



Water quality benchmarking (WQB) and priority control screening (PCS) of persistent toxic substances (PTSs) in China: Necessity, method and a case study



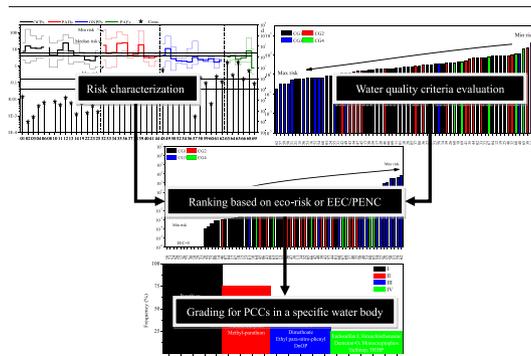
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HIGHLIGHTS

- Predicted no-effect concentrations corrected by P/O medians were credible for WQB.
- China's present WQC underestimated the PTSs' risk to organism in aquatic ecosystem.
- Lake Chaohu confronted high eco-risk from wide usage of pesticides and phthalates.
- Four grades of priority control chemicals were determined in Lake Chaohu.
- Regional PCS was necessary for aquatic ecosystem protection in China.

GRAPHICAL ABSTRACT



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ABSTRACT

The priority control screening (PCS) and water quality benchmarking (WQB) of toxic chemicals in water are key steps to ensure the safety of drinking water and aquatic ecosystem that is the crucial goal of water environment management. Owing to the different levels of social-economic development in different countries and regions, the PCS and WQB of toxic chemicals must be determined in accordance with their specific water environment situations. However, in China, the PCS and WQB of toxic chemicals in water were mainly introduced from the other countries. A method for the PCS and WQB of toxic chemicals in water based on the ecological risks was proposed, and a platform named Bayesian Matbugs Calculator (BMC) was developed. As a case study, the WQB and PCS of sixty-nine PTSs based their ecological risks were performed on the basis of one-year monthly monitoring in Lake Chaohu. The results showed that the current national water quality criteria (WQC) would underestimate the toxicological risk to organisms in this aquatic ecosystem. It appears necessary to develop new WQC for the protection of aquatic organisms in Lake Chaohu. Four grades of priority control chemicals (PCCs) in Lake Chaohu were proposed. The highest priority was assigned to organonitrogen-phosphorus pesticides, including parathion, dichlorvos, malathion, omethoate, and di-n-butyl phthalate. However, the national "blacklist" of toxic compounds only covered 7 of 20 PCCs, indicating that the other 13 PCCs would not be controlled efficiently. Because the pollution pattern of PTSs in various water bodies might be quite different, we appealed to the governments to screen the regional PPC lists or develop a more comprehensive national list for aquatic ecosystem protection in China.

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1. Introduction

China has experienced rapid economic development in the past 30 years. However, an environmental cost was paid for this rapid development, and water pollution events have occurred frequently. For example, 100 tons of benzene, aniline, nitrobenzene and other toxicants were spilled into the Songhua River following a plant explosion in 2005 (Fu et al., 2008). In 2010, 9100 m³ of wastewater were discharged into rivers due to a lack of valid environmental protection facilities in Fujian province, resulting in the death of a large number of fish (Zhang et al., 2011). In January 2013, more than 39 tons of aniline leaked into rivers in Shanxi province, posing a great threat to the safety of drinking water for downstream provinces (Areddy, 2013). Environmental issues have become a major societal concern in China. Although China has been implementing a water quality criteria (WQC) program for the protection of the aquatic environment, the present WQC (GB3838-2002) has several inherent problems. First, water quality grades I–V were established without clear identification of susceptible species to be protected, as only the water body type (including natural reserve, surface drinking water, industrial/recreational water, and agricultural/landscape water) was evaluated for grade classification (Wu et al., 2010). Second, the present WQC grading system lacks scientific support. For example, five grades were established for environmental concentrations of volatile phenols, i.e., 0.002, 0.002, 0.005, 0.01, and 0.1 mg/L, but there was no scientific support provided for this gradation. Third, the assessment of pollutants using surface WQC is limited in scope and not easily adapted for the assessment of multiple pollutants in surface water. For example, nitrobenzene pollution in Shanxi can only be assessed based on the drinking water criteria, which is unsuitable for the evaluation of the hazards presented to aquatic organisms. Thus, it is necessary to assess the ecological risk of nitrobenzene using WQC from other countries (USEPA, 2002), which may not be protective for Chinese waters (Yan et al., 2012). Moreover, there is increasing evidence that they are not protective in the U.S. either (Clements et al., 2000). The reason why we used WQC from other countries is that investment in research and relevant basic science is limited. China has recognized that Chinese surface WQC should be established in the next 20 years (Wu et al., 2010). However, current WQC in China focus on the impact of water pollutants on human health but they do not effectively protect aquatic organisms. WQC development in China has begun to include greater consideration of the protection of aquatic organisms (Yan et al., 2012; Yang et al., 2012).

To develop WQC for aquatic ecosystems, many preliminary studies, such as those of physical and chemical properties of chemicals, toxicant concentrations, bioavailability, bioaccumulation, and water pollution levels are considered. In other countries, predicted no-effect concentrations (PNEC) deduced from ecotoxicity data from various species provide the primary scientific support for WQC and risk assessment (Girling et al., 2000). A risk quotient (RQ), calculated by dividing the PNEC by the environmental exposure concentration (EEC), is often used to assess chemical hazard in the aquatic ecosystem (Hela et al., 2005). When calculating the PNEC, an array of methods, including the assessment factor (AF) method, species sensitivity distribution (SSD) models, and quantitative structure-activity relationship (QSAR) models are often used to contextualize assay data (Cormier et al., 2013; Cormier and Suter Ii, 2013; Hernando et al., 2006; Roelofs et al., 2003; Salvito et al., 2002; USEPA, 2011). Moreover, based on the available toxicity data, preliminary, refined, and comprehensive assessment stages can be implemented (OECD, 1989).

The fundamental purpose of establishing WQC is to effectively, preferentially, and temporally control chemicals that may pose higher hazards and result is a more severe pollution. Although China has a nationwide “blacklist” about the priority pollutants (Zhou et al., 1991), due to China’s diverse regional economic development, pollution sources, and pollution levels, it is unreasonable to implement a plan for the same priority control chemicals (PCCs) for all Chinese waters.

Moreover, the “blacklist” contains only 68 chemicals and was put forwarded 20 years ago, indicating it is too old and limited to protect the aquatic environment. It is therefore necessary to screen and rank PCCs for specific bodies of water, where chemicals that carry higher risks need to be considered and controlled. That is just the first step. It would best to give a name to the “blacklist” that best describes its intent and then consider both a national and local way to prioritize work based on different scale risk assessments. At present, the PCS method includes the Hasse-diagram method (Brüggemann and Münzer, 1993), the chemical scoring and ranking assessment model (Snyder et al., 2000), a principal component analysis method (Timmer et al., 1988; Zitko, 1990), the European Union risk-ranking method (Hansen et al., 1999), the bioconcentration factor method (Nordberg and Rudén, 2007), and ecological risk assessment recommend by USEPA (Suter, 2008). These methods fall into two categories: (1) ranking by the degree of hazard, which is characterized by combining physicochemical properties and ecotoxicity data for various species; and, (2) ranking by the degree of risk, which is evaluated based on EEC, ecotoxicity data and relevant models.

In this study, based on ecotoxicity data, WQC for protecting a freshwater ecosystem were developed using AF values that were (1) directly based on observed toxicity data (AF); (2) based on hazard concentrations that corresponded to adverse effects in 5% of species (HC5), as calculated from SSD models (AF_{SSD}); and (3) based on toxicity data predicted using QSAR (AF_{QSAR}). These WQC were then comparatively analyzed. A typical freshwater body, Lake Chaohu, was chosen for a case study intended to assess the temporal-spatial variation of the ecological risks posed by chemicals. An uncertainty model based on the Bayesian Matbug calculator (BMC) platform, which was constructed using Bayesian inference and SSD models, was used for this assessment. Ecological risk was evaluated by both BMC and RQ based on the WQC, and this risk model was further used to determine the PCCs in Lake Chao, as shown in Fig. 1.

2. Methods

2.1. Study area

Lake Chaohu (117.18° to 117.50°E, 31.25° to 31.42°N) is one of China’s five largest freshwater lakes. This lake is located in Eastern China in a subtropical monsoon climate, has an annual average water depth of 8.37 m, and has a precipitation storage capacity of 1.72 to 3.23 million m³. Most of the aquatic species in Lake Chaohu are similar to those in other bodies of water in China, such as Lake Taihu in the middle and lower reaches of the Yangtze River basin. Given that anthropogenic activities adjacent to the lake are different in the east vs. the west, pollution is high in the west and low in the east. Lake Chaohu is eutrophic (Xu et al., 2001), and many persistent toxic substances (PTSs) have recently been detected (He et al., 2012; Liu et al., 2012; Ouyang et al., 2012; Qin et al., 2013; Yang et al., 2009). During a long-term (August, 2009 to March, 2013) monitoring of PTSs (including polycyclic aromatic hydrocarbons (PAHs), organochlorine pesticides (OCPs), polychlorinated biphenyl (PCB), phthalate esters (PAEs), and organonitrogen-phosphorus pesticides (ONPPs) (He et al., 2012; Liu et al., 2012; Ouyang et al., 2012; Qin et al., 2013), our group measured concentrations of PTSs from May 2010 to April 2011. These observations are as follows: the median concentration of the sum of 16 PAHs ($\Sigma_{16}\text{PAHs}$) was 171.6 ng/L; the median concentration of the sum of 26 OCPs ($\Sigma_{26}\text{OCPs}$) was 9.9 ng/L; the median concentration of the sum of 6 PAEs ($\Sigma_6\text{PAEs}$) was 2624.0 ng/L; and the median concentration of the sum of 15 ONPPs ($\Sigma_{15}\text{ONPPs}$) was 269.4 ng/L. The PTSs are divided into four chemical groups (CGs): Group One (CG1) includes OCPs and PCBs; Group Two (CG2) includes PAHs; Group Three (CG3) includes ONPPs; and Group Four (CG4) includes PAEs.

