Wen *et al. Environmental Sciences Europe* (2024) 36:35
https://doi.org/10.1186/s12302-024-00855-3

Environmental Sciences Europe

RESEARCH **Open Access**

Priority screening on emerging contaminants in sediments of the Yangtze River, China

Yu Wen[1], Siyu Huang[1,2], Zhihao Qin[1], Zhongli Chen[1] and Ying Shao[1,3*]

Abstract

Background Screen the priority of emerging contaminants (ECs) from sediments is essential for risk assessment to aquatic environment and human health. Currently, priority approaches mainly focus on contaminant identification, exposure analysis, risk assessment, and hazard properties. However, there is still far from the reality due to, for instance, limitations on lack of occurrence data and uncertainty analysis. In this study, the multi-criteria screening method on the basis of hazard potential (HP) and exposure potential (EP) integrating with uncertainty analysis was developed for prioritization of 185 ECs, which have been reported to be widely found in the Yangtze River sediment. The HP based on the ecological risk and human health, and the EP according to the occurrence were both quantitatively analyzed. The priority index of these 185 chemicals was the product of the normalized HP and the normalized EP.

Results According to the priority ranking scheme, 20 chemicals were identified as the top-priority, and 58 compounds as high-priority, respectively. After uncertainty scoring for each chemical based on data availability, there were 7 compounds (5 pesticides and 2 PFASs) recommended as the major priority ECs. In addition, the current study also emphasized that necessary for further studying some ECs, such as PFAS alternatives, as the data limitation may lead to reduce accurate prioritization.

Conclusions Overall, this study provides an efficient approach for screening priority ECs, which is useful for river ecosystem health management.

Keywords Emerging contaminants, Prioritization, The Yangtze River, Sediments, Hazard potential, Exposure potential

Background

Emerging contaminants (ECs), such as plasticizers, antibiotics, per- and polyfluoroalkyl substances (PFASs), pesticides, and flame retardants, have caused growing concerns for both environments and human beings. The ECs usually consist all or part of the characteristics, which are great harm, hidden risk, environmental persistence, extensive sources, and complex management [1]. These chemicals are necessary and continually used in industry, agriculture and personal products. ECs access the sediment environment by diverse means, including agricultural production activities [2, 3], municipal waste [4], reclaimed wastewater irrigation [5, 6], and atmospheric deposition [7]. Due to continuous consumption, ECs have been frequently detected in various sediments at 10^{-10} to 10^{-6} g g^{-1} [8–12]. Studies have reported that ECs can induce ecological risk and human health even at concentrations of 10^{-9} $g{\cdot}g^{-1}$ [13–15]. Hence, ECs have received significant attention owing to their harmful effects on ecosystem and human health [16]. However,

---

*Correspondence:
Ying Shao
ying.shao@cqu.edu.cn
[1] Key Laboratory of the Three Gorges Reservoir Region's Eco-Environment, Chongqing University, Chongqing 400030, People's Republic of China
[2] Chongqing Institute for Food and Drug Control, Chongqing 401121, People's Republic of China
[3] College of Environment and Ecology, Chongqing University, 174 Shazheng Street Shapingba, Chongqing 400045, People's Republic of China

most ECs are not regulated in many countries around the world [17].

The Yangtze River is the third longest river in the world and its basin covers about one-fifth of China's total land area [18]. More than 40 percent of China's population life in the watershed area [19]. In recent decades, a large number of treated sewage and industrial wastewater have been discharged into the Yangtze River (25 billion tons/year), accounting for 42 percent of the country's total sewage discharge [20, 21]. The surrounding soil and sediment of the river have been contaminated accordingly. Previous studies indicated that sediment may act as both sink and source of pollutants in aquatic systems [22]. Since water regime, for instance, the fluctuation of water level could cause pollutants such as ECs in sediment either return to the water body or suspend, both of which could bring potential risk to ecological environment and even human health. Therefore, understanding the potential risk of ECs in river ecosystem, in particular for sediments is essential for pollution control and ecosystem health maintain.

Based on the large amount of organic contaminants (about 10^8 chemicals in 2014) in the environment [23], regulated and monitored chemicals, however, are only minor part of those massive amount of the chemicals present in environments [24]. Therefore, it is necessary to prioritize the compounds to ensure efforts on controlling and reducing potential threats. Currently, methods on identifying priority ECs from water bodies have been developed. For instance, the NORMAN network used a decision tree to divided ECs into 6 categories [25], such a decision tree-based approach is difficult to easy-to-implement. The Ministry of Ecology and Environment of China have published "list of key controlled emerging contaminants (2023 version)" [26] by combing semi-quantitative methods and specialist suggestions, leading to subjective influences on the final list [27]. Besides, methods relying on ecotoxicity or human health effects have been established to screen pollutants for priority controlling [28, 29]. At present, the prioritization systems typically include contaminant identification, exposure analysis, risk assessment, and hazard properties [30]. Whereas, these methods have not taken environmental occurrence into consideration [31], which may lead to loss of accuracy on prioritization. To improve prioritization strategies, ideas on ranking pollutants by multi-criteria analysis approach have been recommended [32]. For example, the EU Water Framework Directive (WFD) has developed a screening method relying on a weighted average of diverse effect scores of the exposure and effect index, such as hydrotoxicity, bioaccumulation and human health hazards [33]. By this, determination on the relative materiality of each criterion is possible, while the intrinsic connections among the criteria are ignored. The priority ranking of pollutants in China's water bodies has been studied, in which estimating substance concentrations [34] by non-determinism analysis, and focusing on ecological risks [35] with narrowing scope of pollutant categories [36]. In fact, most of the existing priority screening of ECs are mainly aimed at water bodies, with rare studies focus on sediments and soils [37, 38].

Therefore, to address the limitations on ECs prioritization in sediments, this study developed the multi-criteria screening method that considered both exposure potential (EP) and hazard potential (HP) [30]. The evaluation parameters were persistence, bioaccumulation, ecotoxicity, human health effects, concentration and detection frequency of ECs. The relative materiality of each standard was judged by multiple linear regression model analysis, and the selected ECs were prioritized according to the results of priority analysis and uncertainty analysis. Finally, the ECs (plasticizers, PFASs, pesticides, flame retardants, antibiotics, PCBs) in the Yangtze River sediment were used for multi-class prioritization, which provides useful methodology for ECs management in large rivers worldwide.

Materials and methods

Data collection

Data were collected for six indicators of persistence, bioaccumulation, ecotoxicity, human health effects, concentration, and detection frequency. The detailed workflow for the ECs priority ranking is shown in Fig. 1.

Occurrence data

The occurrence data of ECs in sediments of the Yangtze River during 2013–2023 were obtained from government reports and/or publications by searching in Web of Science with the topic words "phthalates", "Per- and polyfluoroalkyl substances", "pesticides", "flame retardants", "antibiotics" or "PCBs" in combination with "Yangtze River", "soil" or "sediment". The topic words of the ECs belong to six categories, which have been widely detected in the Yangtze River basin, and their ecotoxicity and human health risk effects have been reported [39–44].

Data preprocessing efforts involved [30]: (1) the medians of all concentration and detection frequency, less affected by outliers, are used; (2) the means of concentration and detection frequency are used when median values were incalculable or not detected (ND); (3) employing half of the limit of detection (LOD) or half of the method detection limit (MDL) when ECs were not detected.

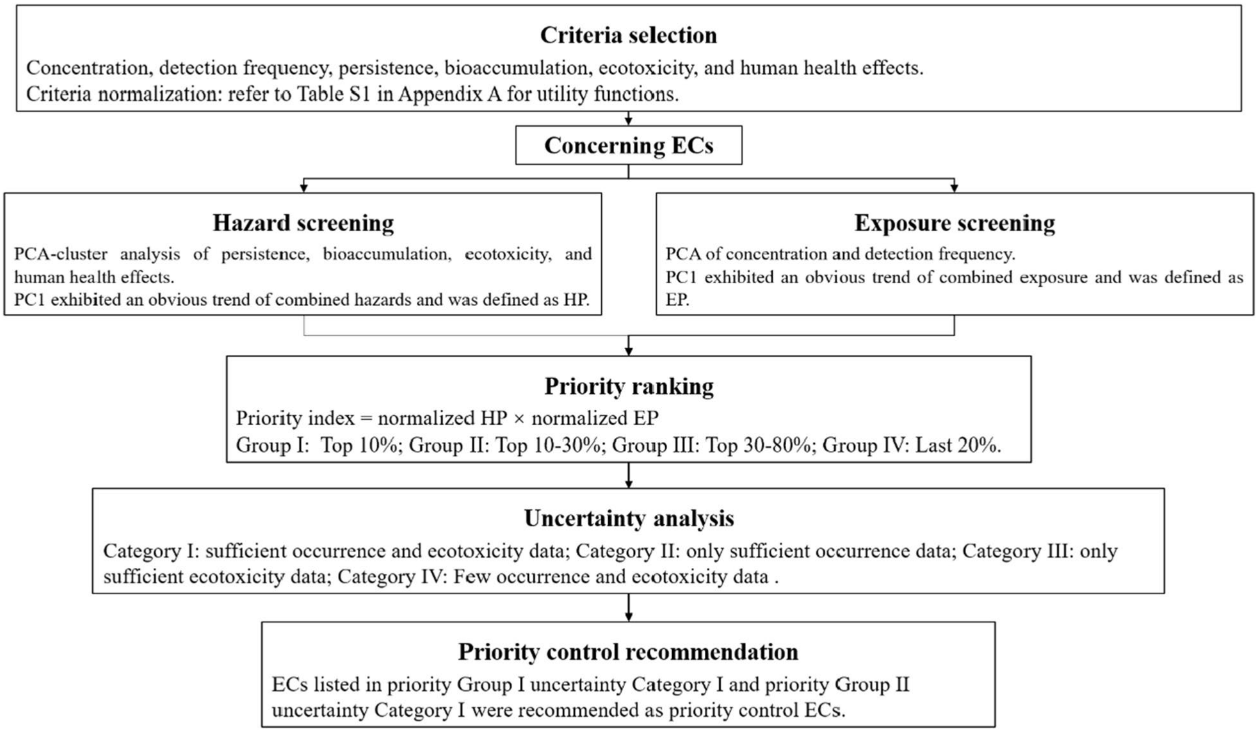


Fig. 1 The flow of the multi-criteria approach for screening priority emerging contaminants (ECs). *PC1* principal component 1, *HP* hazard potential, *EP* exposure potential, *Groups I–IV* top, high, moderate, and low priority group

