

Chapter 18

Computational Tools and Techniques to Predict Aquatic Toxicity of Some Halogenated Pollutants

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ABSTRACT

Halogenated organic compounds are usually xenobiotic in nature and used as ingredients for the synthesis of pesticides, solvents, surfactants, and plastics. However, their introduction to the aquatic ecosystems resulted in ecological danger due to their toxic effects. The usual method of toxicity assessment is by performing the experimental approach by considering some model organism. In this aspect the computational techniques such as QSAR (quantitative structure activity relationship) is considered an effective method. By computing several molecular features and the experimental activity, the toxic effect of a compound can be correlated. This chapter describes the aquatic toxicity of the compounds. The information about different computational resources (databases, tools, and modeling tools) have been given. Also, the application of QSAR to predict aquatic toxicity of different halogenated compounds available in the literature has been reviewed.

INTRODUCTION

From the industry and agriculture sector, huge amount of halogenated organic compounds are produced (Gribble, 1994; Song *et al.*, 2000). Due to their continuous entry into the environment, the propensity for the accumulation of these compounds in the habitats represents a global threatening (Perocco *et al.*, 1983; Damstra, 2002; Dewan *et al.*, 2013). Due to their persistency, many of these compounds are banned. However due to their versatility, long history of formulation and use as major industrial chemicals; these have been detected in soil, sediments as well as in water ecosystems (Persistent, 2000). Another feature in case of the halogenated pollutants is their toxicity increases with an increasing number of halogen

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Table 1. Showing the example of halogenated substances causes aquatic toxicity

S. No.	Common Sources of Halogenated Compounds	Remark
1	Persistent Halogenated compounds	Persistent organic pollutants (POPs) include halogenated compounds as a major component. Important examples are polychlorinated biphenyls (PCBs), dioxins (e.g. TCDD), furans, and organochlorine insecticides.
2	Paper- and pulp-mill effluents	Since chlorinated compounds have disappeared from effluents, the major toxic compounds are natural compounds of trees, such as resin acids from coniferous trees and phenolics from deciduous trees
3	Endocrine-disrupting compounds	These include several types of compounds with various modes of action. Although several different types of hormonal pathways could be targeted, the term is most commonly used for compounds that disturb reproductive hormone cycles
4	Pesticides	Pesticides contain several different types of compounds, including herbicides, insecticides, and fungicides

atoms and number of aromatic rings present in the molecule (Nikinmaa, 2014). Aquatic organisms are frequently faced with periods of exposure to various environmental pollutants, often as the result of the release of chemicals from agricultural and/or industrial activities. Among them, paper and pulp mills were the major sources of halogenated compounds, especially chlorinated compounds because of chlorine bleaching (Walker & Peterson, 1994; Ali & Sreekrishnan, 2001). Different categories of halogenated compounds that are persistent and having ecotoxicological effects are polychlorinated biphenyls (PCBs), dioxins and many organochlorine insecticides (Table 1).

The ecotoxic information is gathered by the study about the effect of pollutant molecules on fish and other aquatic organisms. Most often these results are based on materials tested independently under laboratory conditions in field studies. Therefore, this information may not replicate the realistic measure. The reason is that several toxic substances often occur together in significant amounts in polluted water and are likely to interfere with their actions. For example, the interactions among the substances like dieldrin, DDT, and methoxychlor can cause adverse effects when these substances occur in combination rather than individual effect (Jana, 1994).

The basic application of these toxicity predictions is

1. To study the change the modification of water quality that may affect the aquatic taxa
2. To study genetic impact (mutagenic potential) of aquatic pollutants on aquatic organisms
3. Risk assessment of toxic compounds

Since the experimental methods are difficult to perform for toxicity prediction, as alternative methods, the computational techniques are used. This chapter will basically focus on the importance of computational analytical methods for the prediction analysis of aquatic toxicity of special focus to halogenated substances along with application and challenges exist. In addition to that, different computational tools databases associated with this type of study are to be highlighted by thorough literature survey.

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