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Deriving acute and chronic predicted no effect concentrations of pharmaceuticals and personal care products based on species sensitivity distributions

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ABSTRACT

Pharmaceuticals and personal care products (PPCPs), as emerging contaminants, have been detected in various environmental matrices and caused adverse effects on human health and the ecosystem. But water quality criterias (WQCs) of PPCPs for protecting aquatic environment are lacking, which hinders the environmental management of these emerging contaminants. In the present study, in order to support their WQC derivation, acute and chronic hazardous concentrations for 5% of species (HC_5s) of some frequently detected PPCPs in China were calculated based on acute and chronic species sensitivity distributions (SSDs), respectively, using both parametric (log-normal and log-logistic) and nonparametric bootstrap approaches. The groups of aquatic species used in SSDs included planktons, zooplanktons, invertebrates and vertebrates. Acute and chronic predicted no effect concentrations (PNECs) were derived from the HC_5s. The acute PNECs of the selected PPCPs were in a range from 1.1 to 4993 μg/L. While the chronic PNECs were one or two orders of magnitude lower than the acute PNECs, with a range from 0.02 to 298 μg/L. Among these PPCPs, the compound with the highest acute effect on the aquatic environment was clarithromycin while erythromycin was the one with the highest chronic toxicity effect. Among the studied PPCPs, erythromycin caused a relatively higher aquatic ecological risk in China. This study helps derive WQCs of PPCPs in the aquatic environment, which is essential for environmental managment of these emerging contaminants.

1. Introduction

With increasing production and usage, pharmaceuticals and personal care products (PPCPs) have caused more and more attention among the public and scientists. As trace emerging contaminants, the occurrence or fate of PPCPs have been studied in surface water (Gao et al., 2012; Zhang et al., 2012; Zheng et al., 2012), sediment (Yang et al., 2010; Li et al., 2012), soil (Hu et al., 2010; Chen et al., 2013) and groundwater (Hu et al., 2010) in China. The occurrence of PPCPs reported in wastewater treatment plants (WWTPs) indicates they cannot be completely removed through wastewater treatment process and then are released into aquatic environment (Huang et al., 2011; Dai et al., 2014; Sun et al., 2014). PPCPs residuals in the ecosystem can lead to adverse ecological effects, such as combined cytotoxicity of some synthetic musks to fishes and environmental risk of pharmaceuticals due to increasing pollutions in surface water (Schnell et al., 2009; Zhao et al., 2010). Therefore, it is necessary to assess the potential hazard of PPCPs to organisms in various trophic levels, which is essential for their environmental risk management.

In order to achieve the above goals, toxicity thresholds of PPCPs for the ecosystem are important in ecological risk assessment. Among the toxicity thresholds, predicted no effect concentration (PNEC) is usually adopted for risk assessment (Wang et al., 2013). The estimation of PNECs is mainly based on two methods, including the assessment factor

Abbreviations: ACR, acute to chronic ratio; AF, assessment factor; CAM, clarithromycin; CBZ, carbamazepine; CP, chloramphenicol; DF, diclofenac; EC_{50}, median effect concentration; EM, erythromycin; FAV, Final Acute Value; FCV, Final Chronic Value; GF, gemfibrozil; HC_5, hazardous concentrations for 5% of species; LC_{50}, median lethal concentration; LOEC, lowest observed effect concentration; MECs, measured environmental concentrations; ND, no detected; NOEC, no observed effect concentration; PNECs, predicted no effect concentrations; PPCPs, pharmaceuticals and personal care products; PPN, propranolol; RQ, risk quotient; SD, sulfadiazine; SDM, sulfadimethoxine; SMX, sulfamethoxazole; SSD, species sensitivity distribution; TP, trimethoprim; WQC, water quality criteria; WWTP, wastewater treatment plant

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Table 1
Statistical summary of the toxicity endpoint data of the selected PPCPs and summary of HC_5s derived from SSDs.

Abbr	CAS no.	Endpoint(mg/L)			HC_5(mg/L)		Endpoint/HC_5	ETP
		n	Geomean	GeoSD	Geomean	GeoSD		
LC_{50}/EC_{50}								
SD	68-35-9	9	4.44	16.8	0.047	1.25	93.8	III
SMX	723-46-6	17	3.73	17.4	0.042	1.23	88.0	III
EM	114-07-8	9	5.10	44.1	0.012	1.34	423	III
CAM	81103-11-9	8	1.73	40.6	0.005	1.60	322	III
CP	56–75-7	10	325	6.97	20.6	1.46	15.8	I
GF	25812-30-0	7	26.0	6.02	1.67	1.25	15.5	I
PPN	525-66-6	19	9.12	8.15	0.26	1.14	35.4	II
CBZ	298-46-4	17	61.7	1.79	25.0	1.04	2.47	I
TP	738-70-5	7	84.4	2.44	23.4	1.18	3.61	I
DF	15307-86-5	11	19.2	4.67	2.03	1.28	9.46	I
NOEC/LOEC								
SDM	122-11-2	11	33.8	15.1	0.48	1.26	70.0	I
SMX	723-46-6	10	1.18	23.4	0.007	1.20	167	III
EM	114-07-8	15	0.232	97.9	0.00009	1.43	2584	III
PPN	525-66-6	13	0.286	14.0	0.005	1.22	62.1	III
CBZ	298-46-4	9	2.50	12.7	0.045	1.23	55.7	III
TP	738-70-5	10	18.1	4.53	1.49	1.12	12.1	I
DF	15307-86-5	9	3.20	25.9	0.049	2.78	65.0	III

n: the number of available species of toxicity data; Geomean: Geometric mean; GeoSD: Geometric standard deviation;
ETP: ecological toxicity potential.