Persistence and bioaccumulation

The degradation half-life (DHL), which was determined by the BIOWIN v4.1 module [45], was used to indicate persistence. The sole criterion to judge the persistence time was the ultimate biodegradability, and the values for ultimate biodegradability of each chemical corresponded to the time as follows: five for hours; four for days; three for weeks; two for months; and one for longer period. The bioaccumulation was associated with octanol–water partition coefficient, using KOWWIN v4.1 [45] in the EPI component for calculation.

Ecotoxicity

Ecological environment effects were expressed using predicted no-effect concentrations of ecological ($\mathrm{PNEC_{eco}}$), which was obtained by dividing the using the lowest lethal median concentration ($\mathrm{LC_{50}}$) or half-effect concentration ($\mathrm{EC_{50}}$) by the appropriate assessment factor (AF). The conversion of corresponding data to the PNEC value in the sediment was conducted using Eqs. (1) and (2):

$$\mathrm{PNEC_{sediment}} = f_{\mathrm{oc}} \cdot k_{\mathrm{oc}} \cdot \mathrm{PNEC_{aqua}}, \tag{1}$$

$$\mathrm{PNEC_{aqua}} = \frac{\mathrm{EC50/LC50}}{\mathrm{AF}}. \tag{2}$$

$\mathrm{PNEC_{aqua}}$ represents the PNEC value of water; f_{oc} is the weight fraction of organic carbon in sediment, $f_{\mathrm{oc}} = 0.1$.

Depending on data availability, $\mathrm{EC_{50}/LC_{50}}$ of the chemical was used in this study and AF was set to 1000. The $\mathrm{EC_{50}/LC_{50}}$ values were gained from the US EPA ECOTOX knowledgebase [46], the US Department of Agriculture, Agriculture Research Service Pesticide Properties Database [47], published articles [11, 14, 48–54], and the US EPA Ecological Structure Activity Relationships (ECOSAR) model [45].

The $\mathrm{RQ_{eco}}$ value is calculated as following Eq. (3) [55]:

$$\mathrm{RQ_{eco}} = \frac{\mathrm{MEC}}{\mathrm{PNEC_{eco}}}, \tag{3}$$

where RQ is the ecological risk value of EC compound; MEC is the actually measured EC concentration; and $\mathrm{PNEC_{eco}}$ is the predicted no-effect concentration.

Human health effects

The evaluation of human health effects considered adults exposure through rice and vegetables, utilizing $\mathrm{PNEC_{hum}}$ (ng $\mathrm{g^{-1}}$). Based on Eq. (4), the $\mathrm{PNEC_{hum}}$ values were determined considering acceptable daily intake (ADI, $\mathrm{mg{\cdot}kg^{-1}{\cdot}day^{-1}}$), minimal risk level (MRL) or reference dose (RfD):

$$\mathrm{PNEC}_{\mathrm{hum}} = \frac{1000 \times \mathrm{ADI} \times \mathrm{BW} \times \mathrm{AT}}{(\mathrm{IngRr} + \mathrm{IngRv}) \times \mathrm{BCF} \times \mathrm{EF} \times \mathrm{ED}}, \tag{4}$$

where 1000 was a conversion factor (ng·ug^{-1}); when ADI is unavailable, either RfD or MRL value would be utilized; the body weight (BW) of an average Chinese adult was set at 63 kg [56]. AT was the average exposure time for adults, setting at 10,500 d [14]. IngRr was the adult rice ingestion rate, setting at 279.2 g·d^{-1}, IngRv was the adult vegetable ingestion rate, setting at 92.3 g·d^{-1} [14]. The bioconcentration factor for ECs in terrestrial organism was noted as BCF. In the current study, soil adsorption allocation coefficient (K_{oc}) was used to estimate BCF, deriving from Kenaga and Goring [57], lgBCF = 1.12lgKoc − 1.58, the Koc value is calculated using KOCWIN v4.1 [45] in the EPI component. EF denoted the exposure frequency, which was set at 350 d·a^{-1}, and ED was the exposure duration, setting at 30 years [30].

The ADI values of pesticides were prepared with reference to the national food safety standard (GB 2763–2021) [58], and that for antibiotics were prepared with reference to the national food safety standard (GB 31650–2019) [59]. The other ADI values of plasticizers and PCBs were derived from Zhong et al. [30] and Ossai and Sun et al. [60, 61], respectively. The MRLs of PFASs and flame retardants were acquired from the U.S. Department of Health and Human Services' Agency for Toxic Substances and Disease Registry [62]. Some of the ADI/RfD/MRL values that were not available were replaced by the median values of the category chemicals.

The health risk assessment ($\mathrm{RQ}_{\mathrm{hum}}$) value of the ECs is calculated as following Eq. (5):

$$\mathrm{RQ}_{\mathrm{hum}} = \frac{\mathrm{MEC}}{\mathrm{PNEC}_{\mathrm{hum}}}, \tag{5}$$

where $\mathrm{RQ}_{\mathrm{hum}}$ is the health risk assessment value of each EC; MEC is the actually measured EC concentration; and $\mathrm{PNEC}_{\mathrm{hum}}$ is the predicted no-effect concentration.

Prioritization

Normalization of criteria-specific data

Due to the fact that data sources were from literature, government report or publications, the min–max normalization method was approved to normalize data into dimensionless items in the range of 0–1 (Additional file 1: Table S1). The min–max normalization method, on one hand can maintain the distribution and relative size relationship of the original data, on the other hand, it has less impact on outliers and thus reduces its impact on the overall data. The method is derived from Kumar and Zhong [30, 32]. The respective orders of magnitude for environmental EC concentrations, $\mathrm{PNEC}_{\mathrm{eco}}$ values, and $\mathrm{PNEC}_{\mathrm{hum}}$ terms were 6, 8, and 12. To reduce the data discreteness and facilitate data calculation, the PNEC and concentration values were, respectively, converted to $\log_{10}$- and $\log_2$-due to the wide distributions. In order to supply a logical distribution of values for each particular criterion, the utility function carefully selected the highest and lowest values to ensure the dimensionless utility function terms would cover the range 0 to 1 across all ECs. These utility functions were utilized chemical scores.

Multivariate analysis

Principal component analysis (PCA) is used in this research, in which the largest variation is captured by the PC1, which can be applied as a new cumulative variable for ECs screening and sorting [63]. The degradability of volatile organic pollutants has been explained using the term PC1 in prior research [64], the persistence, bioaccumulation, and toxicity (PBT) characteristics of contaminants [65], and comprehensive aquatic toxicity at different nutrient levels [66, 67]. The current study used PCA to analyze the standardized data related to four hazard indicators: persistence, bioaccumulation, ecotoxicity, and human health effects. The $\mathrm{PC1}_{\mathrm{hazard}}$ was determined as a HP value which the four hazard impacts were evaluated comprehensively. Likewise, standardized criteria-specific data for two exposure factors (pollutant concentration and detection frequency) were analyzed using PCA. The EP was illustrated by utilizing the $\mathrm{PC1}_{\mathrm{exposure}}$.

Scoring

The utility function was used to convert the EP and HP into dimensionless terms within the range of 0–1. By performing the multiplication of the normalized EP and normalized HP, the priority index for pollutant classification was determined. The dimensionless EP, HP value and priority index were calculated according to the following utility functions (6), (7) and (8):

$$U(\mathrm{EP}) = \frac{\mathrm{EP} - \mathrm{EP}_{\mathrm{min}}}{\mathrm{EP}_{\mathrm{max}} - \mathrm{EP}_{\mathrm{min}}}, \tag{6}$$

$$U(\mathrm{HP}) = \frac{\mathrm{HP} - \mathrm{HP}_{\mathrm{min}}}{\mathrm{HP}_{\mathrm{max}} - \mathrm{HP}_{\mathrm{min}}}, \tag{7}$$

$$\text{Priority index} = U(\mathrm{EP}) \times U(\mathrm{HP}), \tag{8}$$

where $\mathrm{EP}_{\mathrm{max}}$ is the maximum EP in the overall list of candidate ECs, $\mathrm{EP}_{\mathrm{min}}$ is the lowest EP value in the overall list of candidate ECs; $\mathrm{HP}_{\mathrm{max}}$ is the maximum HP in the overall list of candidate ECs, $\mathrm{HP}_{\mathrm{min}}$ is the lowest HP value in the overall list of candidate ECs; the priority index determines the priority ranking of chemicals.