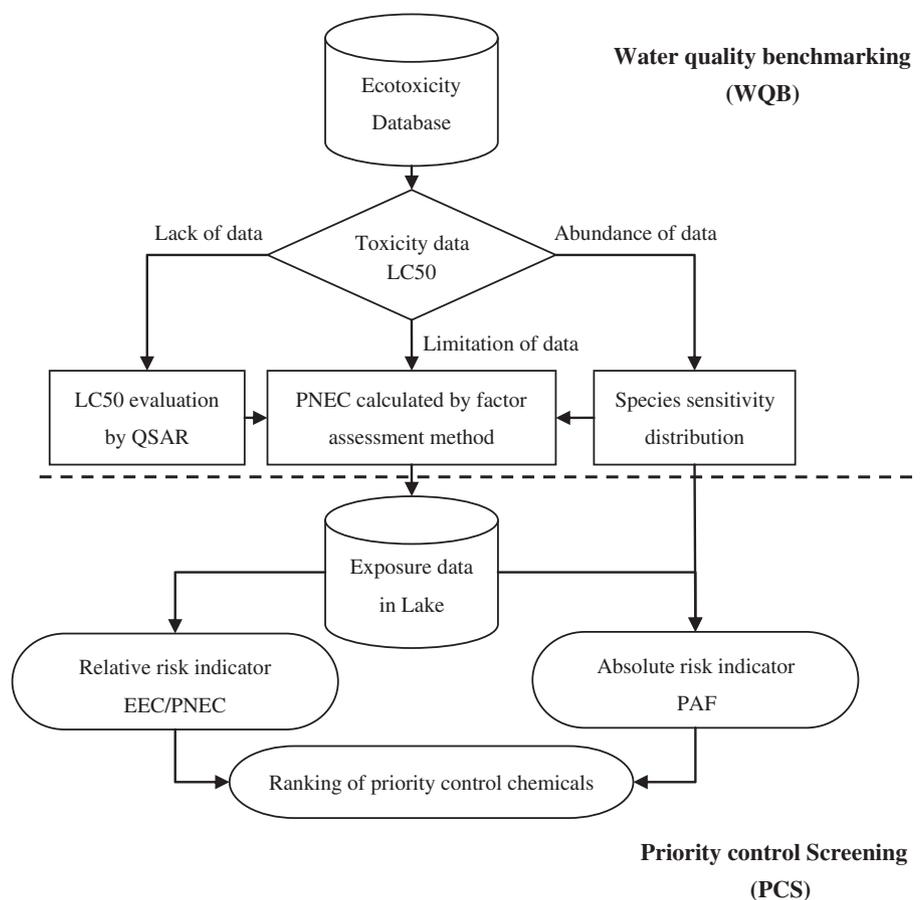


Fig. 1. Technical route for water quality benchmarking and priority control screening of toxic organic chemicals in typical freshwater in Lake Chaohu.

2.2. Measurements of toxic organic chemicals

Four sampling sites, representing the eastern (JC in Fig. S1), the center (ZM and MS in Fig. S1), and the western (TX in Fig. S1) regions of the lake, were selected from May 2010 to April 2011 to investigate the variation in the temporal-spatial concentrations of PAHs, OCPs, PAEs, and ONPPs. Briefly, twenty liters of water was collected monthly, and three parallel samples (1 L aliquot of water per sample) were processed for each type of PTSs using glass fiber membrane filtration, solid phase extraction (SPE), and a gas chromatography tandem-mass spectrometry method. Surrogate standards were added before SPE extraction. The SPE cartridge containing an octadecyl silane-bonded silica (ODS) C18 filler was cleaned twice with elution solvent, activated by methanol, and finally washed using ultrapure water. The elution solvent was dichloromethane for PAHs, OCPs, and ONPPs, and dichloromethane/n-hexane (1:1, v/v) for PAE and an anhydrous sodium sulfate (5 g) cartridge was used to remove water. The extracts were concentrated to approximately 1 mL and internal standard was added to the flask. The samples were sealed in vials and stored at $-20\text{ }^{\circ}\text{C}$ before analysis. PAHs, PAEs, and ONPPs were analyzed by Agilent 6890GC-5973 inert MSD with electron impact (EI) source and OCPs were analyzed by Agilent 7890GC-5975C MSD with negative chemical ionization (NCI) source. More information about measurement of toxic organic chemicals was described in detail in Text S1 of the supplementary data. The fragment ions used for identification and quantification, as well as the instrument limit of detection, the chemical abbreviations, and the method recovery rates of the PTSs are shown in Table S1. Spatio-temporal variation in the PTSs with assigned code numbers in Lake Chaohu from May 2010 to April 2011 is summarized in Table S2; these values were used for risk assessment and PCS.

2.3. The calculation of WQC

The AF method of using toxicity data to derive a PNEC incorporates uncertainty factors or assessment factors and is generally used to calculate WQC (OECD, 1989; USEPA, 2002), as shown in Eq. (1):

$$\text{WQC(PNEC)} = \frac{\text{LC}_{50}\text{ or EC}_{50}\text{ or NOEC or HC}_5}{\prod_{i=1}^n \text{AF}_i} \quad (1)$$

Eq. (1) sometimes uses the LC_{50} and EC_{50} values from short-term toxicity data (US EPA ECOTOX database, <http://cfpub.epa.gov/ecotox/>). However, the LC_{50} and EC_{50} data often rely upon convenient tolerant species and they do not necessarily measure the effect that occurs in the field. These issues, and others, probably should be referenced or briefly noted with respect to the interpretation of the results. Therefore, the no observed effect concentration (NOEC) from long-term toxicity data, the HC_5 as calculated using SSD, and AF_i uncertainty factors that range from 1 to 1000 (Table S3) are often further considered to calculate more credible WQC. 1, 1–5, 10, 50, 100, and 1000 are often assigned as AF values for field data or model ecosystems reviewed on a case by case basis, SSD methods, long-term NOECs from at least three species (normally fish, Daphnia and algae) representing three trophic levels, two long-term NOECs from species representing two trophic levels (fish and/or Daphnia and/or algae), one long-term NOEC (either fish or Daphnia), and at least one short-term L(E)C50 from each of three trophic levels of the baset (fish, Daphnia and algae) (Traas and VanLeeuwen, 2007). Because most chemicals lack field toxicity data, they can only be preliminarily assessed until a refined assessment can be performed when more data are available (Aldenberg and Jaworska,

2000; Traas and VanLeeuwen, 2007; USEPA, 1985). To preliminarily assess chemical risk, the $PNEC_{AF}$ was evaluated by dividing the lowest EC_{50} (LC_{50}) by the product of the AF uncertainty factors ($10 \times 10 \times 10$) (Traas and VanLeeuwen, 2007), as shown in Eq. (2), for a dataset that contained toxicity data for algae (EC_{50}^{algae}), the water flea ($L(E)C_{50}^{water\ flea}$), and fish (LC_{50}^{fish}).

$$PNEC_{AF} = \frac{\text{Min}(EC_{50}^{algae}, L(E)C_{50}^{water\ flea}, LC_{50}^{fish})}{10 \times 10 \times 10} \quad (2)$$

With a set of data from multiple species, if the data for a specific species is abundant, the geometric mean (GM) of $L(E)C_{50}$ values is calculated to reflect the overall toxicity to that species. The toxicity data used for preliminary assessment based on short-term toxicity data are summarized in Table S4. When chemical toxicity data are unavailable, QSAR is often employed to predict short-term toxicity potential, but these predictions may be different from observed data. Therefore, a modified factor or AF, calculated by comparing the predicted to the observed adverse effect concentration, is employed to modify QSAR-predicted toxicity values. We employed Toxicity Estimation Software Tool (TEST), which is a QSAR toxicity model developed by the USEPA (<http://www.epa.gov/nrmrl/std/qsar/qsar.html>), to predict LC_{50} values for the water flea (*Daphnia magna*) and the fathead minnow (*Pimephales promelas*). The P/O ratios that were calculated using the minimum TEST-predicted toxicity value (P) and the minimum observed toxicity data (O) obtained from the ECOTOX database (<http://cfpub.epa.gov/ecotox/>) (Table S5) were used to obtain AF_i^c values. The PNEC based on this modified predicted toxicity value ($PNEC_{QSAR}$) was calculated using Eq. (3), as shown below:

$$PNEC_{QSAR} = \frac{\text{Min}(LC_{50}^{water\ flea}, LC_{50}^{fathead\ minnow})}{10 \times 10 \times 10 \times AF_i^c} \quad (3)$$

If sufficient short-term toxicity data are available, a refined assessment can be completed, and the HC_5 can be obtained by SSD model. After modifying with an acute-to-chronic ratio (ACR, 10) and the AF (values range from 1 to 5, with 5 assigned in this study), the PNEC based on the SSD ($PNEC_{SSD}$) can be calculated using Eq. (4) as shown below (OECD, 1989; Seston et al., 2009):

$$PNEC_{SSD} = \frac{HC_5}{AF \times ACR} \quad (4)$$

The optimum SSD model with appropriate parameters and the mid-level HC_5 value at for each chemical is shown in Tables S6–S7; these values were obtained using the BMC platform that was presented in detail in our another paper (He et al., under review), and described briefly in the Text S2. The HC_5 values shown in Table 1 from the “Median” column in Table S7 were used in Eq. (4) because they were predicted by the SSD curves that best fit the toxicity data.