(AF) method and the statistical extrapolation method based on species sensitivity distributions (SSDs) (Lei et al., 2010; Jin et al., 2012). In the AF method, PNECs are obtained based on the toxicity endpoints divided by an AF (such as 10, 50, 100 and 1000) (ECB, 2003). Both acute toxicities and chronic toxicities have been used as toxicity endpoints, such as the median lethal concentration (LC_{50}), the median effect concentration (EC_{50}) and no observed effect concentration (NOEC). However, due to the uncertainty in AF extrapolation and single species used in the AF method, the hazardous concentration for 5% of the species (HC_5) based on SSDs is suggested to derive PNECs and further formulate the water quality criteria (WQC) (Liu et al., 2016). In the derivation of PNECs, the acute-to-chronic ratio (ACR) can be applied in case of unavailability of enough chronic toxicities.

WQC of the aquatic environment can usually be derived based on PNECs, which is essential to support the environmental protection and managment decision. However, the methods to establish WQC are multifarious in different countries. USEPA recommended to use toxicity percentile rank to derive WQC. The Final Acute Value (FAV) and the Final Chronic Value (FCV) were used to characterize WQC (USEPA, 1985). While in other countries, acute and chronic criteria are usually not well differentiated. In Europe, PNECs were adopted to derive the WQC (Hose, 2005). Other developed countries, such as Australia, Canada, and New Zealand, also have established their own derivation method of WQC (Yan et al., 2012). However, WQC methodology in China is still in the initial stage, especially for PPCPs (Wu et al., 2010). Derivation of aquatic PNECs of 2,4-dichlorophenol was reported to compare the difference between Chinese native species data and non-native species data (Jin et al., 2011). Based on different taxa, a final SSD-based PNEC ranged from 0.008 to 0.045 mg/L. The comparison of different SSD-based HC_5s showed that there was no significant difference between native species and non-native species. The WQC of nonylphenol was established based on SSD in China (Gao et al., 2014). The PNEC of nonylphenol in freshwater and seawater was 0.48 μg/L and 0.28 μg/L, respectively. Though some studies have been conducted, they are still far from meeting the emerging demands of the sound environmental management of emerging contaminants (e.g. PPCPs) (Moermond, 2014), not only in China, but also worldwide.

This study was aimed to develop the PNECs of some frequently detected PPCPs, which can support their environmental risk assessment and WQC derivation. In this study, 10 PPCPs were studied to develop acute SSDs and 7 PPCPs were used to develop chronic SSDs. All the target PPCPs were frequently detected in the aquatic environment. Current derivation of PNECs or WQCs is usually based on single methodology, which might cause uncertainties. In order to obtain robust values, both the acute and chronic HC_5s were calculated using parametric and nonparametric bootstrap methods. Acute and chronic PNECs were derived based on the HC_5s, which could support a comprehensive environmental risk assessment and management of the detected PPCPs.

2. Materials and methods

2.1. Toxicity data of the selected PPCPs

Among the 35 frequently detected PPCPs in our previous study (Ma et al., 2016), we selected the PPCPs with more than 7 species acute or chronic toxicity data to develop SSDs, including sulfadiazine (SD), sulfadimethoxine (SDM), sulfamethoxazole (SMX), erythromycin (EM), clarithromycin (CAM), chloramphenicol (CP), gemfibrozil (GF), propranolol (PPN), carbamazepine (CBZ), trimethoprim (TP) and diclofenac (DF). The species number of available toxicity data was listed in Table S1. The groups of species used in SSDs included planktons, zooplanktons, invertebrates and vertebrates. Both the acute toxicity data ($\leq$ 96 h LC_{50} or EC_{50}) and the chronic toxicity data (NOEC or LOEC) of the selected PPCPs to aquatic species at various trophic levels were collected in Table S2. If there were more than one toxicity value for one species, the arithmetic average or logarithmic mean would be used according to its statistical distribution. Statistics of the toxicity data of the selected PPCPs were summarized in Table 1.

2.2. Development of SSDs with five approaches

In order to ensure a best estimation, both acute and chronic SSDs were developed by two parametric approaches (log-normal and log-logistic) and three nonparametric approaches (basic bootstrap, modified bootstrap and modified bootstrap regression) based on our previous work (Wang et al., 2008). Here, these approaches were detailedly described in SI.