Chemosphere 81 (2010) 177–186

Contents lists available at ScienceDirect

Chemosphere

journal homepage: www.elsevier.com/locate/chemosphere

Aquatic multi-species acute toxicity of (chlorinated) anilines: Experimental versus predicted data

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ARTICLE INFO

Article history:
Received 19 April 2010
Received in revised form 8 June 2010
Accepted 20 June 2010
Available online 15 July 2010

Keywords:
Chlorinated anilines
Multi-species
ECOSAR
Escherichia coli growth inhibition
Species sensitivity distributions
Acute toxicity

ABSTRACT

Aquatic toxicity information is essential in environmental risk assessment to determine the potential hazards and risks of new and existing chemicals. Prediction and modelling techniques, such as quantitative structure activity relationships (QSAR) and species sensitivity distributions (SSDs), are applied to fill data gaps and to predict, assess and extrapolate the toxicity of chemicals. In this study, both techniques (i.e. the ECOSAR programme as QSAR tool and SSDs) were assessed for a set of polar narcotic structural analogues that differ in their degree of chloro-substitution (aniline, 4-chloroaniline, 3,5-dichloroaniline and 2,3,4-chloroaniline). The acute toxicity of these compounds was tested in one prokaryote species (*Escherichia coli*) and three eukaryote aquatic species (*Pseudokirchneriella subcapitata*, *Daphnia magna* and *Danio rerio*). Consequently, the experimental acute toxicity data were compared to the QSAR predictions made by the ECOSAR programme and compared to the species sensitivity modelling results. Large interspecies differences in sensitivity were observed (*D. magna* > *P. subcapitata* > *D. rerio* > *E. coli*). 4-Chloroaniline acted as an outlier in *P. subcapitata* toxicity. Whereas in *D. magna*, toxicity decreased rather than increased with increasing log K_{ow} of the test compounds. In general, large interchemical and interspecies differences in toxicity of these relatively simple chemical structures were observed. Moreover, this species variation could not entirely be characterized by the ECOSAR tool. SSD modelling is particularly focussed on species variations and emphasis is put on protecting those species that are most affected by chemical exposure. Compared to QSARs, SSDs offer broader perspectives regarding species sensitivity ranking, however, in this study they could only be applied for aniline and 4-chloroaniline.

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1. Introduction

Predictive and chemical-read across models are regarded as important and recommended tools in the reduction of animal use in ecotoxicological risk assessment. Consequently, regulatory agencies have invested considerable efforts in the development of general quantitative structure activity relationship (QSARs) models. An example of a QSAR tool that is widely used and freely available, is the ECOSAR (ECOlogical Structure Acivity Relationships) programme, a US EPA QSAR tool that predicts the toxic potency of a wide range of substances to aquatic organisms (Moore et al., 2003; Mayo-Bean et al., 2009). Not only QSARs but also other modelling methods, e.g. species sensitivity distributions (SSDs), are increasingly used to determine hazardous effects of chemicals in probabilistic ecological risk assessment procedures. In SSD modelling, all available (aquatic) toxicity data is used to predict a concentration below which only an acceptably small percentage of (aquatic) species, populations and habitats is affected. This approach is in contrast to the traditional quotient and assessment factor approaches that often only focus on single species acute toxicity data to extrapolate effects to multispecies ecosystems. This improved data usage in SSD modelling is assumed to introduce greater statistical confidence into risk assessment (Wheeler et al., 2002; Newman et al., 2000; Duboudin et al., 2004; Wang et al., 2008).

Aniline (phenylamine, aminobenzene) is an organic compound consisting of a phenyl group to which an amino group is coupled. Aniline and various chlorinated anilines are widely used in the production of polyurethanes, rubbers, cosmetic products, dyes and pesticides. These compounds are present in the environment at detectable levels and they are considered priority pollutants in environmental risk assessment (Abe et al., 2001; Boehncke et al., 2003).

According to the Verhaar classification scheme (Verhaar et al., 1992), they are categorized as polar narcotic compounds. The Verhaar scheme is a frequently used classification scheme which is implemented in the Toxtree software (ECB, 2009) and in the OECD QSAR application toolbox (OECD, 2008). In general, this scheme classifies chemicals based on their physico-chemical properties into one of the four main mode of action (MOA) classes: (1) narcotics, (2) polar narcotics, (3) reactive chemicals and (4) spe-

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0045-6535/$ - see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.chemosphere.2010.06.059

cifically acting reactive chemicals (Verhaar et al., 1992, 2000). The first two classes are described as inert baseline toxicity chemicals by which toxicity is evoked through non-specific mechanisms. The toxic potency of these chemicals correlates strongly with their hydrophobicity (log K_{ow}, the octanol/water partitioning coefficient) and is assumed to be easily predicted by the mathematical QSAR models. Polar narcotics are slightly more toxic than non-polar narcotic compounds due to the hydrogen bond acceptor capacity of these structures. The latter two classes are described as excess toxicity compounds which evoke toxicity through additional, specific mechanisms. The toxic potency of those chemicals cannot always be determined solely based on their hydrophobic properties and is therefore more difficult to predict (Verhaar et al., 2000; Moore et al., 2003; Öberg, 2004; Von der Ohe et al., 2005).

