QSAR GENERATED RANKING SYSTEM FOR ORGANOCHLORINE COMPOUNDS IN THE MARINE ENVIRONMENT

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ABSTRACT

The physical-chemical constants water solubility and vapour pressure in combination with data for acute toxicity towards aquatic organisms have been used as basis for the development of a model for preliminary hazard assessment. The results of such a ranking system for organochlorine compounds provide a helpful tool to predict potential damage to aquatic organisms.

INTRODUCTION

Chlorinated chemicals are a diverse group of substances which play an important economic role in the industrial production. About 35 million tons of chlorine are produced by the chemical industry annually; about 1/10 of this in Germany [1]. Organochlorine compounds find wide application as solvents, starting materials for the production of polymers, catalysts, propellent gases, pesticides, and are used as intermediates in a variety of chemical production processes. Although many of these compounds are used in closed systems, they are capable of entering the environment by a variety of routes; e.g. either directly as solid, liquid or gaseous end-products or they are disposed of as wastes. Furthermore, there is widespread concern that organochlorine compounds have a general potential for producing adverse effects in the environment. Special attention has to be paid on their tendency to enter surface waters and subsequently for bioaccumulation in the aquatic food-chain. Therefore, it is necessary to perform a risk assessment by ranking organochlorine compounds according to their potential to damage the marine environment [2]. By aid of QSARs [3] (Quantitative Structure Activity Relationships) a ranking system of potentially dangerous chlorinated pesticides towards the aquatic environment has been published [4]. We now present a second list of chlorinated chemicals that have been categorized accordingly.

METHODS

On the basis of chemical, physical, and biological data of a substance estimations of its fate in the environment can be made. For a preliminary hazard assessment on surface waters the most important basic data and information are the values for Henry's constant (H) and the lethal concentration values (LC_{50}) for aquatic organisms. Henry's constant is the ratio of a chemical's concentration in air to its concentration in water at equilibrium. The LC_{50} is the concentration of a chemi-

cal in water which causes the death of 50% of the organisms tested over a 96 hrs. period; so, a direct measure of the acute toxicity of a substance.

For the preliminary risk assessment presented in Table I, only experimental data have been used [5-13]. The Henry constant can be calculated as follows:

$$H = \frac{v_p \cdot MW}{S}$$

To get a suitable equation we formed the reciprocal product of H and LC_{50}:

$$F = \frac{1}{H \cdot \min\{LC_{50}\}} \quad (Pa^{-1})$$

v_p Vapour pressure (Pa) S Water solubility ($g \cdot m^{-3}$)
MW Molecular weight ($g \cdot mol^{-1}$) F Toxicity ranking factor (Pa^{-1})
$\min\{LC_{50}\}$ Lethal concentration (using the lowest value reported) ($mol \cdot m^{-3}$).

Thus, a high factor F indicates that the chemical considered has a high potential to damage the aquatic environment: small values of F indicate a little toxic potential.

RESULTS

From more than 600 organochlorine substances (compiled in ref. [2]) measured values for H (or vp and S, resp.) and LC_{50} have been available for only 47 chemicals. The classification of these compounds according to a decreasing hazardous potential towards the aquatic environment is shown in Table I.

DISCUSSION

It can be seen from Table I that based of an evaluation of potential exposure (chemical will preferably be found in the water phase = small value for H) and the effects of that exposure (acute toxicity = high values for LC_{50}) chlorinated aromatic compounds have the highest potential to damage the aquatic environment. Furthermore, the results show that the fully chlorinated compounds are not necessarily the most toxic substances. Within one family of compounds, e.g. the phenols, benzenes, ethanes, etc., the F-value decreases with decreasing number of chlorine substituents in the molecule.

A ranking system as shown above can be used for further risk assessment by combining these data with information on uses, production amounts, degradability, or persistence, respectively.

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Table I: Toxicity Ranking System for Organochlorine Compounds Based on H and LC_{50}

Substance	Toxicity Ranking Factor (F)	Substance	Toxicity Ranking Factor (F)
2,4,5-Trichlorophenoxyacetic acid	6,810,000	1-Chloro-4-nitrobenzene	0.86
2,3,7,8-Tetrachlorodibenzo-*p*-dioxin	4,700,000	1,1,2,2-Tetrachloroethane	0.46
Hexachlorocyclohexane	178,000	Hexachlorobenzene	0.29
4-Chloroaniline	21,700	1,1,2-Trichloroethane	0.24
p,p'-DDD	1,340	1,2,3,5-Tetrachlorobenzene	0.23
Pentachlorophenol	356	1,2,3-Trichlorobenzene	0.22
2,3,4,5-Tetrachlorophenol	331	Pentachloroethane	0.16
3-Chlorophenol	301	1,2,4-Trichlorobenzene	0.14
4-Chlorophenol	244	1,3-Dichlorobenzene	0.086
2,4,5-Trichlorophenol	235	1,3,5-Trichlorobenzene	0.0471
2,4,6-Trichlorophenol	223	Dibromochloromethane	0.037
2,4-Dichlorophenol	7.92	1,1,2,2,-Tetrachloroethene	0.014
Pentachlorobenzene	5.84	Tetrachloromethane	0.014
3-Chloroaniline	5.66	1,1-Dichloroethane	0.00712
1-Chloro-2-nitrobenzene	5.38	Hexachloroethane	0.00564
2,6-Dichlorobenzonitrile	5.22	1,4-Dichloro-2-nitrobenzene	0.00478
1,2,4,5-Tetrachlorobenzene	4.76	Benzylchloride	0.00466
1-Chloro-3-nitrobenzene	3.41	Trichloroethene	0.00462
Cyanogenchloride	2.26	1,2-Dichloroethane	0.0019
1,4-Dichlorobenzene	1.63	1,1,1-Trichloroethane	0.000964
1,2,3,4-Tetrachlorobenzene	1.53	Chloroform	0.0000373
Chlorobenzene	1.49	Chloromethane	0.00000437
2-Chlorophenol	1.22	1,1,1-Trichloro-2,2,2-trifluoroethane	0.000000625
1,2-Dichlorobenzene	0.96		