In this study, a multiple linear regression model was used to quantitatively represent the relationship between concentration, detection frequency and EP. Similarly, multiple linear regression model was used to quantify the relationship between persistence, bioaccumulation, ecotoxicity, human health effects and HP. Standardized values are used for the above parameters.

Uncertainty analysis

Regarding uncertainty analysis, the uncertainty score should be derived from the accessibility of monitoring data (Table 1). The occurrence data of this study were obtained from previous studies, in which when the data of occurrence were obtained from a minimum of 4 provinces and 50 sites, the uncertainty scores of pollutant concentrations and detection frequencies were 0. If data of occurrence were from fewer than 4 provinces or less than fifty sites, the uncertainty scores were set at 0.25. In case of occurrence data were not available, the uncertainty scores were established as 0.5. The lack of experimental data, the model-based toxicity, ADI values, and BCF values provided a significant level of uncertainty regarding ECs. The ecotoxicity and human health effects uncertainty scores were 0 when experimental data were used for PNEC calculations, yet they increased to 0.25 after incorporating model-based evaluations, and further rose to 0.5 without any experimental or evaluated data. As all the data of human health effects were from model calculation, all chemicals had an uncertainty score basis of 0.25 in the human health effect criteria. About the remaining criteria, chemical data availability and unavailable determined the assignment of uncertainty scores as either 0 or 0.5. Finally, the aggregate uncertainty scores were decided by using the arithmetic mean of the each uncertainty scores of the 6 criteria.

Results

Concentration and detection frequency of ECs

Overall, a total of 185 ECs including priority controlled chemicals in China (Additional file 1: Table S2), were selected from 2399 sites in 10 provinces or municipalities (Additional file 1: Figure S1). The median concentration of these 185 compounds ranged from 5×10^{-5} ng g^{-1} to 835 ng g^{-1}, with 4 compounds (DBP, DEHP, TBOEP, 6:2 FTOH) exhibiting median concentration (>100 ng g^{-1}). The plasticizers displayed a higher median concentration (1.8 ng g^{-1}), followed by pesticides (0.89 ng g^{-1}), and PCBs (0.71 ng g^{-1}). The flame retardants and PFASs exhibited low median concentration, with the mean values up to 0.49 and 0.25 ng g^{-1}, respectively. Antibiotics had the lowest median concentration which was below 0.1 ng g^{-1}. The average ECs detection frequency was greater than 35% for all categories except antibiotics (21.9%) (Fig. 2).

Persistence, bioaccumulation, ecotoxicity and human health

The 4 criteria values of 185 ECs can be seen in Additional file 1: Table S4. The DHL values representing persistence for the 185 selected compounds ranged from −2.36 to 3.66, and their $\mathrm{LogK_{ow}}$ values ranged from −3.21 to 12.11. The $\mathrm{PNEC_{eco}}$ value ranged from 0.01 to 1.08×10^{5} ng g^{-1}, while the $\mathrm{PNEC_{hum}}$ value were between 1.36×10^{-7} and 3.29×10^{6} ng g^{-1}. All data are presented in Fig. 3. Overall, plasticizers revealed comparatively high DHL with a median value of 3.11, followed by antibiotics (1.99), flame retardants (1.83), pesticides (1.74), PCBs (1.44) and PFASs (0.74). PCBs displayed higher $\mathrm{LogK_{ow}}$ with a median value of 6.98, followed by flame retardants (5.88). The other categories observed a sequential drop in their median $\mathrm{LogK_{ow}}$ as follows: plasticizers (4.61), pesticides (4.56), PFASs (4.46) and antibiotics (0.43). PCBs and pesticides showed relatively low $\mathrm{PNEC_{eco}}$ with the median values of 60.18 ng g^{-1} and 61.00 ng g^{-1} followed by flame retardants (159.16 ng g^{-1})

Table 1 Split-point values assigned to uncertainty categories I–IV for ECs in the Yangtze River sediment

Uncertainty category	Description	Proportion of chemicals detected in all sample sites	Ecological risks
I	Plenty monitoring data and hazard assessment utilizing experimental toxicity	≥ 4 provinces and ≥ 50 sites	Both effects utilizing experimental data
II	Sufficient monitoring data but hazard assessment utilizing predicted toxicity	≥ 4 provinces and ≥ 50 sites	One or two effects utilizing predicted data
III	Ecological risk assessment utilizing experimental toxicity but few monitoring data	< 4 provinces and ≥ 50 sites	Ecotoxicity effect utilizing experimental data
IV	Few monitoring data and hazard assessment utilizing predicted toxicity	< 4 provinces and ≥ 50 sites	Ecotoxicity effect utilizing predicted values

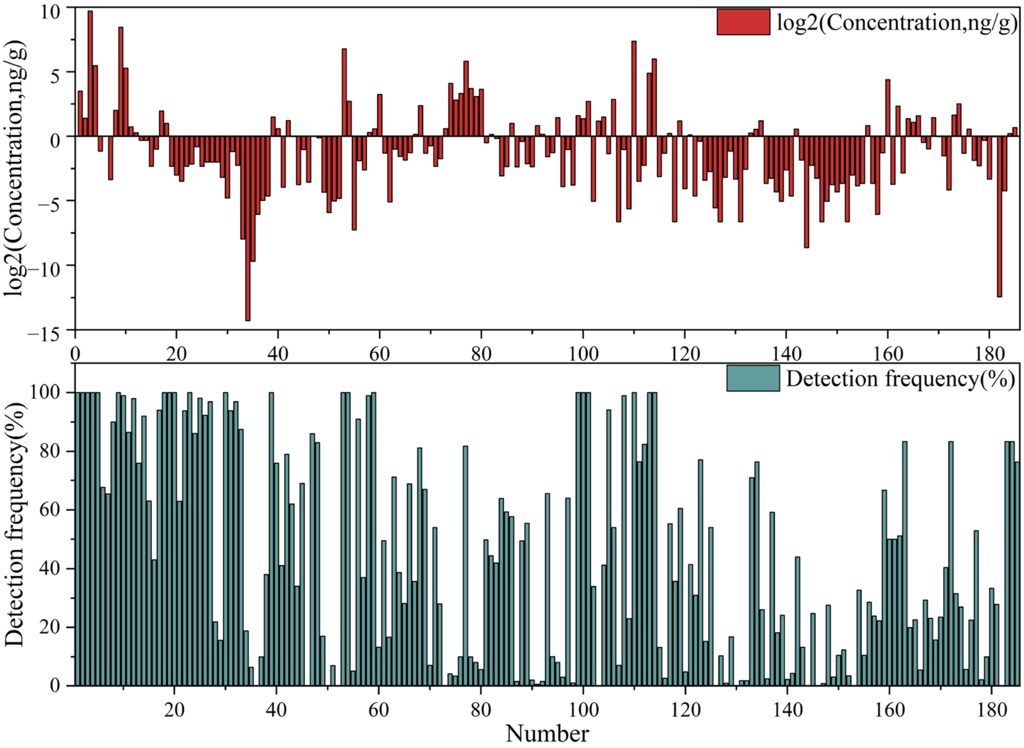


Fig. 2 The $\log_2$concentration and detection frequency of the 185 compounds (the names of these chemicals are listed in Additional file 1: Table S2)

and plasticizers (234.31 ng g^{-1}). The order of increased median $PNEC_{eco}$ of other categories were as follows: antibiotics (670.35 ng g^{-1}), PFASs (1297.53 ng g^{-1}). The PCBs showed relatively low $PNEC_{hum}$ with median values of 0.22 ng g^{-1}, followed by flame retardants (599.05 ng g^{-1}). The progression of increased median $PNEC_{eco}$ for the remaining categories unfolded in the sequence: pesticides (2027.60 ng g^{-1}), PFASs (3614.23 ng g^{-1}), plasticizers (9.8×10^5 ng g^{-1}) and antibiotics (1.27×10^6 ng g^{-1}).

Hazard and exposure assessment

In the current study, a PCA analysis was conducted on these 185 compounds. As shown in Fig. 4, $PC1_{hazard}$ played a major part with an explanation rate of 54.9%, $PC2_{hazard}$ constituted 25.0% and explaining the further hazard parameters. For instance, compounds with greater ecotoxicity and human health effects were located at the top right of the PCA score chart, yet ECs with greater persistence and bioaccumulation were situated in the bottom right of the PCA score chart (Fig. 4a). The 4 hazard criteria completely enhanced with $PC1_{hazard}$, indicating prospective tendencies for the HP parameter. Ranging from −2.65 to 4.37, the HP values of the 185 chemicals are listed in Additional file 1: Table S5. On the whole, PCBs displayed higher median HP value (1.61), followed by flame retardants (0.58) and PFASs (0.33). The median HP value of pesticides (0.20) located in the middle. The plasticizers (−1.12) and antibiotics (−1.55) showed relatively low HP. The relative importance of the 4 hazard parameters to the HP was quantitatively analyzed using a multiple linear regression analysis, and the proportions of DHL, $LogK_{ow}$, $PNEC_{eco}$ and $PNEC_{hum}$ were 2.674, 3.086, 1.292 and 3.109, respectively.