2.4. Screening of PCCs

Many ranking methods for PCCs are based on scoring (Sampaolo and Binetti, 1986; Snyder et al., 2000; Swanson et al., 1997; Timmer et al., 1988; Zitko, 1990). A small number of studies have previously employed a risk assessment approach to rank the PCCs (Hansen et al., 1999). In this study, the mid-level ecological risk values were calculated using the BMC and RQ (EEC/PNEC ratio) and were used to rank the PTSs in Lake Chaohu. Ecological risk values greater than 0.1, between 0.001 and 0.1, between 0.001 and 10^{-6} , and 10^{-6} indicated that PTSs posed a very high, high, potential, and limited risk to the aquatic ecosystem, respectively. An RQ value greater than 1 indicated that a PTS poses a high risk, and an RQ value less than 1 indicated that PTSs pose a low risk to the aquatic

Table 1
Mid-level HC_5 ($\mu\text{g/L}$) calculated using the BMC platform (“Median” column in Table S7).

| No. | Chemicals | HC_5 |
|-----|----------------------------|----------|
| 1 | Aldrine | 3.63 |
| 2 | Endosulfan II | 1.447 |
| 3 | Endrine | 0.381 |
| 4 | γ -HCH | 5.56 |
| 5 | o,p'-DDE | |
| 6 | Heptachlor | 5.921 |
| 7 | o,p'-DDD | |
| 8 | Mirex | 172.719 |
| 9 | o,p'-DDT | |
| 10 | p,p'-DDD | 0.354 |
| 11 | p,p'-DDT | 1.313 |
| 12 | β -HCH | 882.832 |
| 13 | Isodrin | 9.007 |
| 14 | p,p'-DDE | 0.177 |
| 15 | oxy-Chlordane | |
| 16 | Heptachlorepoxyde | 0.035 |
| 17 | trans-Chlordane | |
| 18 | DDMU | |
| 19 | α -HCH | 40.102 |
| 20 | cis-Chlordane | |
| 21 | Dieldrine | 1.947 |
| 22 | Endosulfan I | 0.041 |
| 23 | Hexachlorbenzene | 0.182 |
| 24 | Methoxychlor | 1.005 |
| 25 | δ -HCH | 17.69 |
| 26 | PCB28 | |
| 27 | PCB52 | |
| 28 | PCB101 | 5.232 |
| 29 | PCB137 | |
| 30 | PCB153 | |
| 31 | PCB180 | |
| 32 | Acenaphthylene | 85.861 |
| 33 | Anthracene | 2.178 |
| 34 | Benzo(a)pyrene | 1.085 |
| 35 | Phenanthrene | 106.189 |
| 36 | Benzo(a)anthracene | 7.987 |
| 37 | Fluoranthene | 4.966 |
| 38 | Naphthalene | 324.41 |
| 39 | Pyrene | 3.439 |
| 40 | Acenaphthene | 51.263 |
| 41 | Chrysene | 28.606 |
| 42 | Benzo(b)fluoranthene | 65 |
| 43 | Benzo(k)fluoranthene | 66 |
| 44 | Fluorene | 63.44 |
| 45 | Indeno(1,2,3-cd)pyrene | 68 |
| 46 | Dibenz(a,h)anthracene | 69 |
| 47 | Benzo(g,h,i)perylene | |
| 48 | Atrazine | 23.602 |
| 49 | Chlorothalonil | 6.613 |
| 50 | Parathion | 0.629 |
| 51 | Demeton-O | |
| 52 | Dichlorvos | 1.228 |
| 53 | Monocrotophos | |
| 54 | Malathion | 0.218 |
| 55 | Demeton-S | |
| 56 | Omethoate | 0.679 |
| 57 | Sulfotep | 0.034 |
| 58 | Carbaryl | 15.707 |
| 59 | Dimethoate | 4.793 |
| 60 | Ethyl para-nitro-phenyl | 0.695 |
| 61 | Methamidophos | 3.488 |
| 62 | Methyl-parathion | 5.009 |
| 63 | Dimethyl phthalate | 4801.222 |
| 64 | Diethyl phthalate | 1636.629 |
| 65 | dinbutyl phthalate | 111.396 |
| 66 | Butylbenzyl phthalate | 78.933 |
| 67 | Di(2-ethylhexyl)adipate | |
| 68 | Di(2-ethylhexyl) phthalate | 99.904 |
| 69 | Dinocetyl phthalate | 0.00004 |

ecosystem. After ranking the ecological risk and RQ values from high to low, the PTSs with the highest risk (top 25%) were defined as PCCs.

3. Results and discussion

3.1. WQC of PTSs

3.1.1. Modifying factors for toxicity data predicted by QSAR

Although QSAR was widely used for the evaluation of ecotoxicity data, modifying factors should be considered to reduce the difference

between the predicted and the observed (Salvito et al., 2002). The statistical analysis of the P/O ratios (Table S5) is provided in Table S8. The P/O ratios ranged from 10^{-3} to 10^3 , covering six orders of magnitude. It is therefore necessary to modify the predicted values using the P/O ratios for each CG. When the P/O ratio ranged from 0.1 to 10, the range of variation was considered to be an acceptable, and we determined that 65% of chemicals in CG1, 80% of chemicals in CG2, 67% of

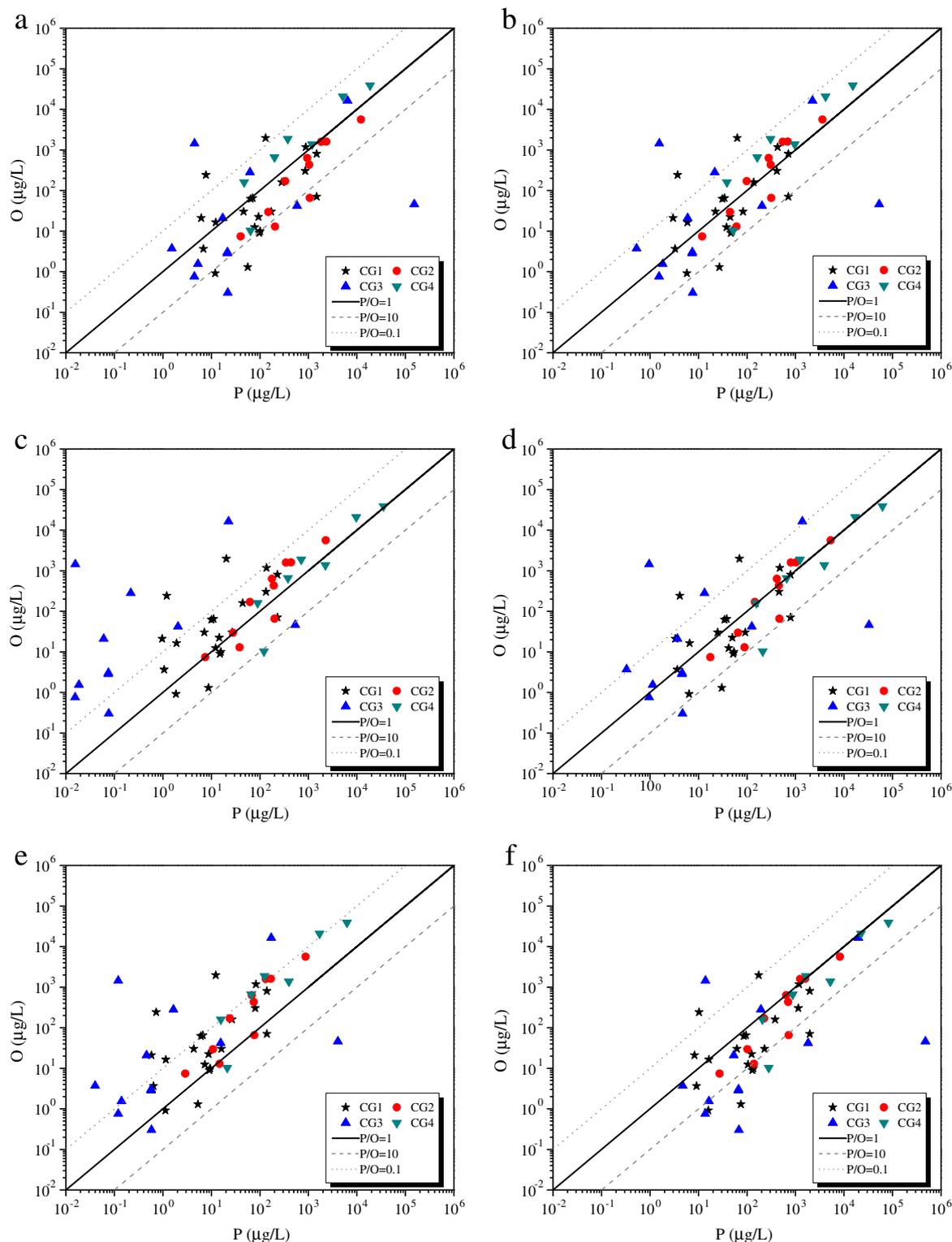


Fig. 2. The LC50 predicted using QSAR, the modified predicted LC50 using QSAR, and the observed LC50 in Table S4 (Chart a: predicted LC50 vs. observed LC50; Chart b–f: predicted LC50 modified by the geometric mean, arithmetic mean, median, 80th centile, and 20th centile of the P/O ratios.).

