Environmental risk assessment of selected organic chemicals based on TOC test and QSAR estimation models

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ABSTRACT

Environmental risks of organic chemicals have been greatly determined by their persistence, bioaccumulation, and toxicity (PBT) and physicochemical properties. Major regulations in different countries and regions identify chemicals according to their bioconcentration factor (BCF) and octanol–water partition coefficient (K_{ow}), which frequently displays a substantial correlation with the sediment sorption coefficient (K_{oc}). Half-life or degradability is crucial for the persistence evaluation of chemicals. Quantitative structure activity relationship (QSAR) estimation models are indispensable for predicting environmental fate and health effects in the absence of field- or laboratory-based data. In this study, 39 chemicals of high concern were chosen for half-life testing based on total organic carbon (TOC) degradation, and two widely accepted and highly used QSAR estimation models (*i.e.*, EPI Suite and PBT Profiler) were adopted for environmental risk evaluation. The experimental results and estimated data, as well as the two model-based results were compared, based on the water solubility, K_{ow}, K_{oc}, BCF and half-life. Environmental risk assessment of the selected compounds was achieved by combining experimental data and estimation models. It was concluded that both EPI Suite and PBT Profiler were fairly accurate in measuring the physicochemical properties and degradation half-lives for water, soil, and sediment. However, the half-lives between the experimental and the estimated results were still not absolutely consistent. This suggests deficiencies of the prediction models in some ways, and the necessity to combine the experimental data and predicted results for the evaluation of environmental fate and risks of pollutants.

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Introduction

Because of the advancement of industrialization, more and more organic chemicals are being discharged into the environment, many of which have become major concerns recently because of their extreme toxicity or persistence in environment (Aksu, 2005). Common organic chemicals are used extensively in the chemical and pharmaceutical industries, food technologies, oil refineries, petrochemical works, dyeing and textile processes, and industrial and agricultural activities (Shahidi et al., 2015), and can exist in different environmental samples with diversified forms (Vörösmarty et al., 2010; Samecka-Cymerman et al., 2009; Elperin et al., 2011). Environmental risk of such compounds has aroused global concern, as they may not only be very persistent and very bioaccumulative (vPvB) and deleterious, but can also be transported through air, water, soil,

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sediment, and other environmental media far away from their original sources (Pavan and Worth, 2008).

Organic pollution owing to such compounds is of great harm to the environment and is a serious issue given their association with many health-related problems (Berezina et al., 2015). Both the fate and behavior of many organic chemicals in the environment depend largely on their physicochemical properties and environmental factors (Reid et al., 2000). Although the exact amount of organic pollutants produced in the world is indeterminate, it has been reported that there are at least 10,000 chemicals in current commercial production, with approximately 1000 being added each year (Mackay et al., 2006). Continuous increase in the production and extensive application of organic pollutants will intensify potential hazards to the environment and human health (Cachada et al., 2012). Organic compounds are distributed in many environmental media, having long half-lives. Pollutants with long half-lives will be present in some environmental media for a long time, which can lead to a wide distribution of such compounds (Schüürmann, 2004). They may accumulate and magnify greatly in the food chain and in individual organisms and have adverse effects on human health and the environment. However, little is known about their potential effects on the environment because of a lack of experimental data. In addition, organic pollutants can vary greatly in physical and chemical characteristics. Although toxicity data are adequate for some noted organic pollutants, data is sparse for most of these compounds and nonexistent for a few. For such chemicals, risk assessment is often impossible because their various toxicities, environmental fates, and health effects are largely undiscovered (Rücker and Kümmerer, 2012).

Furthermore, experimental testing of chemical compounds is usually costly and time-consuming, thus prediction models have played a significant role in remedying the shortage of data (Gramatica and Papa, 2003). Quantitative structure activity relationship (QSAR) models can predict biological activities by using variables of molecular structure (Liaw and Svetnik, 2015) and have the merit of only needing knowledge of chemical structure (Zhao et al., 2008). Such models search for mathematical relationships between chemical structures and activities. QSAR models immediately draw a conclusion that structurally similar chemicals generally show similar biological activities (Bradbury et al., 2004).

