di Toro, D. M., McGrath, J. M., Hansen, D. J., Berry, W. J., Paquin, P. R., Mathew, R., Wu, K. B., & Santore, R. C.

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

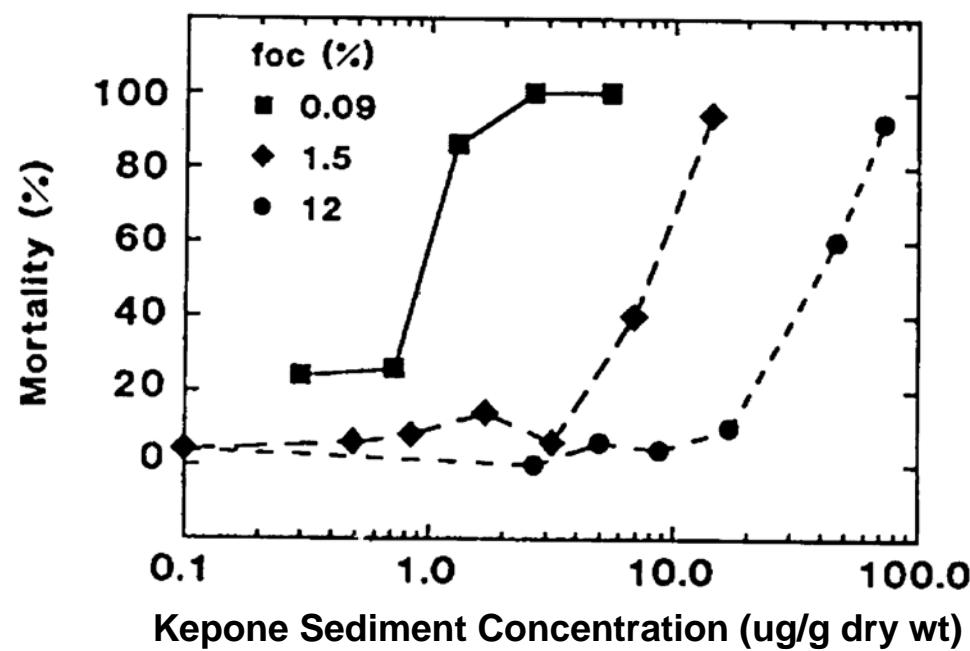
Environ Tox. Chem., (2005).

Bioavailability - Sediment

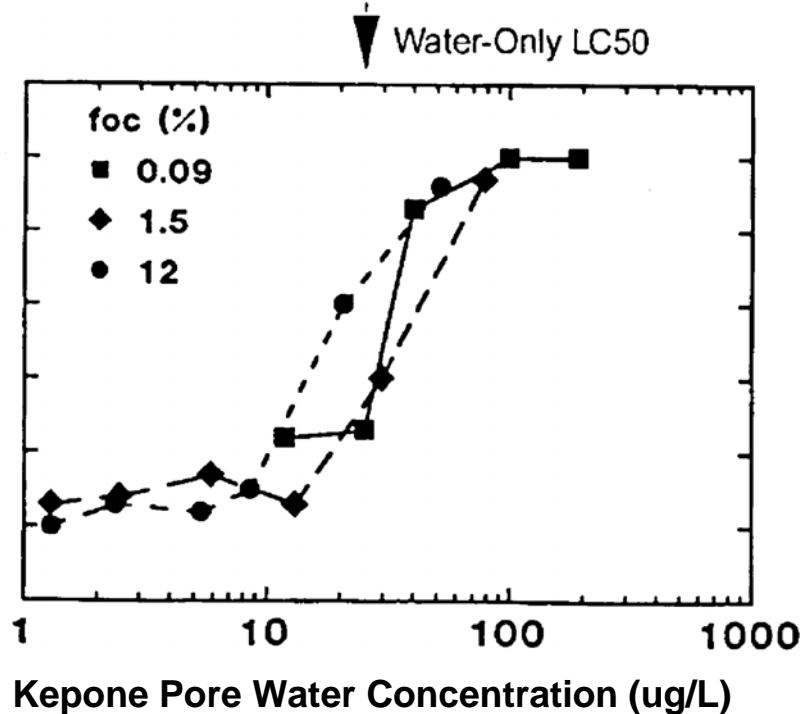


Pore water Concentration Predicts Sediment Toxicity

Dry Weight Normalization



Pore Water Normalization

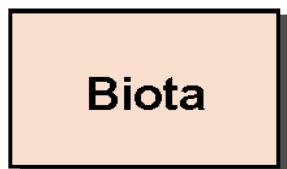


Adams, W. J., Kimerle, R. A., & Mosher, R. G. (1985). In R. D. Cardwell, R. Purdy, & R. C. Bahner (Eds.), Aquatic Toxicology and Hazard Assessment: Seventh Symposium. STP 854 (pp. 429-453). Am. Soc. for Testing and Materials.