The PCA analysis results of the exposure parameters for the 185 ECs could be obtained from Fig. 4b and Additional file 1: Table S6. The explanation of the total variance was divided between $PC1_{exposure}$ (72%) and $PC2_{exposure}$ (27%). The range of EP values of the 185 ECs varied between −3.17 to 3.28. Actually, the EP of plasticizers stood at 1.33, marking the highest median value, followed by PFASs at 0.66. The medium median EP of the categories were pesticides (0.20) and flame retardants (0.20). The lower median EP of the categories were PCBs (−0.03) and antibiotics (−1.11). The relationship between EP and the 2 exposure parameters was investigated through multiple linear regression analysis, and the proportions of concentration and frequency were 4.856 and 1.96, respectively.

Priority index

The listing of the priority indices for the concerning ECs is displayed in Additional file 1: Table S7. The 185

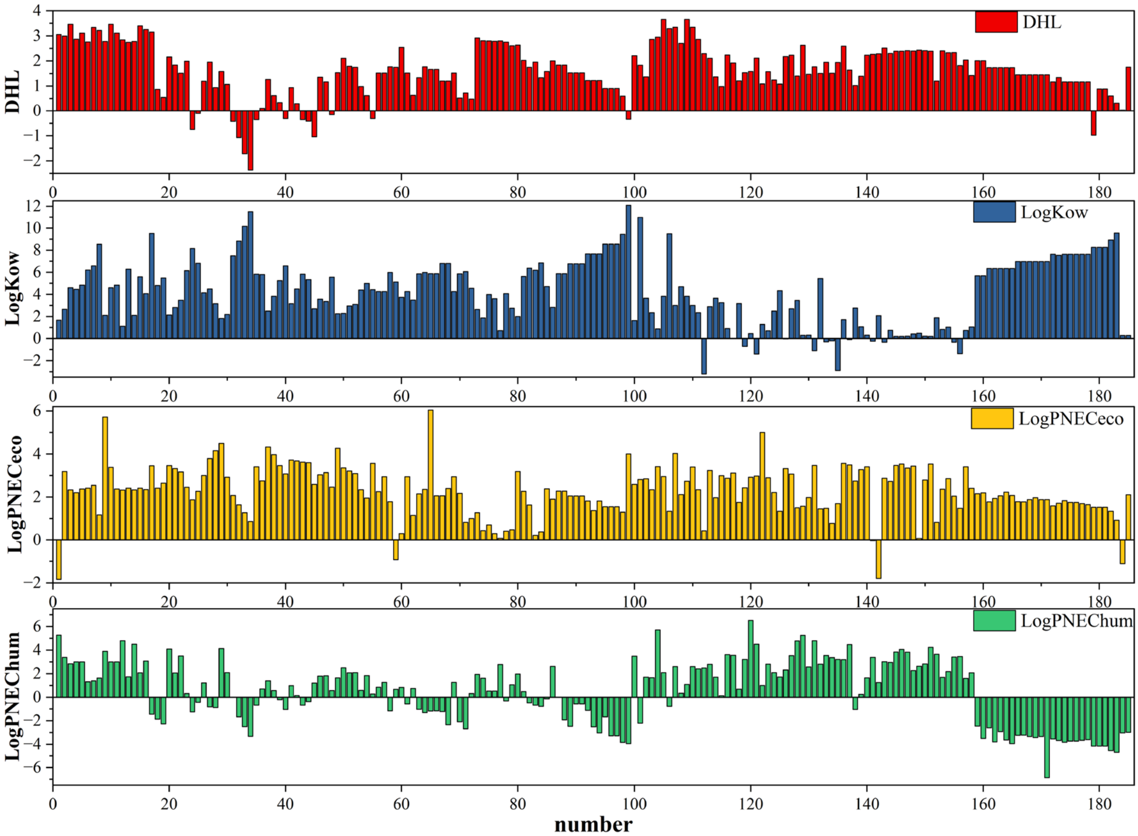
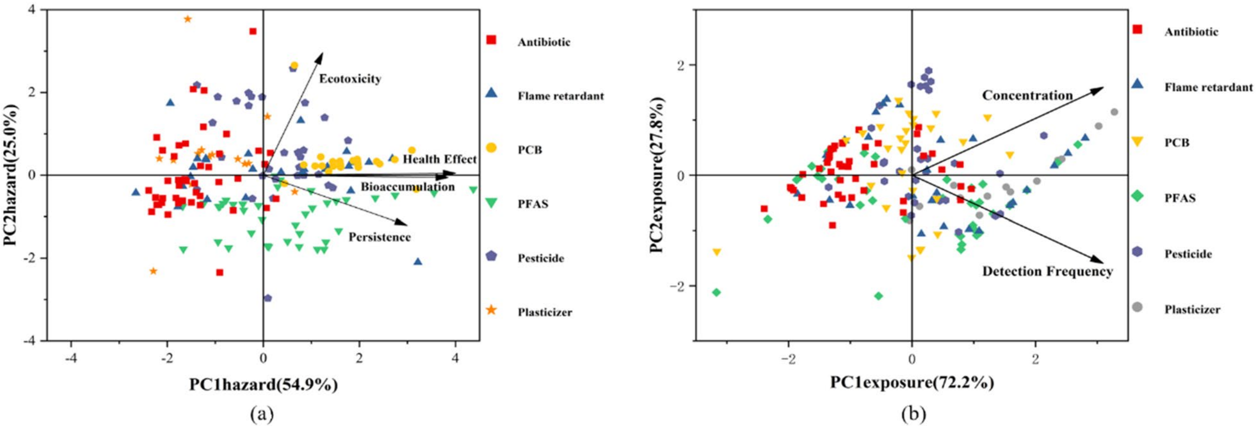


Fig. 3 The persistence, bioaccumulation, $\mathrm{logPNEC_{eco}}$ and $\mathrm{logPNEC_{hum}}$ of plasticizers, pesticides, PFASs, flame retardants, antibiotics and PCBs



(a) (b)

Fig. 4 PCA for the four hazard parameters (**a**) ($\mathrm{PC1_{hazard}}$ denoted the integrated HP) and PCA of the 2 exposed effect parameters (**b**) ($\mathrm{PC1_{exposure}}$ denoted the integrated EP)

concerning ECs were divided into 4 groups based on the priority index distribution (Fig. 5a): Group I (consisting of 20 chemicals in top priority), Group II (comprising 58 chemicals in high priority), Group III (including a total of 69 chemicals in moderate priority) and Group IV (containing 38 chemicals in low priority). Due to the variable threshold size, the distribution of priority index was done on a relative scale. Based on this, the prioritization of the future ecological environment monitoring and regulation should focus on the chemicals in Group I and Group II. Compounds in Group III should also be included when additional data on toxicity and risk assessment are

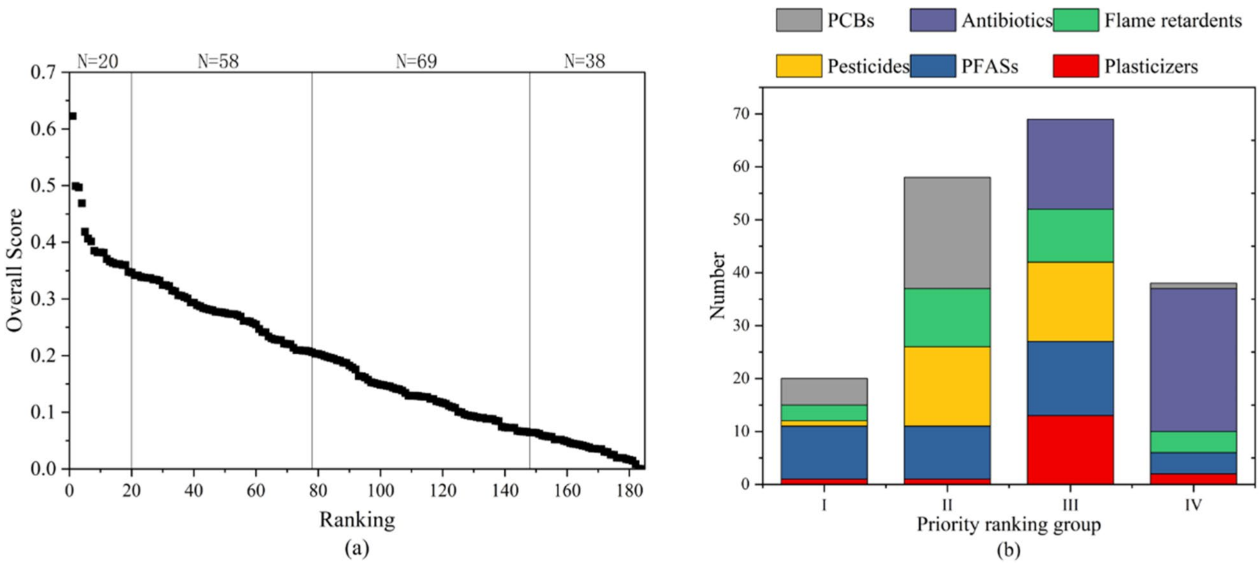


Fig. 5 Priority index and rank of the concerning ECs (**a**) and the numbers of compounds of each category in each ranking group (**b**). The respective priority index split-points for Group I, II, and III were set at 0.35, 0.21, and 0.06

sufficient. Each priority ranking group in Fig. 5b showed the numbers and category of compounds. PFASs, PCBs, flame retardants, pesticides, and plasticizers contributed for 50%, 25%, 15%, 5%, and 5%, respectively, among the compounds in Group I. With Group II, PCBs, pesticides, flame retardants, PFASs and plasticizers contributed for 37%, 26%, 19%, 16% and 2%, respectively. Therefore, PFASs, PCBs, flame retardants, and pesticides were classified as top-priority category, which were chosen for future priority environmental monitoring and pollutant treatment researches with their contamination in Group I and II representing serious human health risks and ecotoxicity.