Table 2Pearson correlation and linear regression analysis between $\lg(\text{PNEC}_{\text{SSD}})$ and $\lg(\text{PNEC}_{\text{AF}})$, $\lg(\text{PNEC}_{\text{QSAR}})$, and $\lg(\text{PNEC}_{\text{QSAR}})$.

| | $\text{PNEC}_{\text{SSD}}^{\text{a}}$ | $\text{PNEC}_{\text{AF}}^{\text{b}}$ | $\text{PNEC}_{\text{QSAR}}^{\text{b}}$ | $\text{PNEC}_{\text{QSAR}}^{\text{c}}$ | | |
|--|---------------------------------------|--------------------------------------|--|--|-------------------------------|-------------------------------|
| | | | | $\text{QSAR}_{80}^{\text{b}}$ | $\text{QSAR}_{50}^{\text{b}}$ | $\text{QSAR}_{20}^{\text{b}}$ |
| N ^c | 48 | 48 | 48 | 48 | 48 | 48 |
| Normal test (p value) | 0.924 | 0.845 | 0.627 | 0.57 | 0.992 | 0.976 |
| AM ^c | 1.97 | 1.75 | 2.13 | 2.32 | 1.84 | 1.02 |
| SD ^c | 1.40 | 1.21 | 0.95 | 0.96 | 1.09 | 1.08 |
| Min ^c | -3.15 | -0.51 | 0.18 | 0.68 | -0.48 | -1.39 |
| Max ^c | 4.98 | 4.79 | 5.18 | 5.68 | 4.79 | 3.80 |
| <i>I. The outlier DnOP was not omitted</i> | | | | | | |
| r ^c | 1.000 | 0.694** | 0.524** | 0.505** | 0.525** | 0.522** |
| B ^c | 0.000 | 0.563 | 1.496 | 1.745 | 1.098 | 0.277 |
| A ^c | 1.000 | 0.619 | 0.402 | 0.384 | 0.456 | 0.451 |
| R ^{2c} | 1.000 | 0.471 | 0.259 | 0.239 | 0.260 | 0.257 |
| Mean of Y - X | - | 0.66 | 0.85 | 0.86 | 0.83 | 1.25 |
| SD of Y - X | - | 0.83 | 0.95 | 1.06 | 0.97 | 0.85 |
| Fraction ^c (%) | - | 77.1 | 66.7 | 68.8 | 70.8 | 43.8 |
| <i>II. The outlier DnOP was omitted</i> | | | | | | |
| r ^c | 1.000 | 0.849** | 0.581** | 0.595** | 0.650** | 0.633** |
| B ^c | 0.000 | -0.093 | 1.201 | 1.386 | 0.598 | -0.187 |
| A ^c | 1.000 | 0.899 | 0.528 | 0.537 | 0.668 | 0.649 |
| R ^{2c} | 1.000 | 0.715 | 0.323 | 0.340 | 0.409 | 0.387 |
| Mean of Y - X | - | 0.56 | 0.76 | 0.76 | 0.73 | 1.18 |
| SD of Y - X | - | 0.48 | 0.75 | 0.80 | 0.70 | 0.71 |
| Fraction ^c (%) | - | 78.7 | 68.1 | 70.2 | 72.3 | 44.7 |

^a PNEC_{SSD} is independent variable (X) in Pearson correlation and linear regression analysis.^b PNEC_{AF} , $\text{PNEC}_{\text{QSAR}}$, $\text{PNEC}_{\text{QSAR}_{80}}$, $\text{PNEC}_{\text{QSAR}_{50}}$, and $\text{PNEC}_{\text{QSAR}_{20}}$ are dependent variable (Y) in Pearson correlation and linear regression analysis.^c N, AM, SD, Min, Max, r, B, A, R², and fraction denote number of chemicals, arithmetic mean, standard deviation, minimum, maximum, Pearson correlation coefficient, constant of linear regression, slope of linear regression, coefficient of determination, and fraction of chemicals when |Y - X| < 1.

** Denotes p < 0.001.

chemicals in CG3, and 100% of chemicals in CG4 demonstrated acceptable differences between the predicted and observed toxicity values. A Kolmogorov–Smirnov test indicated that every CG followed a logarithmic normal distribution. Consequently, GM was more suitable for reflecting the central tendency of the distribution. The GM of the P/O ratios for each CG ranged from 0.5 to 3.4, indicating that differences between the predicted and the observed toxicity values were acceptable.

The GM, arithmetic mean (AM), median, 80th centile, and 20th centile of P/O ratios for each CG were set as the modifying factors for the predicted toxicity values. The LC₅₀ as predicted by QSAR, the modified predicted LC₅₀ based on QSAR, and the observed LC₅₀ are shown in Fig. 2. The predicted toxicity values for most chemicals in CG1 and CG2

were greater than the observed toxicity values, indicating that the QSAR model underestimated the ecotoxicity of these chemicals. The QSAR values for CG3 may have been less predictive, as there were large differences between the predicted and the observed toxicity values for methamidophos (P/O = 3 319) and dimethoate (P/O = 0.003). P/O values for CG4 ranged from 0.1 to 10, and a majority of the chemical ecotoxicity potentials were overestimated. When predicted values were modified by the GM of P/O ratios (Fig. 2b), the number of chemical P/O values within the range of 0.1 to 10 increased, and only six chemicals were outside of this acceptable range. However, many predicted and observed toxicity value data points were still far from the line P/O = 1, indicating that the modified prediction was not ideal. When modified by AM (Fig. 2c), the predicted toxicity values for most chemicals in CG1 and CG3 were much smaller than the observed toxicity values, indicating that the QSAR model overestimated their ecotoxicity potential. In contrast, most of the predicted and observed toxicity value data points in CG2 and CG4 were close to the line P/O = 1, indicating that the modified prediction was ideal. Although fewer chemicals' P/O values fell within the range of 0.1 to 10 when modified by the median than when modified by the GM (Fig. 2d), most predicted and observed toxicity value data points in CG2 and CG4 were near the line P/O = 1, indicating that modifying by the median conferred an advantage over both modified by AM and modified by GM. When the 80th centile and the 20th centile P/O values were used as the modifying factors (Fig. 2e and f, respectively), most of the predicted and observed toxicity value data points were positioned to the left or right of the line P/O = 1. Positioning to the left of the line may have resulted in overestimation of the ecotoxicity potential, and positioning to the right of the line may have resulted in the underestimation of the ecotoxicity potential. If a conservative evaluation strategy was required, modified by the 80th centile would be appropriate. In summary, predictions modified by the 80th centile, median, and 20th centile of the P/O values for each CG reflected conservative, moderate, and optimistic strategies to evaluate ecotoxicity potential. The 80th and 20th centiles also offered an uncertainty scale for this modified prediction. The maximum and minimum P/O values were not considered given that they were most likely outliers. Modifying factors (or AF_i) were

Table 3

Comparison with China's present WQC (ng/L).

| No. | Chemicals | PNEC_{SSD} | PNEC_{AF} | $\text{PNEC}_{\text{QSAR}_{50}}$ | GB3838-2002 | WQC in Our study |
|-----|-----------|----------------------------|---------------------------|----------------------------------|-------------|------------------|
| 11 | p,p'-DDT | 2.63E + 01 | 1.14E + 01 | 4.20E + 01 | 1.00E + 03 | 1.14E + 01 |
| 16 | HCP | 6.91E - 01 | 1.90E + 01 | 4.14E + 00 | 2.00E + 02 | 6.91E - 01 |
| 23 | HCB | 3.64E + 00 | 4.93E + 00 | 1.18E + 02 | 5.00E + 04 | 3.64E + 00 |
| 26 | PCB28 | | 1.60E + 02 | 1.52E + 02 | 2.00E + 01 | 1.52E + 02 |
| 27 | PCB52 | | 3.00E + 01 | 9.21E + 01 | 2.00E + 01 | 3.00E + 01 |
| 28 | PCB101 | 1.05E + 02 | 1.00E + 01 | 5.41E + 01 | 2.00E + 01 | 1.00E + 01 |
| 29 | PCB137 | | | 3.07E + 01 | 2.00E + 01 | 3.07E + 01 |
| 30 | PCB153 | | 1.30E + 00 | 3.02E + 01 | 2.00E + 01 | 1.30E + 00 |
| 31 | PCB180 | | | 1.17E + 01 | 2.00E + 01 | 1.17E + 01 |
| 34 | BaP | 2.17E + 01 | 9.56E + 00 | 1.75E + 01 | 2.80E + 00 | 9.56E + 00 |
| 48 | Atz | 4.72E + 02 | 1.73E + 02 | 1.38E + 03 | 3.00E + 03 | 1.73E + 02 |
| 49 | Ctn | 1.32E + 02 | 4.80E + 01 | 1.34E + 01 | 1.00E + 04 | 1.34E + 01 |
| 50 | Pt | 1.26E + 01 | 1.25E + 00 | 1.14E + 00 | 3.00E + 03 | 1.14E + 00 |
| 51 | Dmo | | 5.00E + 03 | 2.55E + 00 | 3.00E + 04 | 2.55E + 00 |
| 52 | Dcv | 2.46E + 01 | 1.15E + 01 | 4.59E + 00 | 5.00E + 04 | 4.59E + 00 |
| 54 | Mlt | 4.35E + 00 | 8.33E - 01 | 4.61E + 00 | 5.00E + 02 | 8.33E - 01 |
| 55 | Dms | | 1.00E + 01 | 1.02E + 01 | 3.00E + 04 | 1.00E + 01 |
| 59 | Dmt | 9.59E + 01 | 1.78E + 03 | 9.64E - 01 | 8.00E + 04 | 9.64E - 01 |
| 62 | Mpt | 1.00E + 02 | 8.57E - 01 | 3.28E - 01 | 2.00E + 03 | 3.28E - 01 |
| 65 | DnBP | 2.23E + 03 | 1.83E + 03 | 3.93E + 03 | 3.00E + 03 | 1.83E + 03 |
| 68 | DEHP | 2.00E + 03 | 9.60E + 02 | 1.56E + 02 | 8.00E + 03 | 1.56E + 02 |

Notes: WQC in our study was minimum among PNEC_{SSD} , PNEC_{AF} , and $\text{PNEC}_{\text{QSAR}_{50}}$.

derived based on the analysis described above and are summarized in Table S3.