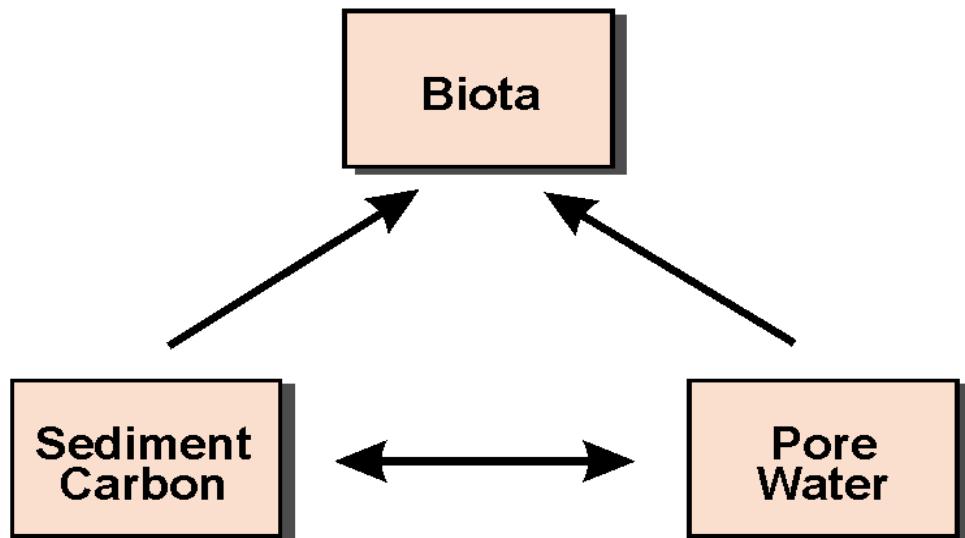
Di Toro, D. M., C. S. Zarba, D. J. Hansen, W. J. Berry, R. C. Swartz, C. E. Cowan, S. P. Pavlou, H. E. Allen, N. A. Thomas, P. R. Paquin. (1991). *Environ. Toxicol. Chem.* 11(12): 1541-1583.

Equilibrium Partitioning Model of Sediment Toxicity

**Water Only
Exposure**



**Sediment - Pore Water
Exposure**

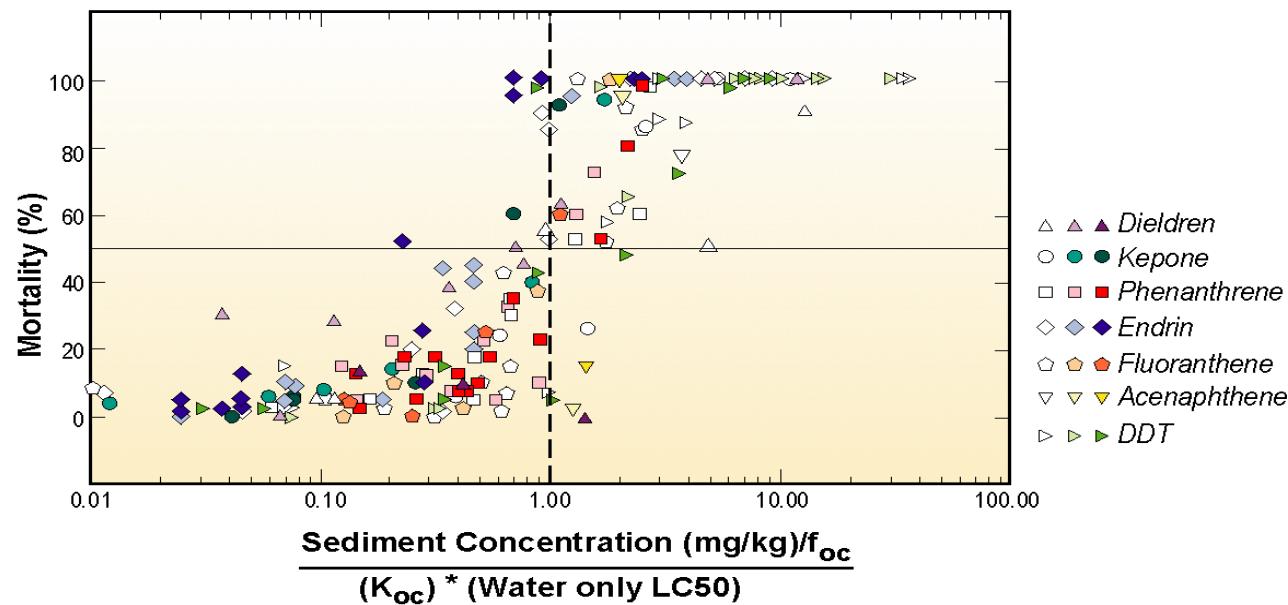
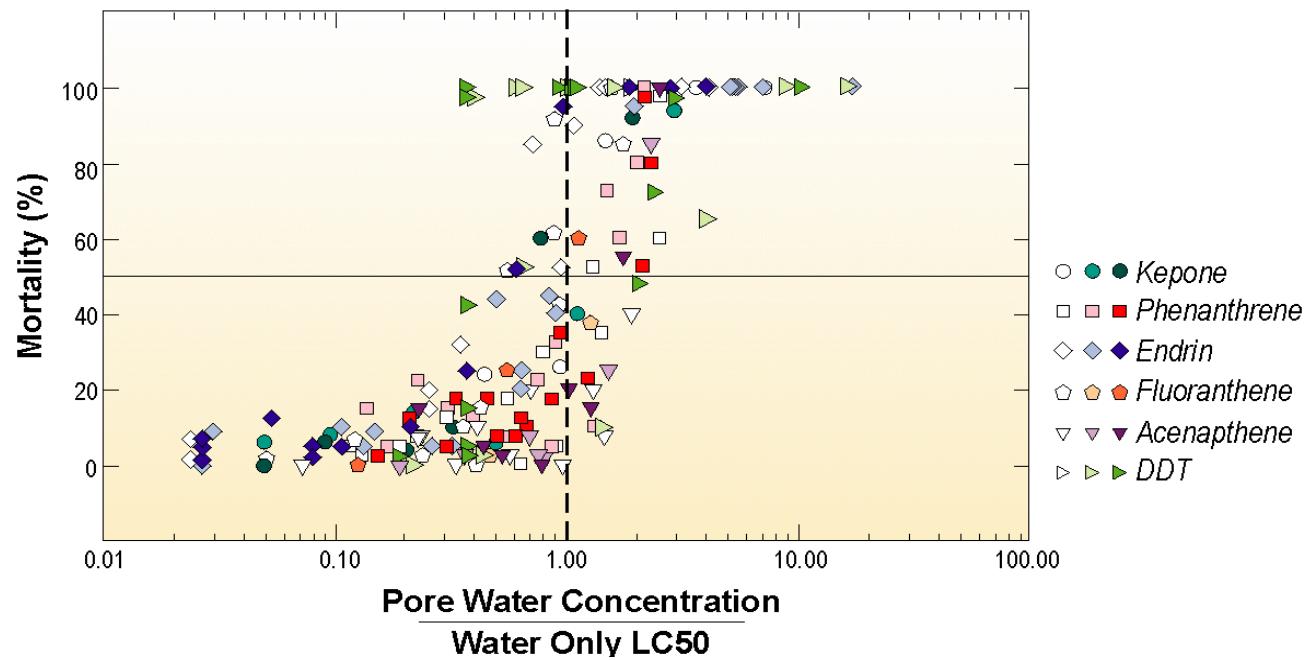