Structurally comparable chemicals with a non-specific MOA (i.e. narcotics and polar-narcotics) normally show relatively small interspecies toxicity differences. Moreover, the toxicity of these chemicals is in most cases easily predictable by their hydrophobicity (Vaal et al., 1997a). However, Vaal et al. (1997b) compared the toxicity of aniline to other Verhaar class 2 compounds among multiple species and illustrated that aniline showed an unexpectedly high level of interspecies toxicity variability. This large interspecies variability in species sensitivity suggests that anilines do not behave as typical Verhaar class 2 compounds. In fact, MOA class categorization of these simple structural analogues is apparently not that straightforward: different class categorization methods do not result in comparable classification results. Although the general Verhaar classification scheme categorizes the chlorinated anilines as polar narcotics, another more specific classification scheme, developed by Von der Ohe et al. (2005) and based on the usage of "structural alerts" for daphnia toxicity in particular, ranked some of the (chlorinated) anilines as excess toxicity compounds. Predicting the toxicity of substituted aniline(s) in different species solely based on their hydrophobicity is therefore likely to result in inaccurate estimates. Moreover, assessing the hazards and risks of these potential pollutants in populations and ecosystems becomes very challenging.

This study examines the relative sensitivity of four test species and the interspecies differences after exposure to four anilines which differ in their degree of chloro-substitution (aniline, 4-chloroaniline, 3,5-dichloroaniline and 2,3,4-trichloroaniline). One prokaryote species *Escherichia coli* and three eukaryote aquatic species representing different trophic levels (*Pseudokirchneriella subcapitata*, *Daphnia magna* and *Danio rerio*) were tested. The experimental toxicity data are compared to the toxicity calculations made by ECOSAR in order to assess the prediction accuracy of the ECOSAR programme for chlorinated aniline toxicity. Since species sensitivity distributions are an appropriate method to describe variation in toxicity of compounds among a set of species, SSDs are constructed to assess the interspecies variation in (chlorinated) aniline toxicity and to evaluate the relative differences in experimental and ECOSAR predicted toxicity data.

2. Materials and methods

2.1. Chemicals

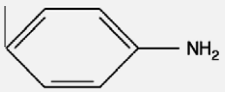
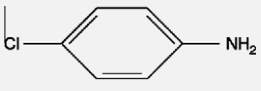
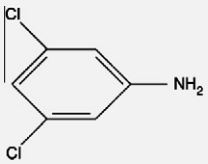
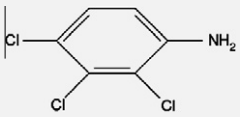
Four anilines (aniline, 4-chloroaniline, 3,5-dichloroaniline and 2,3,4-trichloroaniline) were selected for acute toxicity testing. Aniline (99%) and 4-chloroaniline (98%) were purchased from Sigma Aldrich (Bornem, Belgium). 3,5-Dichloroaniline (98%) and 2,3,4-trichloroaniline (>98%) were purchased from Acros (Geel, Belgium) and TCI Europe (Antwerp, Belgium) respectively. Table 1 displays the chemical structures and characteristics of the four test chemicals. A solvent was used when the water solubility threshold was reached. In *E. coli* and *P. subcapitata* exposures, methanol was used as the standard solvent whereas in *D. magna* and *D. rerio* exposures, ethanol was used. Whenever solvents were used, a solvent control was included in the experimental setup. The maximum acceptable limit of 0.05% solvent for acute toxicity testing (OECD, 2000) was never exceeded.

2.2. Acute toxicity testing in standardized aquatic test organisms

2.2.1. EC_{50} determination in P. subcapitata

P. subcapitata (formerly known as *Selenastrum capricornutum*) is a uni-cellular green freshwater algae (Chlorophyta; Chloropyceae;

Table 1
Overview of chemical characteristics, experimental toxicity data and ECOSAR prediction of the four test compounds. Log K_{ow} is predicted by KOWWIN implemented in the EPI Suite models of US EPA. 95% CI: 95% confidence interval; ChV: chronic toxicity value; ∗: calculated EC50 values using an acute-to-chronic ratio of 4 (Mayo-Bean et al., 2009).

	Aniline	4-Chloroaniline	3,5-Dichloroaniline	2,3,4-Trichloroaniline
Chemical characteristics				
Structure				
CAS number	62-53-3	106-47-8	626-43-7	634-67-3
Molecular weight	93.13	127.57	162.02	196.46
Log K_{ow}	1.08	1.72	2.37	3.01
Water solubility (mg L^{-1})	3593	1095	302	82
Experimental toxicity data				
Pseudokirchneriella subcapitata EC_{50} (72 h) (95% CI) (mg L^{-1})	87.9 (69.0–118)	2.91 (2.65–3.20)	14.5 (12.3–17.1)	4.77 (4.40–5.17)
Daphnia magna EC_{50} (48 h) (95% CI) (mg L^{-1})	0.160 (0.130–0.190)	0.221 (0.192–0.255)	0.600 (0.494–0.728)	2.55 (2.01–3.04)
Danio. rerio LC_{50} (96 h) (95% CI) (mg L^{-1})	116 (104–128)	35.5 (31.0–40.7)	9.38 (8.48–10.4)	4.74 (4.02–5.60)
Escherichia coli EC_{50} (90 min) (95% CI) (mg L^{-1})	2360 (1960–2850)	544 (429–689)	121 (104–140)	41.2 (31.1–54.7)
ECOSAR prediction (aromatic amines)				
Green algae (ChV) (mg L^{-1})	8.38	4.82	2.54	1.29
Green algae (acute toxicity value) (mg L^{-1})*	33.5	19.3	10.2	5.16
Daphnids EC_{50} (48 h) (mg L^{-1})	1.13	1.04	0.88	0.72
Fish EC_{50} (96 h) (mg L^{-1})	134	61.8	26.0	10.6

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