Flame retardants (i.e., BDE-209, TCPP, and BDE-154), PFASs (i.e., PFTeDA, PFTrDA, PFDoDA, 8:2Cl-PFAES, PFOA, 6:2FTOH, PFNA, PFUnDA, 6:2Cl-PFAES, PFHxDA), PCBs (i.e., PCB206, PCB153, PCB28, PCB52, PCB138), pesticides (i.e., *p,p'*-DDT), plasticizers (i.e., DNP) were the top-priority chemicals in Group I. Specific category ranking displayed of the 185 concerning ECs were manufactured by priority indices in Additional file 1: Table S8. The list of chemicals in each category belonging to top-priority Group was as follows: dinonyl phthalate (plasticizer), perfluorotetradecanoic acid (PFAS), dichlorodiphenyltrichloroethane (pesticide), decabromodiphenyl ether (flame retardant), styrene (antibiotic), nonachlorobiphenyl (PCB).

Comparison between the ranking approaches

The ranking of the top 78 ECs in the 5 different prioritization schemes (RQ_{hum}, RQ_{eco}, EP, HP, priority index) is shown in Table 2. All the ranking lists are accessible through Additional file 1: Table S9. The Pearson's correlation (Fig. 6) varied between -0.084 (RQ_{eco} and HP) to 0.778 (HP and priority index) for these 5 ranking approaches, and the priority index correlated greatly with HP and EP (0.511).

Four prioritization strategies selected 6:2 FTOH, TCPP, PCB61, PFOA, *p,p'*-DDT, *p,p'*-DDE, PCB28, PFTrDA, PFTeDA, TEHP, PCB52, HCB, BDE-154, PCB153, BDE-99, PCB138, cypermethrin in the top 78 chemicals. Three prioritization schemes included DBP, TDCIPP, 8:2 FTOH, BDE-209, 6:2Cl-PFAES, DNP, chlorpyrifos, 6:2 FTS, PFNA, PFDoDA, 8:2Cl-PFAES, PFUnDA, 8:2 FTS, *p,p'*-DDD, PCB66, PCB18, disulfoton, parathion, thionazin, BDE-28, phorate, PCB180, PCB206, PCB126, PCB189, PCB157, PCB156, PCB167, PCB169, BDE-138, BDE-100, PCB118, PCB123, PCB114, PCB105, PCB101, PCB81, PCB77, BDE-85, cyhalothrin, *o,p'*-DDT, deltamethrin, PCB209, ROX, aldrin, BDE-71 in their ranking of the top 78 chemicals. According to the 5 different prioritization schemes, the ranking on the top of 78 ECs consist of 14 plasticizers, 28 PFASs, 30 pesticides, 24 flame retardants, 13 antibiotics and 27 PCBs, amounting from 29.55% (antibiotics) up to 100% (PCBs) of the selected chemicals in each types. Hence, different prioritization scheme can result in different ranking patterns of chemicals.

Uncertainty score

The whole uncertainty scores of concerning ECs are displayed in Additional file 1: Table S10. On the basis of the

Table 2 Top 78 priority ECs according to the 5 disparate prioritization schemes, namely EP, HP, RQ_{eco}, RQ_{hum} and priority index

No.	EP	HP	RQ_{eco}	RQ_{hum}	Priority index
1	DBP	PFODA	DMP	PCB126	BDE-209
2	DEHP	PFHxDA	SDM	PCB28	PFTeDA
3	TBOEP	BDE-209	Dimethoate	PCB153	TCPP
4	6:2FTOH	PCB180	Chlorpyrifos	PCB52	PFTrDA
5	TDCIPP	PCB206	Thionazin	BDE-209	PCB206
6	DIBP	PFTeDA	Disulfoton	PCB81	*p,p′*-DDT
7	DnBP	PCB195	Phorate	PCB138	PFDoDA
8	PFPA	BDE-183	Parathion	PCB189	8:2Cl-PFAES
9	TCIPP	PCB126	DBP	PCB61	PFOA
10	Dimethoate	PCB189	Methyl parathion	PCB77	BDE-154
11	DMP	PCB187	Sulfotep	PCB180	6:2FTOH
12	8:2FTOH	PFTrDA	TDCIPP	PCB157	PFNA
13	TCPP	BDE-154	Deltamethrin	PCB118	PFUnDA
14	BDE-209	BDE-153	6:2FTOH	PCB101	PCB153
15	6:2Cl-PFAES	PCB153	PCB209	PCB206	PCB28
16	DEP	PCB157	TEHP	PCB123	PCB52
17	DNP	PCB156	DIBP	PCB156	6:2Cl-PFAES
18	TCEP	PCB167	DNOP	PCB187	PFHxDA
19	PCB61	PCB169	OFL	PCB167	DNP
20	PFOA	PCB128	PCB28	PCB105	PCB138
21	DNOP	PCB138	PCB61	PCB114	PCB180
22	Chlorpyrifos	BDE-138	PCB153	*p,p′*-DDT	*p,p′*-DDE
23	*p,p′*-DDT	TCPP	*O,O,O*-Triethylphosphorothioate	TCPP	PCB189
24	*p,p′*-DDE	BDE-100	TMPP	BDE-154	BDE-99
25	DMEP	Aldrin	BDE-138	PCB169	PCB128
26	PFOS	BDE-99	8:2FTOH	BDE-183	PCB126
27	PCB28	PFDoDA	TBOEP	BDE-100	HFPO-TA
28	BBP	PCB118	SMX	PCB128	8:2FTOH
29	6:2FTS	PCB123	PCB138	PFOA	Chlorpyrifos
30	PFDA	PCB114	PCB52	BDE-138	PCB61
31	PFTrDA	PCB105	TC	BDE-153	PCB167
32	DEEP	PCB101	Cyhalothrin	PCB66	8:2FTS
33	TPhP	8:2Cl-PFAES	PCB101	PCB18	TEHP
34	BzBP	PFUnDA	OTC	BDE-99	PCB157
35	PFNA	PCB81	SD	DNP	PCB66
36	HFPO-DA	Heptachlor	PFPA	Aldrin	TDCIPP
37	PFTeDA	PCB52	NFX	PFNA	Aldrin
38	TEHP	PCB77	Aldrin	Heptachlor	6:2FTS
39	PFDoDA	*p,p′*-DDT	HEPX	BDE-47	PCB118
40	8:2Cl-PFAES	BDE-85	PCB118	BDE-28	BDE-138
41	OFL	PFNA	PCB189	TEHP	PCB81
42	HFPO-TA	PFDS	PCB157	PCB209	HCB
43	TnBP	BDE-47	Cypermethrin	PCB44	DNOP
44	PCB52	Cyhalothrin	Atrazine	6:2FTOH	PCB77
45	PFUnDA	8:2FTS	PCB180	Disulfoton	PCB105
46	NFX	PCB66	*p,p′*-DDT	PFTrDA	PCB123
47	PFBA	PCB44	*p,p′*-DDE	PFTeDA	BDE-47
48	PFHxA	*o,p′*-DDT	PCB81	*o,p′*-DDT	PCB187
49	EFX	10:2FTS	TCIPP	*p,p′*-DDE	PCB101

Table 2 (continued)

No.	EP	HP	RQ_{eco}	RQ_{hum}	Priority index
50	BMPP	PCB28	BDE-85	8:2Cl-PFAES	PCB18
51	CTC	HFPO-TA	DnBP	BDE-85	Cyhalothrin
52	PFHpA	PFOA	PFTrDA	PFOS	*o,p'*-DDT
53	α-HCH	FOSA	BDE-71	*o,p'*-DDE	PFDA
54	Atrazine	Deltamethrin	PCB77	BDE-71	*p,p'*-DDD
55	DCHP	BDE-71	BDE-99	PCB195	PFNOBS
56	8:2FTS	BDE-66	BDE-154	*p,p'*-DDD	PCB114
57	HCB	HCB	PCB123	HCB	BDE-28
58	TMPP	PCB18	LIN	8:2FTS	PFOS
59	PFNOBS	HEPX	PCB105	6:2Cl-PFAES	Deltamethrin
60	CFX	BDE-28	PFTeDA	Deltamethrin	Cypermethrin
61	TEP	TEHP	TPrP	*o,p'*-DDD	PFPA
62	*p,p'*-DDD	*p,p'*-DDE	TCPP	Cypermethrin	PCB156
63	PCB66	6:2Cl-PFAES	*o,p'*-DDT	Phorate	BDE-100
64	PCB18	*p,p'*-DDD	PFOA	Sulfotep	PCB44
65	BDE-154	F-53B	CTC	PFHxS	PCB209
66	β-HCH	Cypermethrin	Famphur	6:2FTS	α-HCH
67	PCB153	*o,p'*-DDE	BBP	γ-HCH	BDE-85
68	SDM	PFNOBS	PCB156	Parathion	Heptachlor
69	BDE-99	DNP	ETM-H2O	PFHxDA	PFHpA
70	PCB138	PCB209	PCB114	TDCIPP	*o,p'*-DDE
71	Disulfoton	Chlorpyrifos	TCEP	DBP	TPhP
72	Parathion	6:2FTS	PCB206	Methyl parathion	PCB169
73	Thionazin	PCB61	BDE-100	BDE-66	HEPX
74	Cypermethrin	Endosulfan I	MON	Cyhalothrin	BDE-183
75	BDE-28	BDE-17	DMEP	ROX	BDE-71
76	Fenpropathrin	8:2FTOH	PCB167	PFUnDA	HFPO-DA
77	Phorate	6:2FTOH	PCB169	PFDoDA	Fenpropathrin
78	Famphur	ROX	PCB126	Thionazin	HCBD

origin of uncertainty, compounds were divided into 4 categories: Category I (26 chemicals with plenty ecotoxicity and occurrence data); Category II (65 chemicals with incomplete toxicity data); Category III (36 chemicals with incomplete human health effect and occurrence data); Category IV (58 chemicals with insufficient data on both occurrence and toxicity).