Equilibrium Partitioning

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.

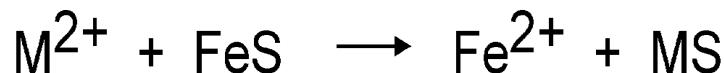
Sediment Toxicity Prediction

Pore Water
Organic Carbon
Normalized



SEM – AVS Model of Metal Bioavailability

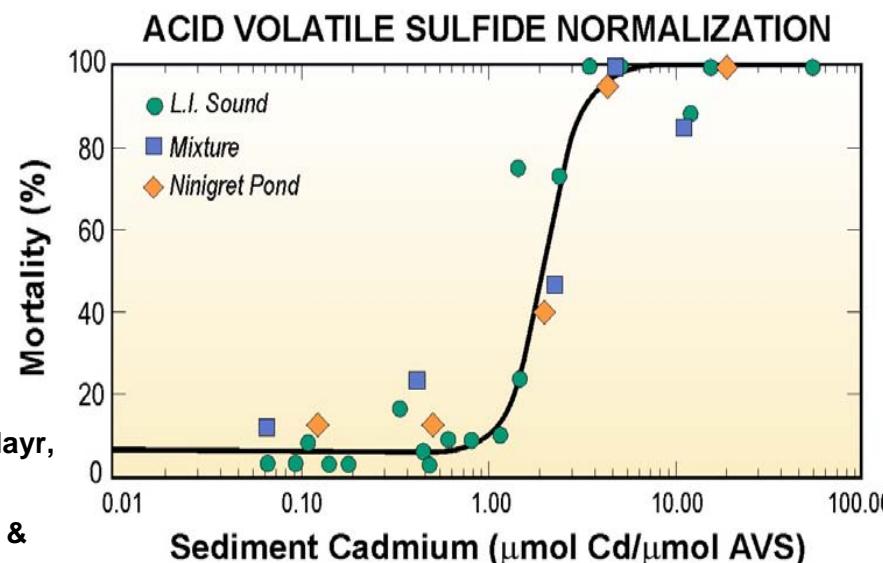
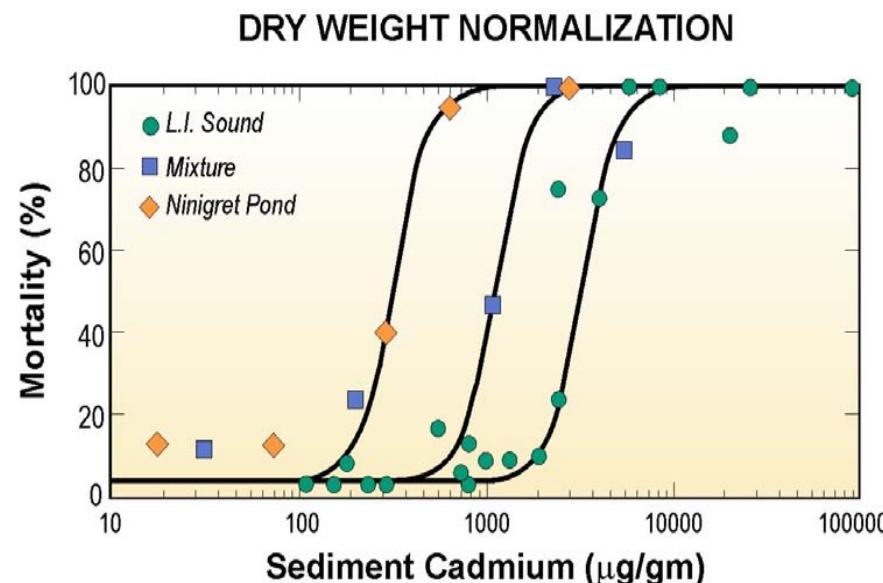
Metals are precipitated by reacting with iron monosulfide (AVS)