3.1.2. The comparison of PNEC values as calculated using the AF, AF_{SSD}, and AF_{QSAR} methods

According to the method described in Section 2.3, PNEC values were calculated using the AF, AF_{SSD}, AF_{QSAR}, and AF_{QSAR} methods (including AF_{QSAR80}, AF_{QSAR50}, and AF_{QSAR20}) (Table S9). The results indicated that the PNEC_{SSD}, PNEC_{AF}, and PNEC_{QSAR} accounted for 70%, 87%, and 100% of the PTSs in the present study. A normality test demonstrated that the data followed a logarithmic normal distribution. We also observed that the toxicity values for di-n-octyl phthalate (No. 69) were outliers. Thus, Pearson correlation and linear regression analyses between lg(PNEC_{SSD}) and either lg(PNEC_{AF}), lg(PNEC_{QSAR}), or lg(PNEC_{QSAR'}), with or without di-n-octyl phthalate, were completed using SPSS software (Table 2, Figs. S2, and S3). Because PNEC_{SSD} was calculated using the SSD, which was a refined assessment strategy, this value was assigned as an independent variable (X). The other PNEC values were analyzed as dependent variables (Y). The results indicated that there were significantly positive correlations between lg(PNEC_{SSD}) and lg(PNEC_{AF}), lg(PNEC_{QSAR}), and lg(PNEC_{QSAR'}), with or without di-n-octyl phthalate. That is, there were significantly positive correlations for a data set that included a broad range of values. The average order of magnitude of the PNEC data sets ranged from 1.02 to 2.32. PNEC_{SSD} included data that ranged over eight orders of magnitude, while both PNEC_{AF} and PNEC_{QSAR} demonstrated a span of five orders of magnitude. The absolute

value of Y minus X ($|Y - X|$) yielded large differences between PNEC_{SSD} values and PNEC values derived by other calculation methods. The PNEC_{AF} values approached the PNEC_{SSD} values, followed by PNEC_{QSAR50}. We also observed that over 70% of the $|Y - X|$ values for chemicals were lower than 1 for PNEC_{AF} and PNEC_{QSAR50}, indicating that the difference between the preliminary assessment and refined assessment results were minor.

3.1.3. Comparison with China's present WQC

China has not set WQC for aquatic ecosystems. This government document (standard number: GB3838-2002) provides WQC for 69 organic chemicals, and the majority of these WQC were obtained from other countries. The objective of GB3838-2002 was the protection of water sources for anthropogenic use. After comparing the WQC (or PNEC) calculated in this study with China's present WQC (which include 21 chemicals in the present study) (Table S10), we determined that 81% of the chemical WQC values in GB3838-2002 were higher than those we derived, indicating that China's present WQC may underestimate the risk to organisms in aquatic ecosystems. For example, China's WQC for atrazine was 50.0 µg/L, but the WQC in this study was 0.2 µg/L. Atrazine may not be harmful at 50.0 µg/L for humans; however, the growth of sensitive species in the aquatic environment would be inhibited at this concentration as indicated by the ecological risk. In conclusion, it is necessary to develop WQC for the protection of aquatic organism in Chinese surface waters because of the underestimation of current WQC (Table 3).

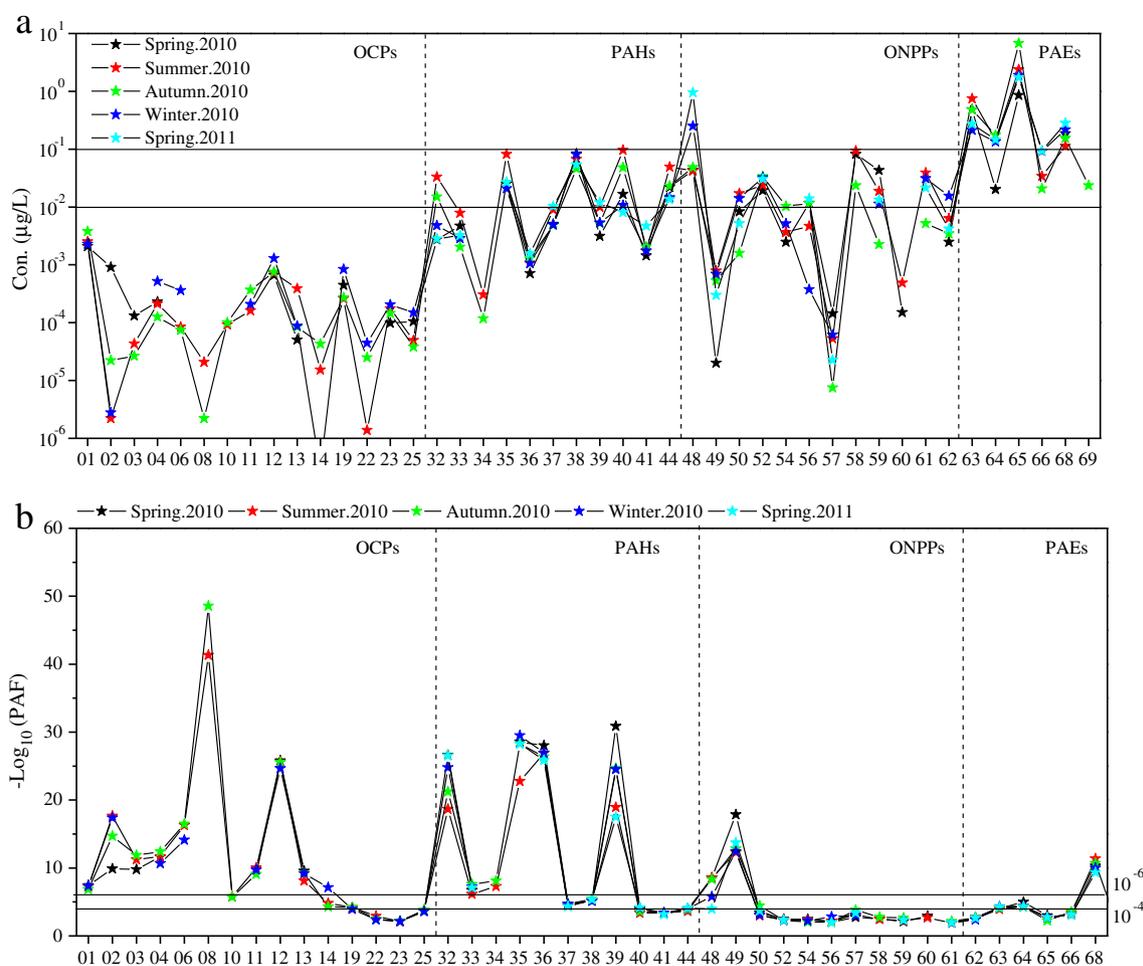


Fig. 3. Seasonal variation in chemical concentrations (Chart a) and ecological risks (Chart b) at the mid-level of the typical organic toxicant load in Lake Chaohu. The numbers along the x-axis represent the chemicals in Table 1. The variations observed for the majority of chemicals were not significant, except for endosulfan II, mirex, acenaphthylene, phenanthrene, pyrene, atrazine, and chlorothalonil.

3.2. The concentration and ecological risk of typical PTSs in Lake Chaohu

3.2.1. Seasonal variance

Concentrations and ecological risks at low-, mid-, and high-levels of the typical organic toxicant load from spring 2010 to spring 2011 in Lake Chaohu are shown in Figs. S4–S8 and summarized in Fig. 3. In CG1, the concentrations of β -HCH and aldrine were higher than the concentrations of other chemicals and were highest in the autumn and the lowest in the spring. Concentrations in the autumn were also at their peak values. In CG2, the concentrations of naphthalene, fluorine, and phenanthrene were at the same order of magnitude across different seasons but were present at higher concentrations than other PAHs. Little variance was observed for naphthalene in samples collected from different seasons. Concentrations of acenaphthene, fluorine, and phenanthrene first increased and then decreased, and peak values were observed in the summer. Benz(a)anthracene was only detected in the summer and autumn. In CG3, dichlorvos, carbaryl, atrazine, and methamidophos were detected at higher concentrations than other ONPPs. Concentrations of atrazine increased with time, and the peak value was observed in spring 2011 of the sampling period. Concentrations of dichlorvos and carbaryl first increased and then decreased, and their peak values were observed in the autumn and summer, respectively. The concentration of methamidophos decreased first and then increased, and its lowest measured concentration was in the autumn. In CG4, dimethyl phthalate and di-*n*-butyl phthalate were detected at higher concentrations than other chemicals in multiple seasons. Dimethyl phthalate and di-*n*-butyl phthalate concentrations both increased first and then decreased, and their peak values were observed in the summer and autumn,

respectively. The lowest measured concentrations for di(2-ethylhexyl) phthalate were detected in the summer. For any specific chemical, the variance in the ecological risk was similar to the seasonal variance in the concentration. However, the degree of variance observed was different with different SSD models. As shown in Fig. S10b, the variation observed for the majority of chemicals was not significant, except for endosulfan II, mirex, acenaphthylene, phenanthrene, pyrene, atrazine, and chlorothalonil. According to our previous study (He et al., 2013), we considered that meteorological and hydrological factors were only driving factors for the variation of various PTSs, and the real reasons were that human's agricultural, industrial, and daily activities varied with the seasons. More human's activities in warm seasons might increase the discharge of the PTSs. Some PTSs like pesticide, including heptachlor, mirex, p,p'-DDD, p,p'-DDT, p,p'-DDE, endosulfan I, methamidophos, were used at the middle of the spring and until the end of the summer. The runoff, carrying lots of pesticides, increased because of rainfall during the warm seasons. With the increase of human activities, PAH like benzo(a)pyrene and PAE like butylbenzyl phthalate would be detected.

