

Frontiers of Chemical Bioaccumulation Modeling with Fish

A seminar presented by Dr. John W. Nichols to students and faculty at the University of
Minnesota, Duluth
March 27, 2105

Predictive models for chemical accumulation in fish have been provided by numerous authors. Historically, these models were developed to describe the accumulation of neutral hydrophobic compounds which undergo little or no biotransformation. In such cases, accumulation can be predicted with acceptable accuracy using a simple lipid partitioning paradigm. More recently, modelers have begun to address chemicals that exhibit more “complex” behaviors. This presentation will describe two such efforts. The first addresses the issue of biotransformation, and involves the development of in vitro-to-in vivo extrapolation procedures which can be used to predict in vivo rates of metabolism from measured levels of in vitro activity. The second involves compounds that ionize at environmental pH values, including a number of pharmaceuticals. Accurate predictions for these compounds require the use of a model that accounts for acidification of the gill surface caused by elimination of metabolically-derived acid.