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

AVS > SEM No toxicity possible

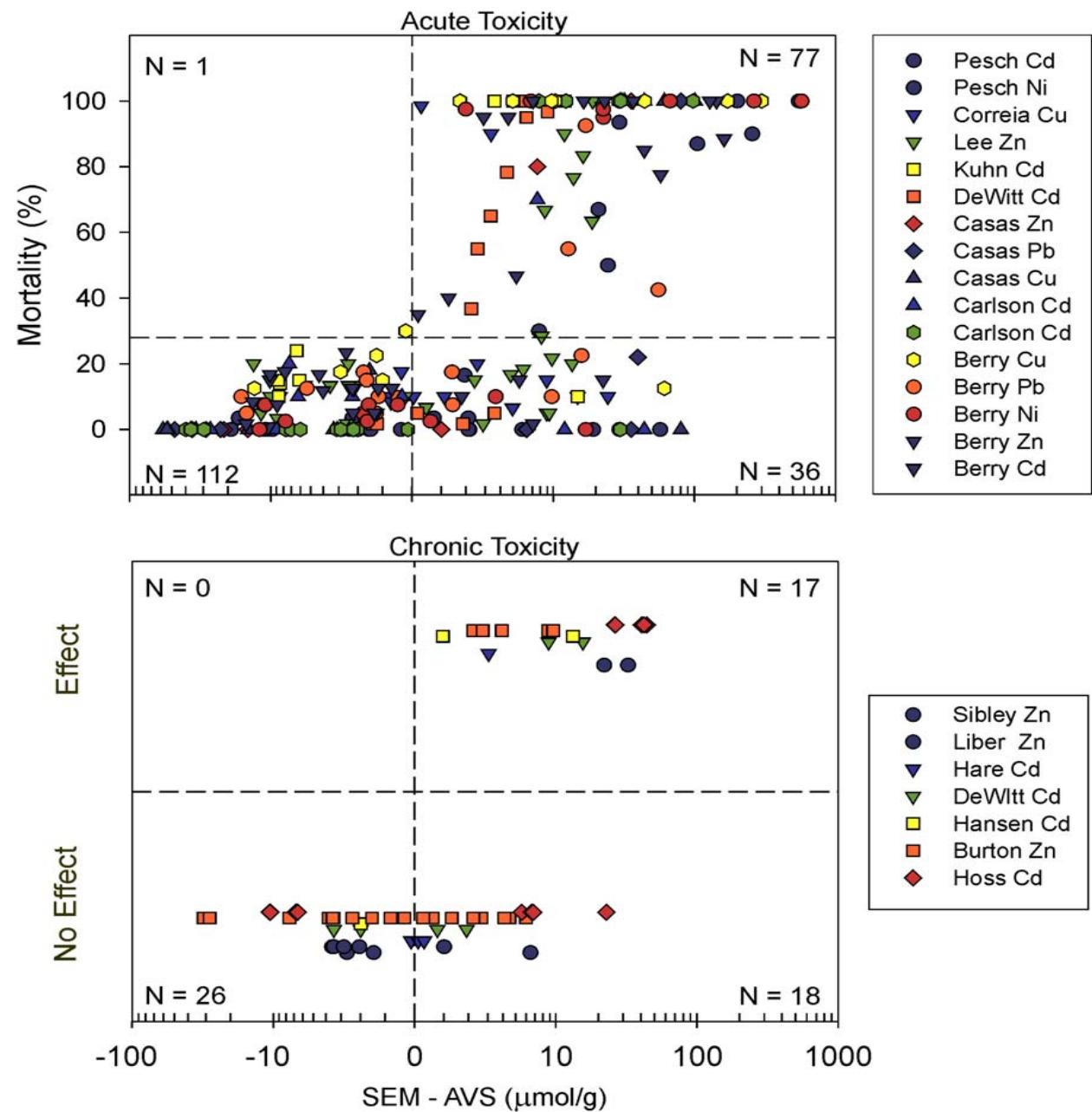
AVS < SEM Toxicity possible



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

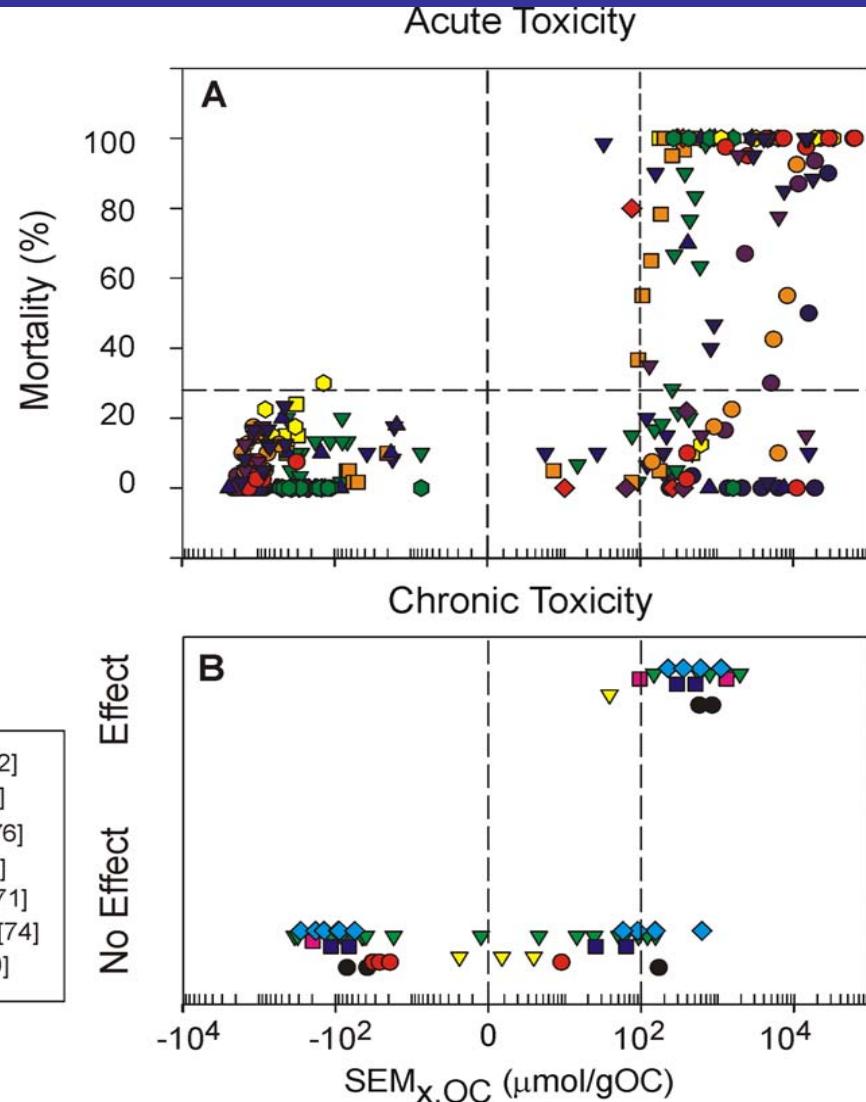
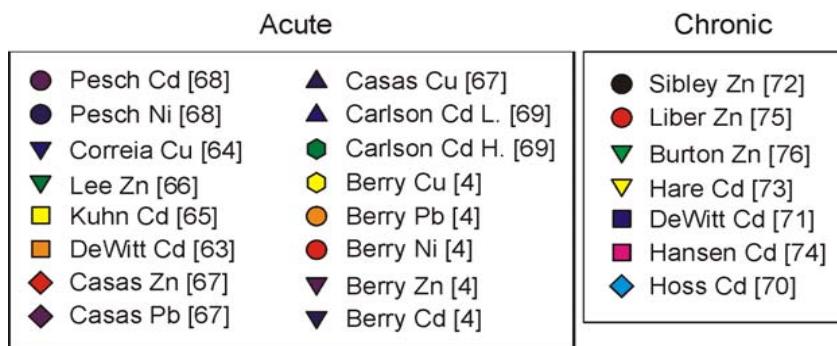