3.2.2. Spatial variance

The concentration and ecological risk at low-, mid-, and high-levels of the typical organic toxicant load in various regions of Lake Chaohu are shown in Figs. S9–S11 and summarized in Fig. S12. Most of the OCPs were detected at higher concentrations in the western region of the lake. The concentration distributions for aldrine, p,p'-DDT, and endosulfan I were highest in the western region of the lake, followed by the center and eastern regions. There was limited spatial variance for

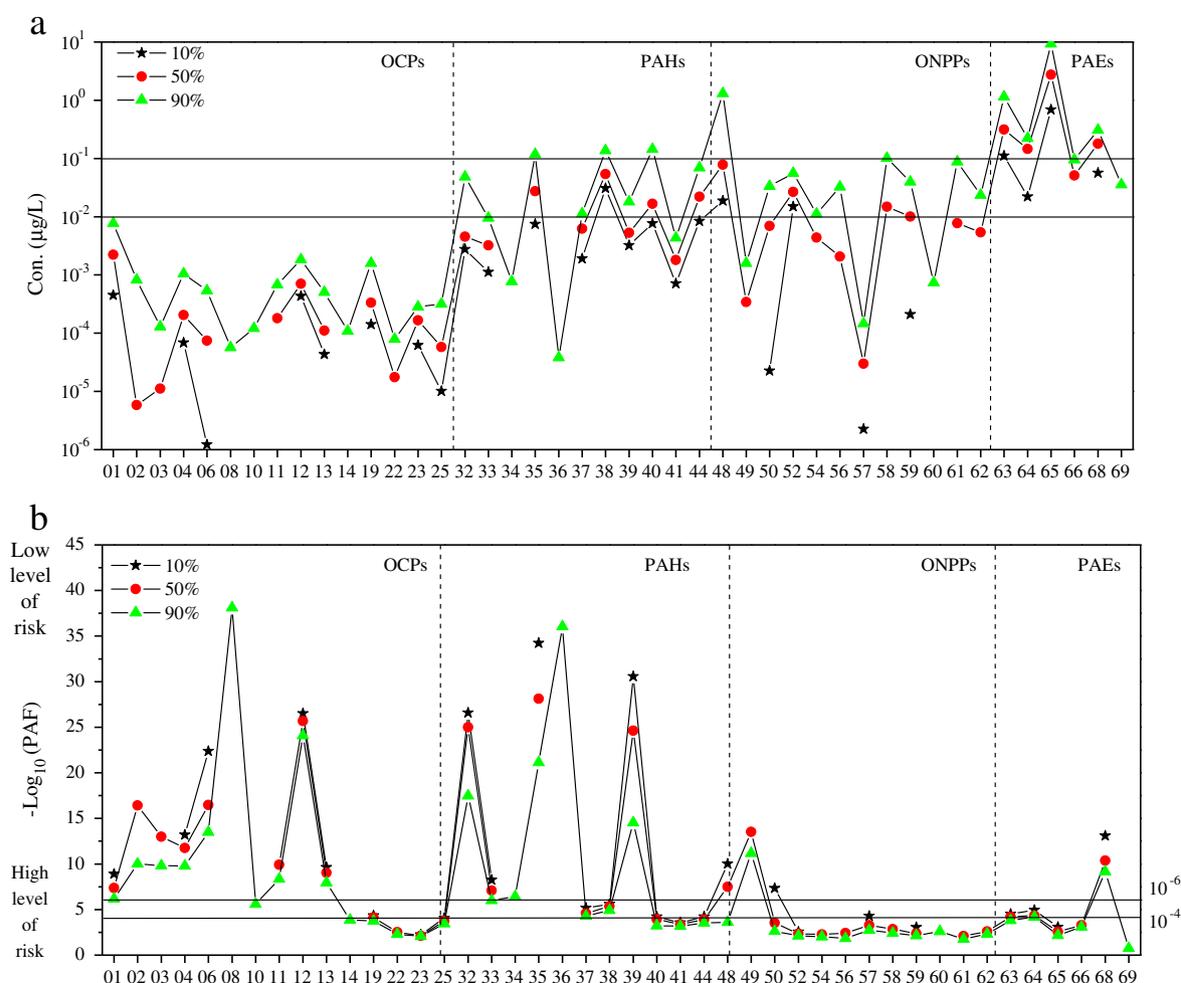


Fig. 4. The 10th, 50th, and 90th centiles of chemical concentrations (Chart a) and their associated ecological risks (Chart b) at mid-level as evaluated using the BMC platform.

PAH concentrations. The concentration distributions for atrazine and malathion were highest in the western region of the lake, followed by the center and the eastern regions. The spatial variance for chlorothalonil was the opposite of that for atrazine and malathion. Dimethyl phthalate was detected at higher concentrations in the eastern region of the lake, and di-n-butyl phthalate was detected at higher concentrations in the western region. Similar to temporal ecological risk, variations in spatial ecological risk varied for chemicals were limited, except for chlorothalonil.

3.2.3. The characterization of PTSs' concentration and ecological risk in the entire lake

To characterize the concentration of PTSs and the ecological risks posed in the entire lake, the 10th, 50th, and 90th centile of chemical concentrations and their associated ecological risks (Fig. 4b) at the mid-level were evaluated using the BMC platform (Fig. S13, summarized in Fig. 4). The results indicated that most of the OCPs were present at low concentrations and posed limited ecological risk, except for α -HCH, cis-chlordane, and hexachlorbenzene. Most of the PAHs were at the mid-level of measured concentrations and predicted ecological risk, except for acenaphthylene, phenanthrene, benz(a)anthracene, and pyrene, which demonstrated ecological risk even at low concentrations. Most of the ONPPs were at the mid-level of concentration and posed a high level of ecological risk, except for chlorothalonil. Most of the PAEs were measured at high concentrations and were associated with a high level of ecological risk, except for di(2-ethylhexyl) phthalate. Because OCPs have been banned for many years, the ecological risk posed by these chemicals was more limited (Feng et al., 2003). However, ONPPs are still used for agriculture and have become a new threat to aquatic ecosystems (Honeycutt and Schabcker, 1994). PAEs are endocrine-disrupting

chemicals (Okamoto et al., 2011) and have been a focus of attention in China because they are frequently detected in wines and food (Zhu, 2012). PAE residue was not observed to be high in these food items, and its health risk was very low (Guo et al., 2012). However, our study showed that some aquatic organisms in Lake Chaohu were confronted with high-level of ecological risk from PAEs on the basis of SSD models.

3.3. PCCs in Lake Chaohu

3.3.1. Ranking and screening using PNEC

If EEC is not considered for screening PCCs, we can employ a PNEC-based approach to rank and screen. A lower PNEC value indicates higher hazard for a specific chemical. A ranking of toxic organic chemicals in Lake Chaohu based on $PNEC_{SSD}$, $PNEC_{AF}$, $PNEC_{QSAR}$, and $PNEC_{QSAR50}$ is shown in Figs. S14 and 5. $PNEC_{SSD}$ offered a more consistent evaluation of chemical hazard than $PNEC_{AF}$ and $PNEC_{QSAR}$, but only 48 PTSs could be ranked because of a lack of available data for this approach. The ranking results shown in Fig. 5a indicated that most PAEs, except di-n-octyl phthalate, were associated with low toxicity. Di-n-octyl phthalate appeared to be the most toxic chemical among the examined PTSs. Twenty-five percent of the examined PTSs were pesticides, but di-n-octyl phthalate is not a pesticide. Certain OCPs belong to a class of chemicals known as POPs, such as p,p'-DDE, hexachlorbenzene, p,p'-DDD, and endrine. Other OCPs included organophosphate pesticides, including dichlorvos, sulfotep, carbaryl, dimethoate, and parathion. Benzo(a)pyrene, anthracene, and pyrene were more toxic than other PAHs. $PNEC_{QSAR}$ was a useful tool with which to evaluate all of the PTSs investigated in Lake Chaohu (Fig. 5b). We also observed that pesticides, which accounted for the top 25% of PTSs, posed a larger threat than other PTSs. Most OCPs and PCBs exhibited moderate levels of risk. PAHs