Antibiotics were distributed across all the 4 uncertainty categories, accounting for 57.7%, 23%, 16.7%, and 13.8% of Category I to IV, respectively. Flame retardants are mainly distributed in categories II and III, accounting for 17% and 33.3% of Category II and III, respectively. PCBs were generally included in Category II, accounting for 26.2%. Most pesticides were identified into Category III, accounting for 50%. PFASs and plasticizers were representative greatly in Category IV, accounting for 39.7% and 13.8%, respectively. The PFASs in Category IV were mainly substitutes for PFASs. In general, 31.35% of the ECs were included into Category IV. (Fig. 7).

Results for priority control

Combining the results of 4 priority groups and 4 uncertainty categories, the selected 185 ECs were separated to 16 subgroups for comprehensive ranking. These chemicals were ranked using a priority index in each uncertainty category, and the results are available from Additional file 1: Table S11. The uncertainty categories I, II, III, and IV exhibited respective amounts of 26, 66, 36, and 57 chemicals. Finally, 7 chemicals were selected as the final priority ECs, which are *p,p'*-DDT, PFOA, *p,p'*-DDE, *p,p'*-DDT, *p,p'*-DDD, PFOS, and α-HCH. The detailed uncertainty categories of chemicals showed in the priority groups can be found in Table 3.

Discussion

Occurrence, fate and bioaccumulation

Plasticizers (PAEs) could be degraded by light [68], therefore, the highest median concentration might be related to the widespread detection campaigns in the

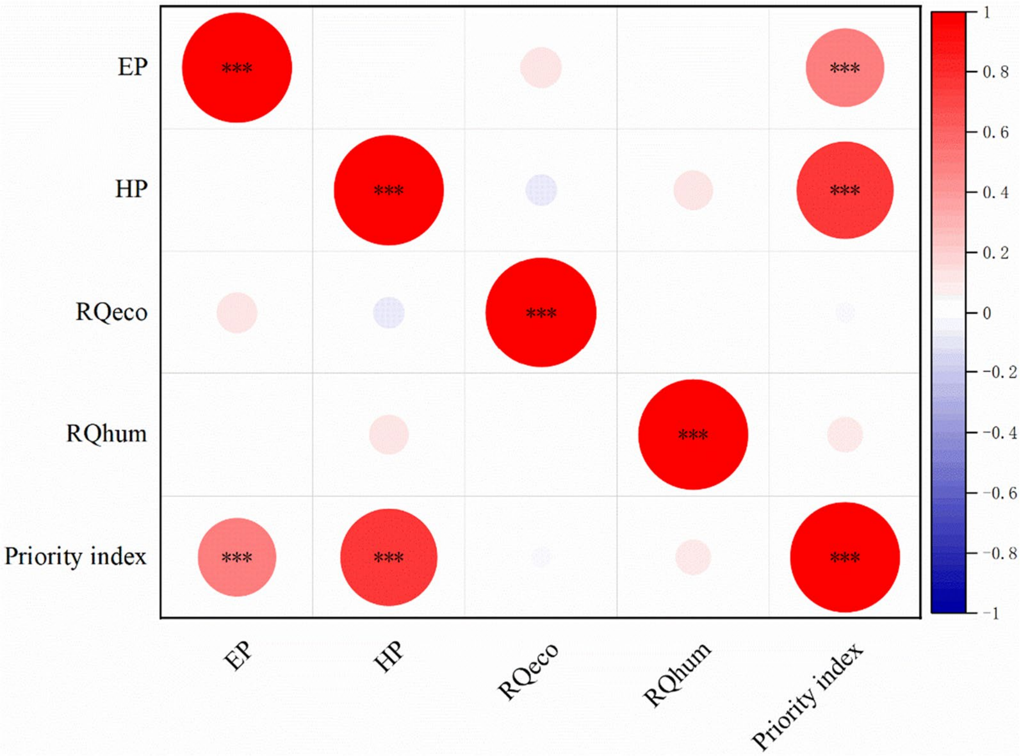


Fig. 6 Correlation among the five ranking methods (EP, HP, RQ_{eco}, RQ_{hum}, and Priority index)

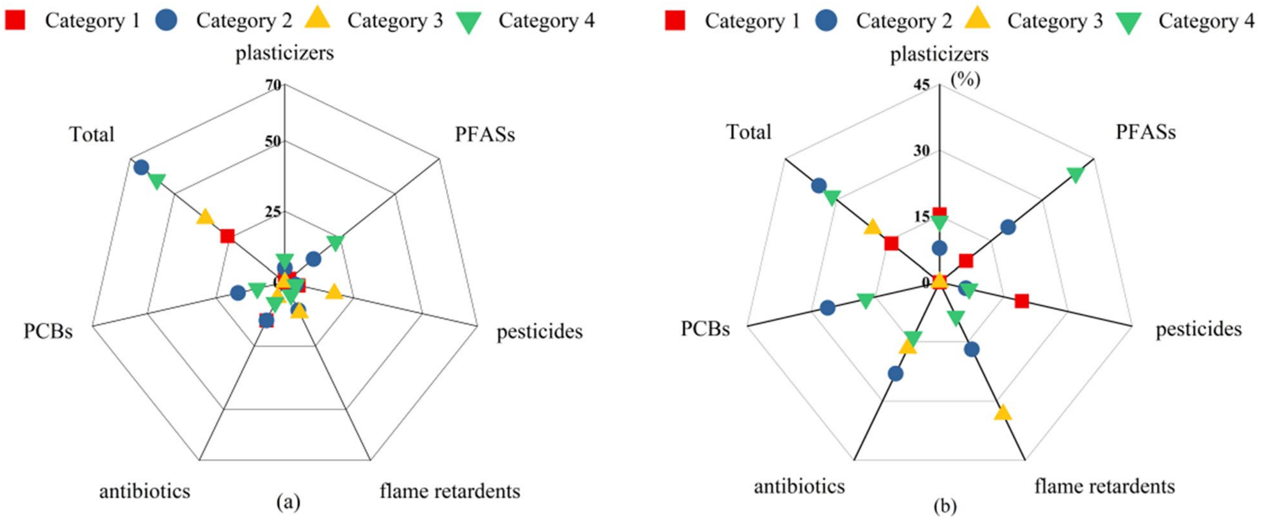


Fig. 7 The quantity (**a**) and percentum (**b**) of compounds through each EC category in the uncertainty category

Yangtze River Basin [44]. The high intensity of agricultural activities in the Yangtze River Basin resulting in pesticides detectable in high concentrations [69, 70]. Previous studies mainly focused on long-chain PFASs (PFOA and PFOS), while their alternatives with short-chain structures were rarely studied, hence the lowest median concentration of PFASs were found [42]. It is also possible that PFASs in surface water mainly come from Waste Water Treatment Plant [71], and the concentration of PFASs would be reduced after treatment. The ECs categories of the current study were widely distributed in environment [72], having high detection

Table 3 The detailed uncertainty categories of chemicals showed in priority groups

	Uncertainty I	Uncertainty II			Uncertainty III		Uncertainty IV	
Priority I	*p,p′*-DDT PFOA	PFTeDA PFTrDA PFDoDA PFNA PFUnDA	BDE-154 PCB153 PCB28 PCB52 PCB138		BDE-209 TCPP		PCB206 8:2Cl-PFAES 6:2 FTOH 6:2Cl-PFAES PFHxDA DNP	
Priority II	*p,p′*-DDE *o,p′*-DDT *p,p′*-DDD PFOS α-HCH	PCB180 PCB189 BDE-99 PCB126 PCB157 PCB118 PCB81 HCB	DNOP PCB77 PCB105 PCB123 BDE-47 PCB101 PFDA PCB114	BDE-28 PCB156 BDE-100 BDE-85 PFHpA *o,p′*-DDE PCB169 BDE-183 BDE-71	Chlorpyrifos TEHP TDCIPP Aldrin Cyhalothrin Deltamethrin Cypermethrin Heptachlor TPhP	HEPX Fenpropathrin	PCB128 HFPO-TA 8:2FTOH PCB61 PCB167 8:2FTS PCB66 6:2FTS BDE-138	PCB187 PCB18 PFNOBS PFPA PCB44 PCB209 HFPO-DA HCBD
Priority III	DnBP ROX ATM OFL DMP ERY DEP CTC NFX TYL	DCHP DIBP DBP BDE-153 ETM-H2O *o,p′*-DDD BDE-66 PFHxS PFHxA BBP	δ-HCH BDE-17 PFPeA EFX MON CLA PFBA LCM PFDS CFX		γ-HCH Disulfoton SDM Parathion TCIPP Phorate Sulfotep Methyl parathion Atrazine Dimethoate	Thionazin TBOEP Endosulfan I TCEP TnBP DIF TMP	10:2FTS β-HCH DNHP BzBP PFHpS 4:2FTS DPP F-53B TDCPP FOSA	Famphur TPP *O,O,O*-Triethylphosphorothioate DBEP ADONA TPrP SARA PFEESA DEEP PFPeS PF5OHxA
Priority IV	TC SMX DEHP SD OTC SMZ SDZ SMM LIN	SX PFBS SCP CAP SMTZ FF DC SPD	DAN MAR		LOM TMPP SQX TAP TBEP TEP		3,6-OPFHpA TIP SPI DMEP PER PF4OPeA FLU OXA	SMP SIM SMR PCB195 PFODA