Predicting Sediment Metal Toxicity

Organic Carbon Normalized
Excess SEM

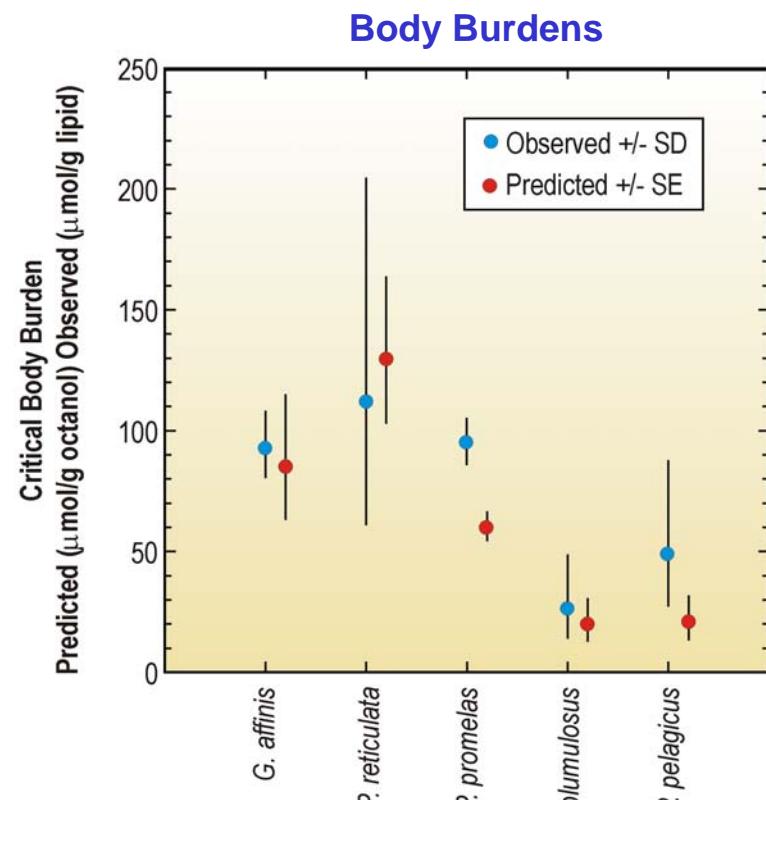
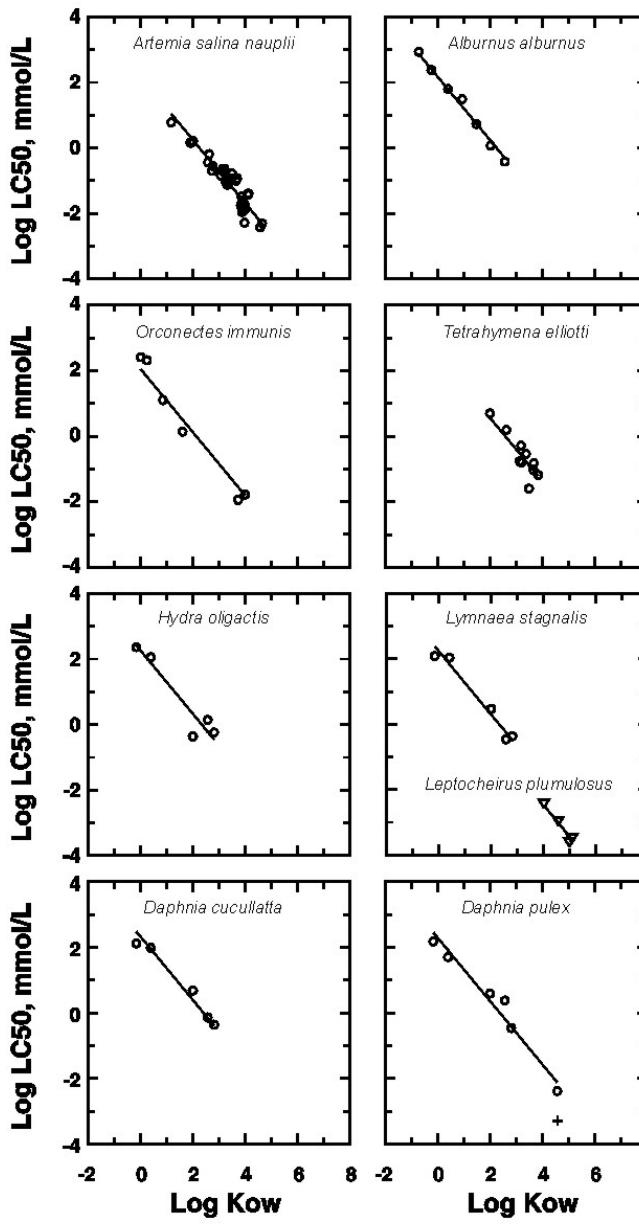
$$SEM_{x,OC} = (SEM - AVS)/f_{OC}$$