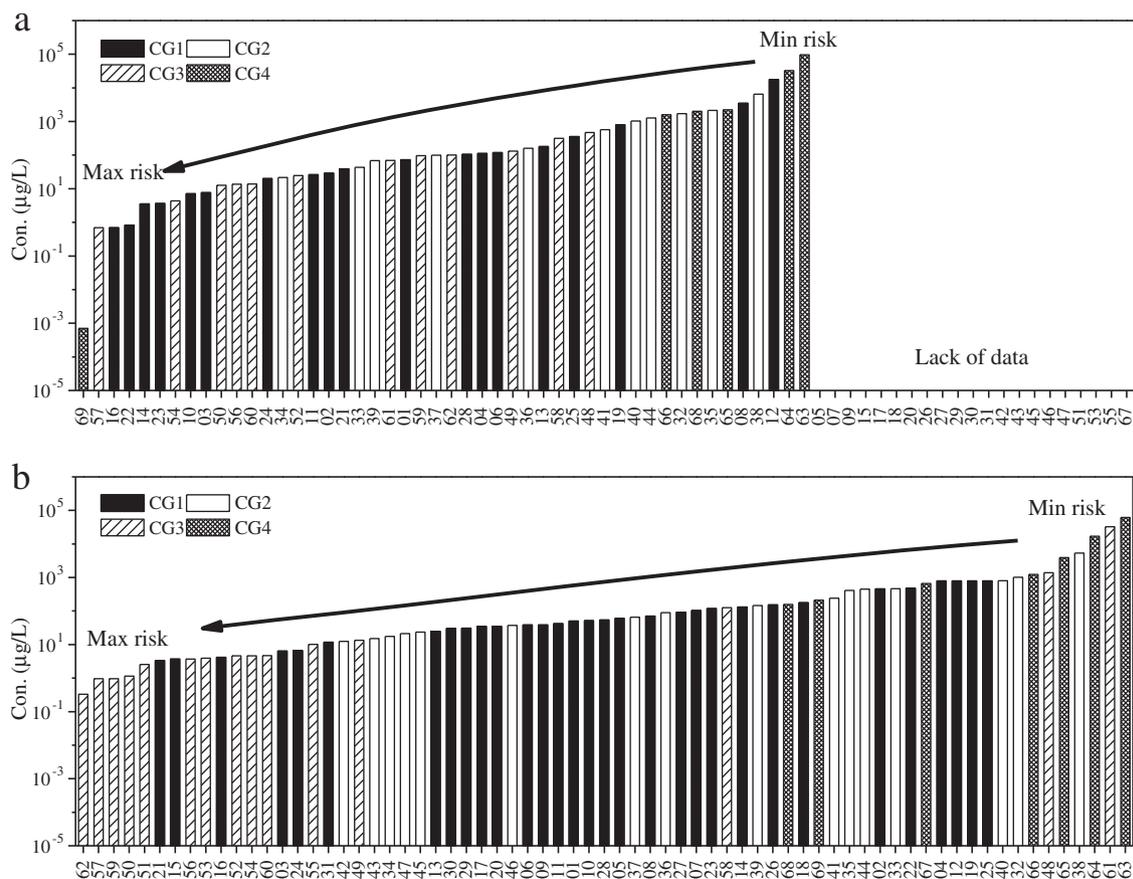


Fig. 5. The ranking of toxic organic chemicals in Lake Chaohu based on $PNEC_{SSD}$ (Chart a) and $PNEC_{QSAR50}$ (Chart b) (The PTSs are divided into four chemical groups (CGs): Group One (CG1) includes OCPs and PCBs; Group Two (CG2) includes PAHs; Group Three (CG3) includes ONPPs; and Group Four (CG4) includes PAEs).

with multiple rings in their structure, such as benzo(b)fluoranthene, benzo(k)fluoranthene, benzo(a)pyrene indeno(1,2,3-cd)pyrene, and benzo(ghi)perylene, were ranked at the top of the prioritization list for Lake Chaohu, indicating a high risk potential. In contrast, PAHs with fewer rings in their structure, such as naphthalene, acenaphthene, and acenaphthylene, were ranked toward the bottom of the list, indicating a low risk. Most of the PAEs were ranked toward the bottom of the list, indicating a low risk.

3.3.2. Ranking and screening using ecological risk as calculated using BMC

Chemical ranking using PNEC values was only a preliminary sorting method, and ecological risk as evaluated by combining EEC and toxicity data enabled a refined assessment. According to the ecological risk that was calculated using BMC, 48 PTSs, each with their own SSD models, were ranked (Fig. 6). When the 50th centile of chemical concentrations was assigned, the 50th centile value for certain PTSs was zero because these PTSs, such as benzo(a)pyrene and di-n-octyl phthalate, were not detected during most of the sampling events. When 90th centile value was assigned, 48 PTSs could be ranked. We obtained similar results no matter which centile was chosen. Most of the ONPPs were at the top of the ranking, and their associated ecological risks were 0.1 to 0.001, indicating that they posed high risk to the Lake Chaohu ecosystem. OCPs, such as endosulfan I and hexachlorbenzene, posed high potential risks, as did chrysene. Di-n-octyl phthalate and di-n-butyl phthalate posed high risk because di-n-octyl phthalate is highly toxic, and di-n-butyl phthalate was detected at high frequency. If very high or high risk criteria (<0.001) were set, the PCCs would be ranked as follows: di-n-octyl phthalate, methamidophos, omethoate, malathion, hexachlorbenzene, dichlorvos, dimethoate, di-n-butyl phthalate, endosulfan I, methylparathion, carbaryl, ethyl para-nitro-phenyl, parathion, and sulfotep. If potential risk was considered, more PTSs would be included in the

ranking, as follows: butylbenzyl phthalate, chrysene, acenaphthene, PCB28, fluorine, atrazine, α -HCH, dimethyl phthalate, p,p'-DDE, diethyl phthalate, fluoranthene, naphthalene, and p,p'-DDD. In summary, ONPPs, endosulfan I, hexachlorbenzene, di-n-butyl phthalate, and di-n-octyl phthalate should be given more attention than the other PTSs for PCC in Lake Chaohu.

3.3.3. Ranking and screening using EEC/PNEC

Although ranking using ecological risk gave absolute risk values for PTSs, many chemicals could not be included because of a lack of available data. Moreover, the RQ method, which is based on the PNEC and EEC values, incorporated the toxicity of chemicals and their concentrations in the environment. Although environmental workers without comprehensive mathematical knowledge still require training for this method, it's easier for them to master it than other assessment methods. The rankings of toxic organic chemicals in Lake Chaohu based on EEC values are presented in Table S2, and those rankings based on PNEC values are presented in Table S9. These values are shown in Figs. S15–S16 and illustrated in more detail in Fig. 7. Regardless of the EEC or PNEC values were selected for the analysis, we found that ONPPs posed a high potential risk, as indicated by their low EEC and PNEC values; OCPs posed low risk, indicated by their high EEC and PNEC values; and PAH-associated risks were also low, as indicated by their EEC/PNEC values of less than 1 and their middle-position in the chemical ranking. PAHs are not very soluble. The light weight ones easily evaporate and heavy weight ones tend to be detected in tissue and bile (Cormier et al., 2000; Lin et al., 1996; Norton et al., 2002). PAHs' ecological risks would be corrected when considering their bioaccumulation in the organism in the future study. PAEs such as di-n-butyl phthalate and di(2-ethylhexyl) phthalate posed a high potential risk, whereas the other PAEs posed relatively low risks. The 90th centile

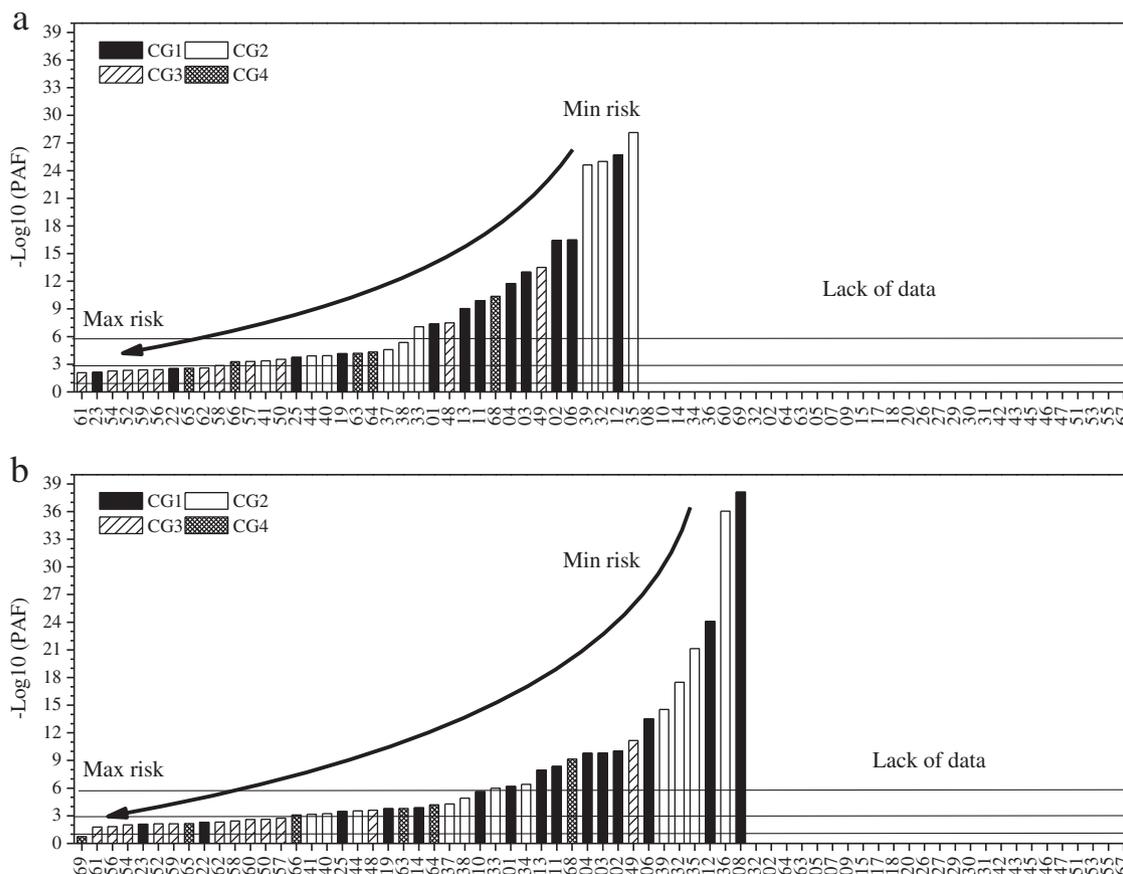


Fig. 6. Ranking of toxic organic chemicals in Lake Chaohu based on associated ecological risk at the mid-level as evaluated by BMC, with the 50th (Chart a) and 90th (Chart b) centiles of chemical concentrations.