frequency. The median DHL value of plasticizers was 3.11, indicating that the duration of completely mineralization last for weeks. While the median DHL values of pesticides, flame retardants, PCBs and antibiotics were closed to 2, revealing the complete mineralization lasted for months, and that for PFASs (DHL = 0.74) were for many years. Overall, PFASs, have been categorized as persistent organic pollutants, showing the strongest environmental persistence [73]. Comparing the median LogK$_{ow}$ values of these six categories, it was found that the value of PCBs (6.98) was the highest. Previously study had shown that the enrichment factor of PCBs was higher [74]. Due to the fact that chemical properties of each compounds varied significantly, the priority ranking based on multiple criteria is of importance. The PNEC$_{eco}$ values and PNEC$_{hum}$ values of PCBs were in the lowest level, indicating that the toxicity of PCBs were the strongest ones.

The potential effects on exposure and hazard

As could been seen from Fig. 4a, PCBs were generally situated at the higher PC1$_{hazard}$ values, representing the greatest integrated hazard and hence should be considered to be the most concerning EC category. Pesticides and PFASs were situated at the mid-range PC1$_{hazard}$ values. Nevertheless, pesticides were primarily composed of positive PC2$_{hazard}$ values, in contrast to PFASs which had PC2$_{hazard}$ values were primarily negative. These results demonstrated higher ecotoxicity and human health effect for pesticides, while higher persistence and bioaccumulation potential for PFASs, as compared to the other selected ECs. Antibiotics were situated at the lower PC1$_{hazard}$ values, indicating the minimal hazard influences. However, antibiotics might still represent primary concerns. Flame retardants and plasticizers were widely scaled, nearly one half were in positive PC1$_{hazard}$ which indicated human health effect and bioaccumulation potential. The study [30] also showed that PFAS and pesticide had the higher HP values, and plasticizer and antibiotic had the lower HP values; whereas, the higher HP value of flame retardants in the current study was in contrast, which might be due to the $\mathrm{PNEC}_{\mathrm{hum}}$ derived from simulation and existed differences with experimental data.

As $\mathrm{PC1}_{\mathrm{exposure}}$ raised, there was a corresponding rise in the cumulative exposure potential. ECs categories included a broad variety of characteristics, for instance, PFASs, pesticides, and flame retardants were widely dispersed across the $\mathrm{PC1}_{\mathrm{exposure}}$ range, suggesting that their properties varied widely in the environment. Antibiotics and PCBs were principally situated at the lower $\mathrm{PC1}_{\mathrm{exposure}}$ values, manifesting most of them were absence of detection in the actual monitoring or the existing methods were insufficient to detect. Plasticizers were mainly situated at higher $\mathrm{PC1}_{\mathrm{exposure}}$ position which was related to higher concentration and detection. A study also showed that plasticizers and flame retardants had the higher EP values, and antibiotic had a lower EP value [75]. The EP data for PFASs and pesticides in this research were in contrast, which might be related to industry and agriculture distribution differed in the Yangtze River basin.

Priority index

Due to the fact that 50% compounds in Group I were PFASs, indicating that PFASs might be the most hazardous. The DNP, *p,p'*-DDT and PCB138 were also listed at the top level in a previously study [27]. Evidence has shown that the *p,p′*-DDT is harmful with health risk to human [76]. For other chemicals in Group I such as BDE-209, special focus should be given because its high concentration and detection frequency in environment, causing endocrine disorders, hepatotoxicity and cardiovascular toxicity [77, 78]. BDE-154 was detected in various environment and showed high bioaccumulation [79]. Nowadays, the global concern for PFASs has gained widely recognition [75]. Compared with the study [30], it is found that PFOA was also listed in the Group I. Simultaneously, PFOA is a group of chemicals that used for industrial production with strong persistence, bioaccumulation, and toxic effects. In 2013, the International Agency for Research on Cancer (IARC) included PCBs as Group 1 carcinogens for humans [80]. BDE-209, PCB206, PFOA, PCB153, PCB28, PCB52, and PCB138 are included into Stockholm Convention on Persistent Organic Pollutants [81] and China's List of Key Emerging Contaminants under Control (2023) [82]. BDE-154 is contained in China's List of Key Emerging Contaminants under Control (2023) and *p,p'*-DDT is involved into EU POPs Control List [83]. Insides, the EU is considering PFNA, PFUnDA, PFDoDA, and PFTrDA as potential candidates for the control of POPs under the Stockholm Convention [81]. Importantly, TCPP, PFTeDA, 8:2 Cl-PFAES, 6:2 FTOH, 6:2 Cl-PFAES, PFHxDA, DNP, which were not contained in any list so far, were identified as the top-priority ECs in our study. Dinonyl phthalate, perfluorotetradecanoic acid, dichlorodiphenyltrichloroethane, decabromodiphenyl ether, styrene, and nonachlorobiphenyl, which are the compounds ranked first in each category, may be classified as priority pollutants for the future environmental monitoring and estimate of sediment treatment process. Therefore, the current approach provide new insights to priority the ECs.

Methodology feasibility and uncertainty analysis

The HP and EP showed a strong correlation with the priority index (0.778 and 0.511), implying that the advantage of our approach considered effects of ECs to both human health and ecological risks. The identification of 78 ECs in Groups I or II based on priority index highlighted the availability for explaining both occurrence and toxicity factors.

The distribution of antibiotics in uncertainty categories showed that there was a lack of research on certain classes of antibiotics. The main distribution of flame retardants in categories II and III indicated a lack of simultaneous monitoring campaigns and toxicity evaluation of the same chemical. The general distribution of PCBs in Category II suggested data gaps related to ecotoxicity. Most pesticides were identified into Category III, indicating the necessary for strengthen monitoring programs in the Yangtze River sediment. PFASs and plasticizers were representative greatly in Category IV, suggesting the urgent need to strengthen monitoring campaigns and hazard assessments. The PFASs in Category IV were mainly substitutes for PFASs, indicating that there was a major need to strengthen research on alternatives to PFASs. The greater mobility and equivalent persistence of short-chain PFASs, as opposed to legacy PFASs, resulting in stronger long-range transport availability [84]. The plasticizers in Category IV were not included in the priority control contaminants [85], and the DNP was in the priority Group I, thus further studies is needed to narrow this gap. In general, there are many ECs were included into Category IV, which indicated principal study gaps for occurrence and toxicity of ECs in the Yangtze River sediment.

Recommendations for priority control

Rigorous hazard assessments of the 65 compounds in uncertainty Category II are recommended, while the 65 compounds in uncertainty Category III require an intensive monitoring. Simultaneously, additional monitoring activities and hazard assessments for the 58 compounds in uncertainty Category IV are recommended.

About the 7 priority ECs shown in priority group I/uncertainty Category I and priority group II/uncertainty Category I, the chemical number only accounting for 8.9% without uncertainty analysis, routine environmental monitoring, setting relevant emission standards, and establishment of control measures are suggested. Similarly, especial concern should also be given to the 19 ECs in the priority group III/uncertainty Category I and the priority group IV/uncertainty Category I. Chemicals of remaining uncertainty categories should be the candidates for subsequent environmental monitoring and toxicity tests. When new occurrence and toxicity data become available, these ECs should be included for re-evaluation of the priority control list.

Conclusion

In the current study, a multi-criteria analysis approach on the basis of HP and EP was developed to rank the priority of 185 selected ECs in the Yangtze River sediment, belonging to plasticizers, PFASs, pesticides, flame retardants, antibiotics and PCBs. Of which, an integrated priority index of concerning chemicals was computed by combining their hazard index and exposure index. The results showed that PCBs, flame retardants and PFASs exhibited higher HP values, however, plasticizers and antibiotics were with low HP values. Additionally, the plasticizers and PFASs showed relatively high EP values, while that for PCBs and antibiotics were low, as revealed by exposure analysis. The priority index listed 20 chemicals that were top-priority and 58 chemicals as high-priority, in which PFASs amounted the highest proportion at both top-priority and high-priority groups. The PCBs, pesticides, and flame retardants were within the high-priority groups. After uncertainty analysis and categorization, a total of 7 ECs were recognized as priority chemicals and suggested to be controlled as the first target. Hence, the study highlights the necessary to provide priority screening on emerging contaminants in different regions. Besides, further studies are needed for the alternatives of PFASs and plasticizers, which could overcome data limitation and thus optimize the approach.