Observed Toxicity Boundary
 $SEM_{x,OC} = 100 \mu\text{mol/gOC}$



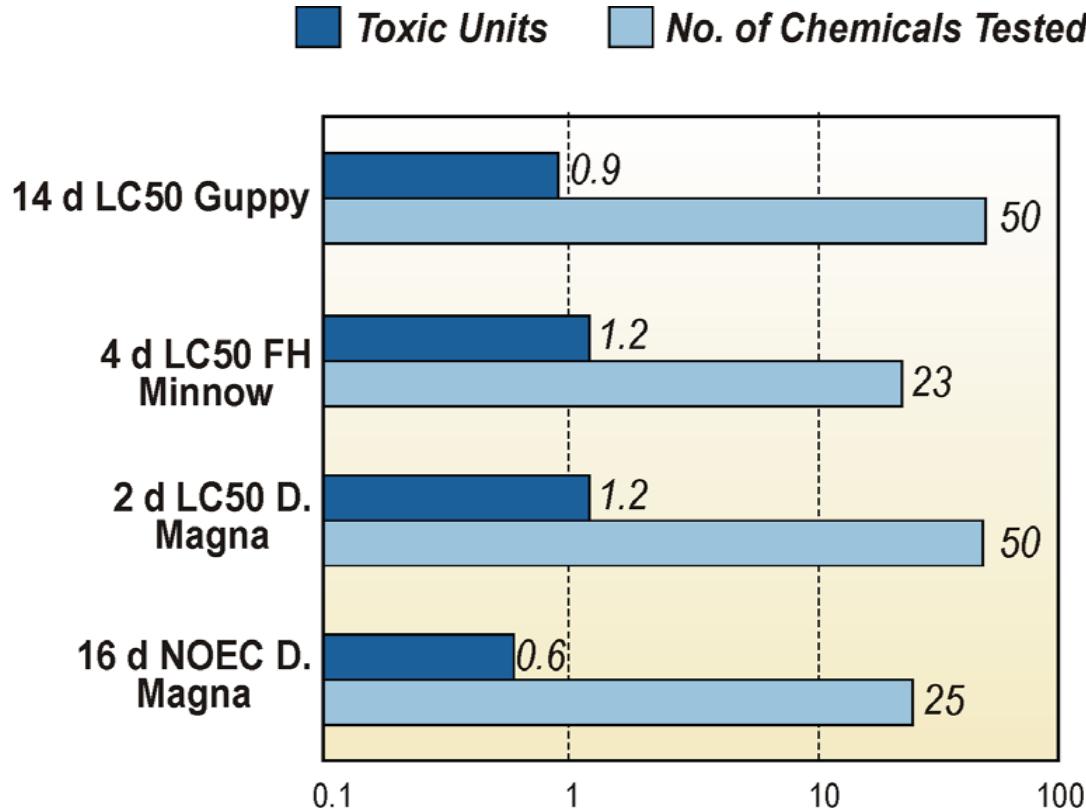
Narcosis Target Lipid Model

LC50s for Various Species



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



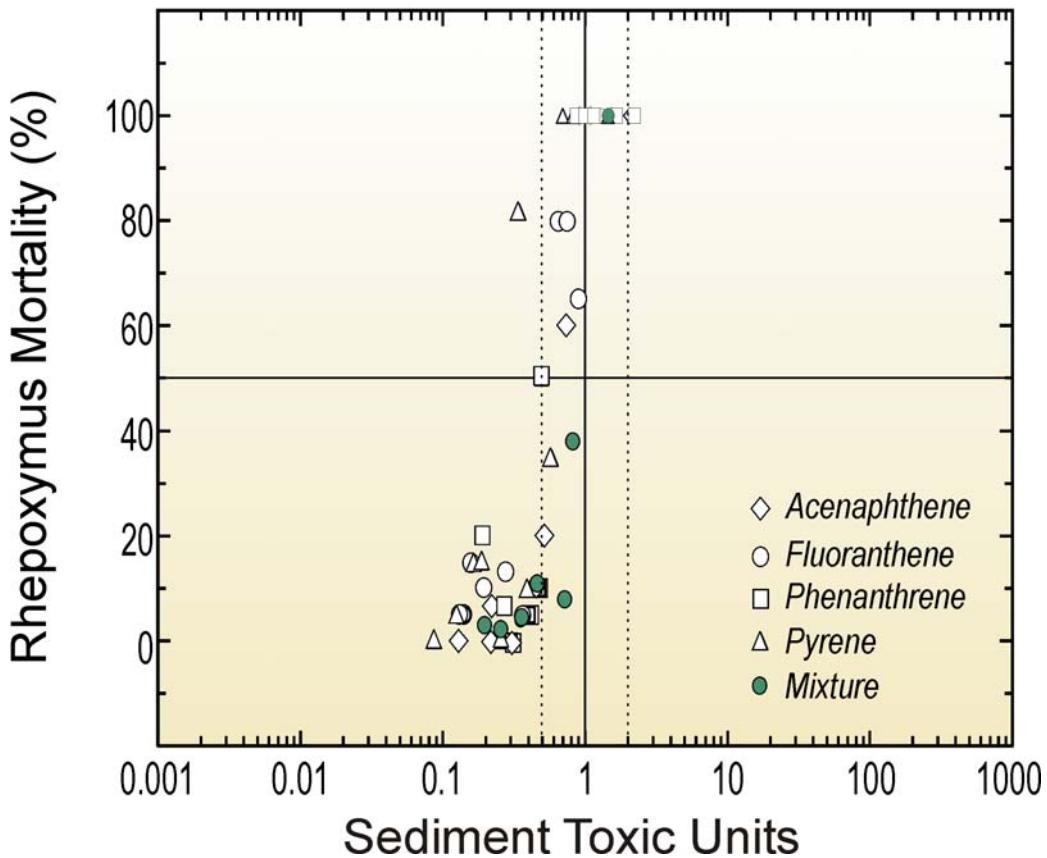