EEC value was greater than the detected EECs in 90% of the sampling events. For maximum protection of aquatic organisms, the $EEC_{90}/PNEC$ quotient was chosen to rank and screen PPCs in Lake Chaohu. Based on this $EEC_{90}/PNEC_{SSD}$ quotient, PCCs was ranked as follows: di-n-octyl phthalate, di-n-butyl phthalate, atrazine, parathion, malathion, omethoate, dichlorvos, methamidophos, and anthracene. Based on the $EEC_{90}/PNEC_{AF}$ quotient, the PCCs were ranked as follows: methyl-parathion, parathion, malathion, atrazine, di-n-butyl phthalate, dichlorvos, demeton-s, carbaryl, ethyl para-nitro-phenyl, omethoate, methamidophos, and anthracene. Lastly, based on the $EEC_{90}/PNEC_{QSAR50}$ quotient, the PCCs were ranked as follows: methyl-parathion, dimethoate, demeton-o, parathion, dichlorvos, demeton-s, omethoate, malathion,

di-n-butyl phthalate, di(2-ethylhexyl) phthalate, monocroptophos, atrazine, and carbaryl.

3.3.4. PCC list in Lake Chaohu and its comparison with China's present PCC list

Based on the frequency of any specific chemical in the four PPC lists (Figs. 6b and 7), PPCs in Lake Chaohu were screened and ranked as follows (Fig. 8): (1) the PPCs with the highest priority included parathion, dichlorvos, malathion, omethoate, and di-n-butyl phthalate; (2) the PPCs with the second highest priority included atrazine, carbaryl, methamidophos, and methyl-parathion; (3) the PPCs with the third highest priority included anthracene, demeton-s, dimethoate, ethyl

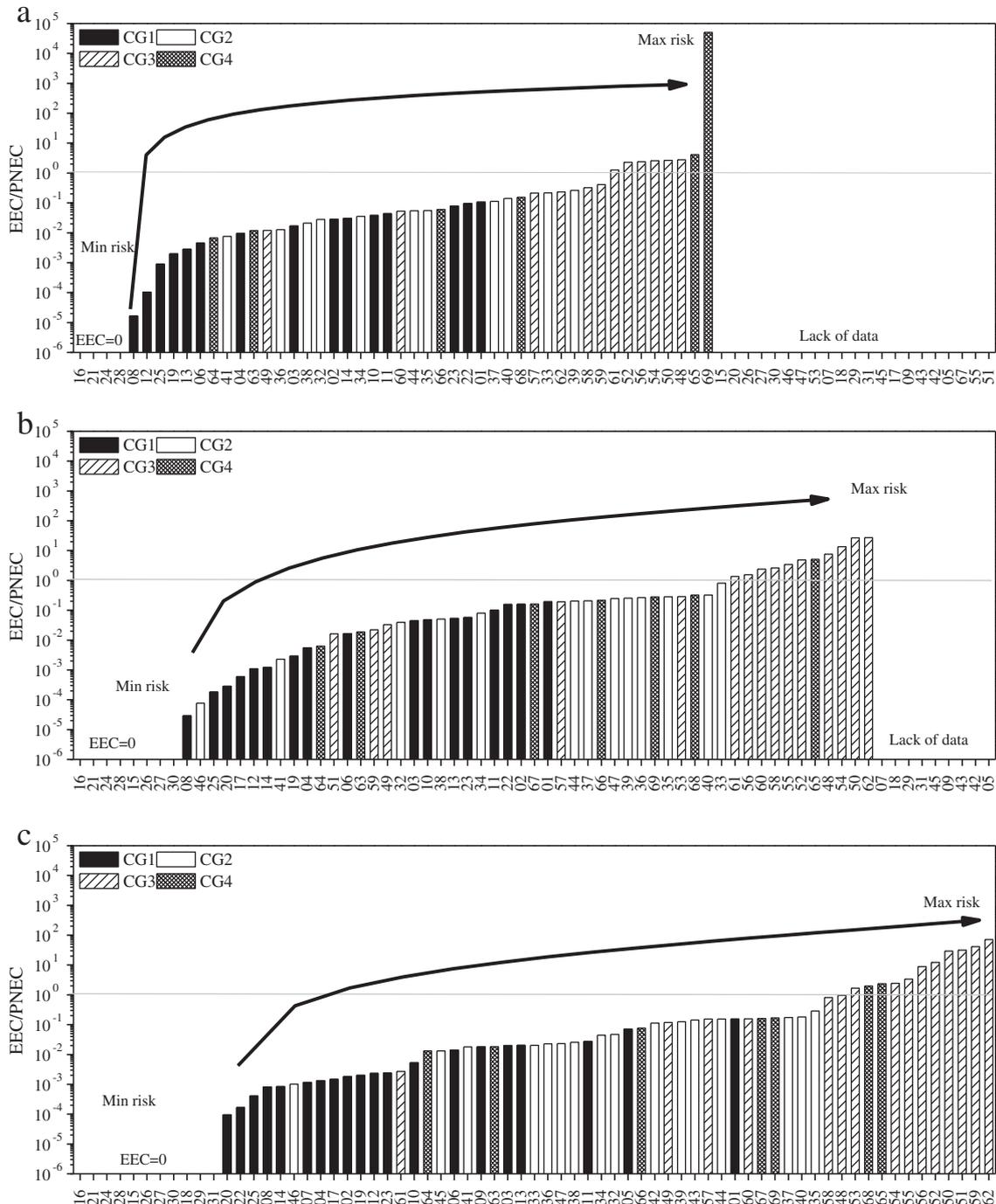


Fig. 7. Ranking of toxic organic chemicals in Lake Chaohu based on the $EEC_{90}/PNEC_{SSD}$, $EEC_{90}/PNEC_{AF}$ and $EEC_{90}/PNEC_{QSAR50}$ quotients.

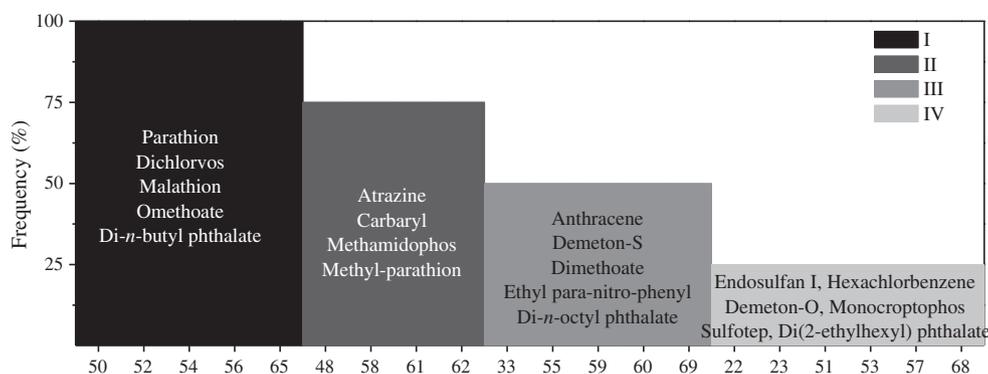


Fig. 8. The frequency of specific chemicals in the four PPC lists from Figs. 5b and 6 It indicates the relative risk; that is, most frequent on the left are likely to be causing adverse effects in Lake Chaohu and those on the far right less so.

para-nitro-phenyl, and di-n-octyl phthalate; and (4) the PPCs with the fourth highest priority included endosulfan I, hexachlorbenzene, demeton-o, monocrotophos, sulfotep, and di(2-ethylhexyl) phthalate.

In the 1990s, China's National Environment Monitoring Station (NEMS) established a priority pollutant list that included 58 toxic organic pollutants, 1 cyanide compound, and 9 heavy metals (Zhou et al., 1991). This list was only a guide for controlling priority chemicals throughout China, but different regions in China had specific pollution challenges. PPCs should also be regulated based on their priority grades; however, the national "blacklist" of priority pollutants did not provide a grading strategy. In the present study, only 7 of 20 PCCs in Lake Chaohu were listed on the national "blacklist" of toxic compounds. If this list were used for chemical pollutant regulation of Lake Chaohu, the risk of certain PTSs, such as malathion, omethoate, atrazine, carbaryl, and methyl-parathion, may be overlooked. Hence, governments should screen the regional PPC lists or develop a more comprehensive national list for aquatic ecosystem protection in China.

4. Conclusions

QSAR was utilized as a preliminary method for developing WQC, especially for organic compounds that have only recently been developed. Our study demonstrated that modified by median of P/O values had the advantages of both modified by arithmetic mean and by geometric mean and was chosen to calculate PNEC. Differences between the preliminary assessment results ($PNEC_{AF}$ or $PNEC_{QSAR50}$) and the refined assessment results ($PNEC_{SSD}$) were minor. China's present WQC underestimate the risk to organisms in aquatic ecosystems. It is necessary to develop a new standard for developing WQC to protect aquatic organisms. Our assessment showed that aquatic organism in Lake Chaohu was confronted by high-level of ecological risk from PTSs such as ONPPs and PAEs. Because those chemicals were used widely, determined at the mid-to-high-level of concentrations, and associated with a high level of ecological risk. On the contrary, OCPs have been banned for many years, and the ecological risk posed by these chemicals was more limited. Four grades of PCCs, including 20 PTSs, were measured in Lake Chaohu, and the highest priority chemicals identified were primarily ONPPs, including parathion, dichlorvos, malathion, omethoate, and di-n-butyl phthalate. However, the national "blacklist" of toxic compounds only covered 7 of 20 PCCs, indicating that the other 13 PCCs would not be controlled efficiently. Because the pollution pattern of PTSs in various water bodies might be quite different, we appealed to the governments to screen the regional PPC lists or develop a more comprehensive national list for aquatic ecosystem protection in China.

Conflict of interest

There is no any conflict of interest.

Acknowledgments

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <http://dx.doi.org/10.1016/j.scitotenv.2013.11.119>.

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