THE NEED AND REQUIREMENTS FOR QUANTITATIVE STRUCTURE-ACTIVITY RELATIONS (QSAR) IN THE GREAT LAKES WATER QUALITY PROGRAM

Douglas J. Hallett

Ontario Region
Environment Canada
55 St. Clair Avenue West
Toronto, Ontario M4T 1M2
CANADA

INTRODUCTION

Under Annex 12 (Persistent Toxic Substances) of the Great Lakes Water Quality Agreement of 1978 between the United States and Canada, Section 5: Early Warning System, a) "Development and use of structure-activity correlations to predict environmental characteristics of chemicals", is a clearly defined requirement. The need for Quantitative Structure-Activity Relations (QSARs) and the complexity of the environmental chemical matrix present in the Great Lakes was well described by Dr. G. Veith of the U.S. Environmental Protection Agency to the Great Lakes community in a presentation at the annual meeting on Great Lakes Water Quality of the International Joint Commission in Windsor in July 1977.

Scientists in the Great Lakes area are developing tests to predict the toxicity of a compound based on the relationship of the toxicity of known compounds and their structures. Caution should be exercised in the reliability of these predictive tests since many of the compounds that are used today and occur as environmental contaminants had some lesser form of test applied to them that indicated they should not be harmful to the environment. There is therefore a great responsibility in developing these tests to ensure that they are
accurate, predictive and that there is no danger that a chemical that appears environmentally sound is not oversold before it has been thoroughly tested. This cautious approach should not overshadow the need for developing faster and more accurate tests with which to establish QSARs. There are many compounds already present in the Great Lakes which require testing for toxic potential.

A framework for toxic chemicals management was first set out by the senior management committee of DOE. This scheme has also been adopted by the International Joint Commission (IJC) as shown in SCHEME 1 (First Report of the IJC Toxic Substances Committee 1980). The scheme involves the development of a hazard and risk assessment from an information base, control actions, and the evaluation of the effectiveness of that action. QSAR fits in at the information base, where there is the greatest expenditure of time, expertise and money. QSAR is one means of expediting the process of screening compounds which have potentially hazardous characteristics.

Herring gulls (Larus argentatus) and coho salmon (Oncorhynchus kisutch), both of which feed on alewives (Alosa pseudoharengus) and rainbow smelt (Osmerus mordax), provide an example of the ecosystem foodweb and bioaccumulation of toxic chemicals within Lake Ontario. TABLE 1 gives the concentrations of PCB's and other contaminants found in Lake Ontario herring gull eggs and coho salmon, and in alewives and smelt removed from their guts (Norstrom et al. 1978). PCB concentrations were a factor of approximately 20 lower in coho salmon and lower still in alewives and smelt when compared to concentrations found in herring gulls. It can be concluded that their common food source, alewives and smelt, are also the source of these contaminants for both coho salmon and herring gulls.

The results of studies on PCB concentrations in herring gulls (Struger et al. 1983), lake trout, rainbow smelt (GLWQB 1981; Whittle and Fitzsimons 1983) and spottail shiners (Ontario Ministry of the Environment, unpublished data, 1981) of Lake Ontario are summarized in FIGURE 1. Although an initial decline in PCB levels between 1974 and 1979 has been found, since that time, there has been a consistent increasing trend of PCB's in this ecosystem. Municipal and industrial effluents cannot account for the total loading to Lake Ontario. The major sources also include atmospheric deposition and contaminated groundwater in the Lake Ontario basin.