TU = Measured Concentration / LC50 Concentration

$$TU_{mixture} = \sum TU$$

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.

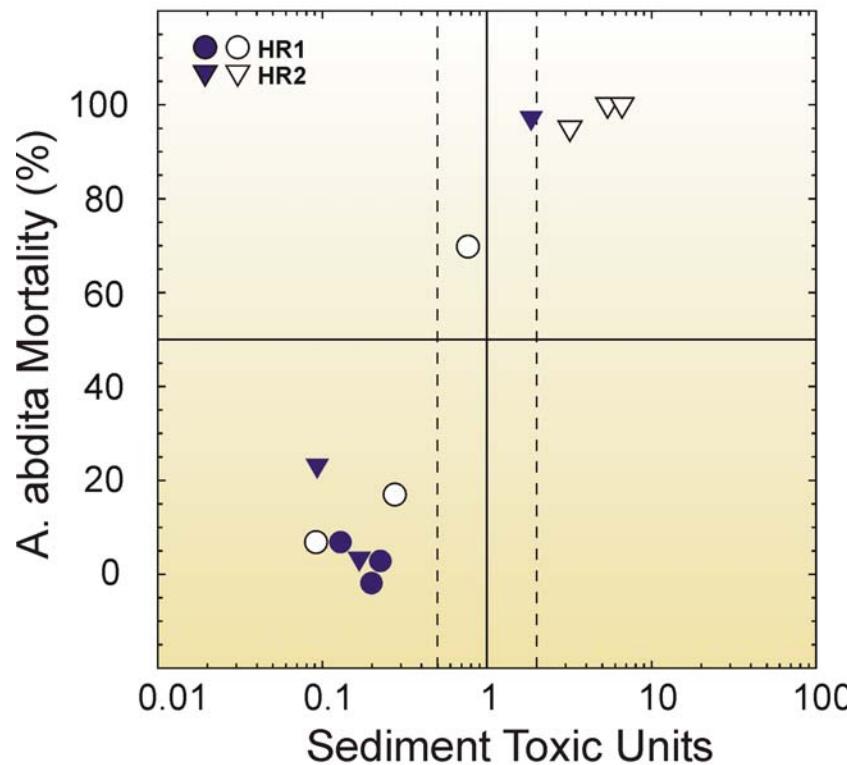
Predicted Sediment Toxicity for Single PAHs and PAH Mixtures Narcosis Target Lipid Model