Bioconcentration is a process by which a specific chemical is absorbed by an organism from the surrounding environment merely via its respiratory and dermal surfaces. The degree to which bioconcentration occurs can be defined by the bioconcentration factor (BCF) (Arnot and Gobas, 2006). BCF is a crucial ecotoxicological indicator describing the trend of chemical compound concentration in a living organism and is an important parameter in environmental assessment (Gramatica and Papa, 2003). The BCF serves as the criteria for bioaccumulation when identifying pollutants that are hazardous to the environment (McGeer et al., 2003).

The fate of chemicals in the environment is constrained principally by their physical and chemical parameters (Mackay and Callcott, 1998), such as the octanol–water partition coefficient (K_{ow}) (Banerjee et al., 1980) and sediment sorption coefficient (K_{oc}) (Lu et al., 2008). K_{ow} can reflect the environmental fate of chemicals; the higher a chemical's K_{ow} value, the greater is the tendency for that chemical to partition to the organic phase. K_{oc} can appraise the relative tendency of chemicals to adsorb onto solid phases and the partitioning degree (Sun et al., 2016). K_{ow} and K_{oc} are of eminent importance for assessing the behavior and fate of organic pollutants in the environment, and they can be estimated using models based on quantum chemical descriptors (Dai et al., 1999).

Total organic carbon (TOC) concerns any chemical that contains carbon atoms except carbon dioxide and other related inorganic carbon substances and is the energy substrate for many microorganisms (Mook et al., 2012). The reaction kinetics could be calculated according to TOC results and be measured by Langmuir–Hinshelwood equation, and then the half-life for first-order kinetics could be calculated by TOC results (Da Silva et al., 2015).

The aim of this study was to assess the environmental fate and risk of select compounds using a combination of QSAR models and TOC-based half-life. According to the trophic magnification factors (TMFs) of the aquatic food web in Bohai in northern China, 39 compounds were selected. These compounds were screened using in vitro assays that measured the intrinsic clearance of liver microsomes from fish (weevers) and birds (quail) (Zheng et al., 2016). All 39 compounds showed significant trophic magnification in the food web.

Herein, prediction of water solubility (S_w), K_{ow}, K_{oc}, BCF, chronic toxicity value (ChV), and half-lives for the compounds in air, water, soil, and sediment was performed via two authoritative and widely used models, EPI Suite and persistence, bioaccumulation, and toxicity (PBT) Profiler. We compared the half-life results obtained from the two models with the laboratorial TOC half-lives. In addition, predictive parameters were compared between the two models for accuracy evaluation.

1. Materials and methods

1.1. Chemicals and devices

Environmental QSAR analysis models developed by the United States Environmental Protection Agency (US EPA) were used in this study. The Estimation Programs Interface suite of models (EPI Suite™, Version 4.10, US EPA, Washington DC, USA) and the PBT Profiler (PBT Profiler™, Version 2.000, US EPA, Washington DC, USA, 2012) were freely available at http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm and http://www.pbtprofiler.net, respectively. TOC was measured using an automatic TOC analyzer (TOC-Vcph, Shimadzu Corporation, Kyoto, Japan). Ultrapure water derived from a Millipore Milli-Q Gradient A10 (with TOC detector) purification system (Millipore, Billerica, MA, USA) was used for the preparation of all solutions. All reagents were of highest purity available and used without further purification. The organic chemicals (Appendix A Table S1) used in this study were purchased from J&K Scientific Ltd. (Beijing, China).

1.2. Estimation models

EPI Suite and PBT Profiler from the US EPA were employed to estimate the physicochemical properties and environmental fate data of organic pollutants for QSAR analyses