Laboratory Spiked Data



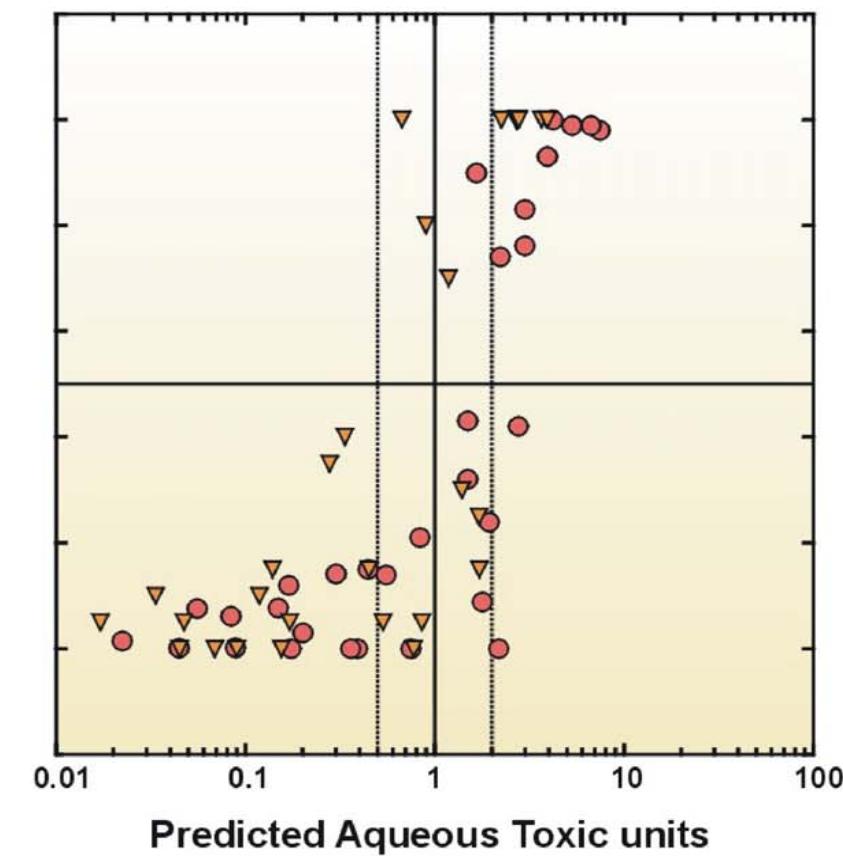
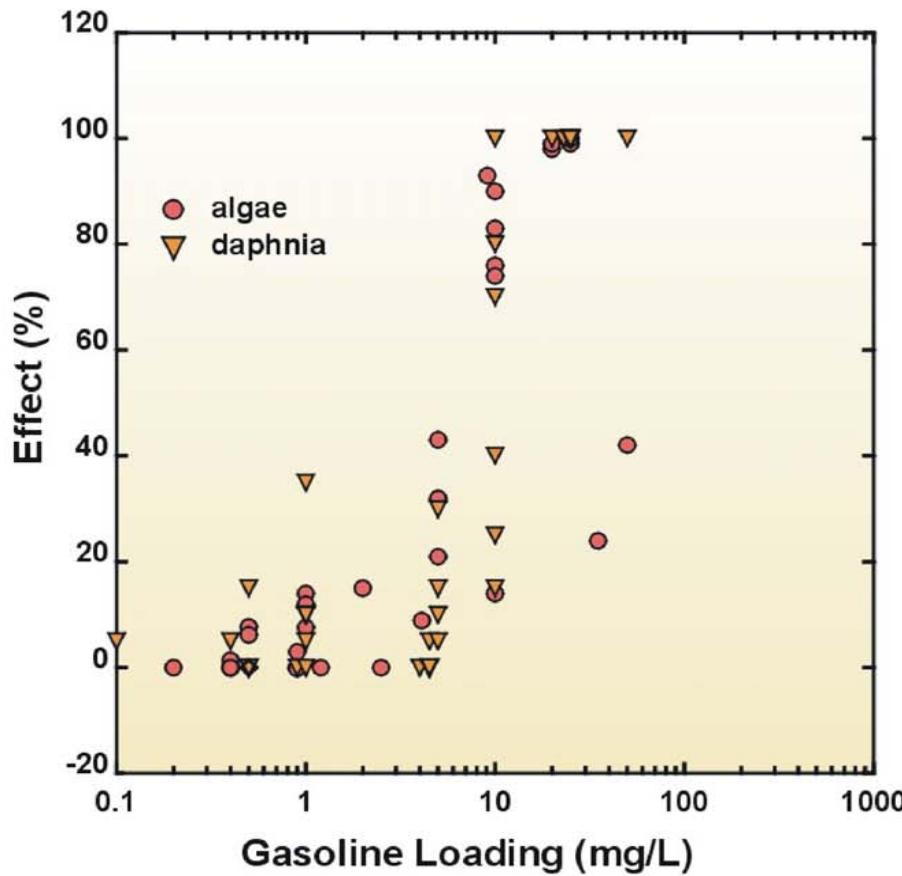
Oil Spill Data

Open symbols < 100 days post spill
Filled symbols > 100 days post spill



(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.