Abbreviations

ECs	Emerging contaminants
PCA	Principal component analysis
PC1	Principal component
HP	Hazard potential
EP	Exposure potential
ND	Not detected
LOD	Limit of detection
MDL	Half of the method detection limit
LC_{50}	Lowest lethal median concentration
EC_{50}	Half-effect concentration
AF	Assessment factor
MEC	The measured EC concentration
BCF	Bioconcentration factor
ADI	Acceptable daily intake
MRL	Minimal risk level
RfD	Reference dose
BW	Body weight
DHL	Degradation half-life
PNEC	Predicted no effect concentration
POPs	Persistence organic pollutants
PFASs	Per- and polyfluoroalkyl substances
PCBs	Polychlorinated biphenyls
BDE	Polybrominated diphenyl ethers
DBP	Dibutyl phthalate
DEHP	1,2-Benzenedicarboxylicacid, 1,2-bis(2-ethoxyethyl) ester
DBP	Dibutyl phthalate
DNP	Dinonyl phthalate
TBOEP	Tris(2-butoxyethyl) phosphate
TCPP	Meso-tetra(4-carboxyphenyl) porphine
TEHP	Tris(2-ethylhexyl) phosphate
TDCIPP	Tris(1,3-dichloro-2-propyl) phosphate
6:2 FTOH	1H,1H,2H,2H-Perfluoro-1-octanol
PFTeDA	Perfluorotetradecanoic acid
PFTrDA	Perfluorotridecanoic acid
PFDoDA	Perfluorolauric acid
PFOA	Perfluorooctanoic acid
PFNA	Perfluorononanoic acid
PFUnDA	Perfluoroundecanoic acid
PFHxDA	Perfluorohexadecanoic acid
8:2 FTOH	8:2 Fluorotelomer alcohol glucuronide
6:2 FTS	1H,1h,2h,2h-Perfluorooctanesulfonic acid
8:2 FTS	1H,1H,2H,2H-Perfluorodecanesulfonic acid
6:2 Cl-PFAES	Perfluoro(2-((6-chlorohexyl)oxy)ethanesulfonic acid)
8:2 Cl-PFAES	11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid
HCB	Hexachlorobenzene
p,p′-DDT	2,2-Bis(*p*-chlorophenyl)-1,1,1-trichloroethane
p,p′-DDD	1-Chloro-4-[2,2-dichloro-1-(4-chlorophenyl)ethyl]benzene
p,p′-DDE	2,2-Bis(4-chlorophenyl)-1,1-dichloroethylene
o,p′-DDT	1-Chlor-2-[2,2,2-trichlor-1-(4-chlorphenyl)ethyl]benzol
α-HCH	1,2,3,4,5,6-Hexachlorocyclohexane
ROX	Roxithromycin

Supplementary Information

The online version contains supplementary material available at https://doi.org/10.1186/s12302-024-00855-3.

Additional file 1: Table S1. Utility functions (U) used to evaluate the six prioritization criteria, hazard potential and exposure potential. **Table S2.** ECs occurrence data, including detection frequency and concentration. **Table S3.** The comparisons between KOWWIN v4.1 and experimental data of logK_{ow}. **Table S4.** The primitive and normalized criteria (persistence, bioaccumulation, toxicity, human health effects) values for candidate ECs. **Table S5.** The hazard potential for candidate ECs. **Table S6.** The exposure potential of candidate ECs. **Table S7.** The ranked list of ECs by priority index. **Table S8.** Category-specific lists of ECs ranked by priority index. **Table S9.** Ranked lists of ECs using five prioritization schemes (e.g., exposure potential, hazard potential, risk quotient for human health effects, risk quotient for Ecotoxicity, and priority index). **Table S10.** Uncertainty values of candidate ECs. **Table S11.** Uncertainty category lists of ECs ranked by priority index. **Fig. S1.** The number of data collecting sites in each province and municipality along the Yangtze River.

Acknowledgements

Not applicable.

Author contributions

YW: data collection and analysis, writing—original draft preparation. ZHQ: data collection. SYH: data analysis. ZLC and YS: supervision, writing—review and editing.

Funding

This work was supported by the National Natural Science Foundation of China (No.: 51909015), the Fundamental Research Funds for the Central Universities (No.: 2019CDCGHS310) and Special Project for Performance Incentive and Guidance of Research Institutes in Chongqing (cstc2021jxjl130011).

Availability of data and materials

The datasets used and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

All authors agreed to publish the paper.

Competing interests

The authors declare that they have no competing interests.

Received: 27 December 2023 Accepted: 30 January 2024

References

1. Four questions emerging contaminants treatment authority interpretation of the ministry of ecological environment. https://www.gov.cn/zhengce/2022-03/30/content_5682516.htm. Accessed 20 May 2023.
2. Bayabil HK, Teshome FT, Li YCC (2022) Emerging contaminants in soil and water. Front Environ Sci 10:8
3. Ondon BS, Li SN, Zhou QX, Li FX (2021) Sources of antibiotic resistant bacteria (ARB) and antibiotic resistance genes (ARGs) in the soil: a review of the spreading mechanism and human health risks. Rev Environ Contam Toxicol 256:121–153
4. Li WC (2014) Occurrence, sources, and fate of pharmaceuticals in aquatic environment and soil. Environ Pollut 187:193–201
5. Penserini L, Cantoni B, Gabrielli M, Sezenna E, Saponaro S, Antonelli M (2023) An integrated human health risk assessment framework for alkylphenols due to drinking water and crops? food consumption. Chemosphere 325:9
6. Vodyanitskii YN, Yakovlev AS (2016) Contamination of soils and groundwater with new organic micropollutants: a review. Eurasian Soil Sci 49:560–569
7. Sharifan H, Bagheri M, Wang D, Burken JG, Higgins CP, Liang YN, Liu JX, Schaefer CE, Blotevogel J (2021) Fate and transport of per- and polyfluoroalkyl substances (PFASs) in the vadose zone. Sci Total Environ 771:20
8. Wang LJ, Liu MM, Tao WD, Zhang WJ, Wang L, Shi XM, Lu XW, Li XP (2018) Pollution characteristics and health risk assessment of phthalate esters in urban soil in the typical semi-arid city of Xi'an, Northwest China. Chemosphere 191:467–476
9. Zhou B, Zhao LX, Sun Y, Li XJ, Weng LP, Li YT (2021) Contamination and human health risks of phthalate esters in vegetable and crop soils from the Huang-Huai-Hai region of China. Sci Total Environ 778:10
10. Tang L, Liu XR, Yang GJ, Xia JF, Zhang N, Wang DB, Deng HW, Mao M, Li XM, Ni BJ (2021) Spatial distribution, sources and risk assessment of perfluoroalkyl substances in surface soils of a representative densely urbanized and industrialized city of China. CATENA 198:7
11. Li M, Yang L, Yen H, Zhao FK, Wang XM, Zhou TH, Feng QY, Chen LD (2023) Occurrence, spatial distribution and ecological risks of antibiotics in soil in urban agglomeration. J Environ Sci 125:678–690
12. Li WL, Liu LY, Zhang ZF, Song WW, Huo CY, Qiao LN, Ma WL, Li YF (2016) Brominated flame retardants in the surrounding soil of two manufacturing plants in China: Occurrence, composition profiles and spatial distribution. Environ Pollut 213:1–7
13. Wang H, Liang H, Gao DW (2017) Occurrence and risk assessment of phthalate esters (PAEs) in agricultural soils of the Sanjiang Plain, northeast China. Environ Sci Pollut Res 24:19723–19732
14. Wang Y, Zhang ZH, Bao MJ, Xu Y, Zhang LJ, Tan F, Zhao HX (2021) Characteristics and risk assessment of organophosphate esters and phthalates in soils and vegetation from Dalian, northeast China. Environ Pollut 284:7
15. Xie LN, Wang XC, Dong XJ, Su LQ, Zhu HJ, Wang C, Zhang DP, Liu FY, Hou SS, Dong B, Shan GQ, Zhang X, Zhu Y (2021) Concentration, spatial distribution, and health risk assessment of PFASs in serum of teenagers, tap water and soil near a Chinese fluorochemical industrial plant. Environ Int 146:13
16. Yadav D, Rangabhashiyam S, Verma P, Singh P, Devi P, Kumar P, Hussain CM, Gaurav GK, Kumar KS (2021) Environmental and health impacts of contaminants of emerging concerns: Recent treatment challenges and approaches. Chemosphere 272:19
17. Naidu R, Jit J, Kennedy B, Arias V (2016) Emerging contaminant uncertainties and policy: The chicken or the egg conundrum. Chemosphere 154:385–390
18. Yang YJ, Chen ZL, Zhang JL, Wu SQ, Yang L, Chen L, Shao Y (2021) The challenge of micropollutants in surface water of the Yangtze River. Sci Total Environ 780:9
19. Guiding Opinions of the State Council on Promoting the Development of the Yangtze River Economic Belt by Relying on the Golden Waterway. https://www.gov.cn/zhengce/content/2014-09/25/content_9092.htm. Accessed 10 May 2023.
20. Li XH, Zhang RH, Tian T, Shang XC, Du X, He YY, Matsuura N, Luo TL, Wang Y, Chen JW, Kadokami K (2021) Screening and ecological risk of 1200 organic micropollutants in Yangtze Estuary water. Water Res 201:10
21. China Association of Environmental Protection Industry. http://www.caepi.org.cn/epasp/website/webgl/webglController/view?xh=1519369165389017223680. Accessed 11 Jan 2024.
22. Liu JJ, Wang PF, Wang C, Qian J, Hou J (2017) Heavy metal pollution status and ecological risks of sediments under the influence of water transfers in Taihu Lake, China. Environ Sci Pollut Res 24:2653–2666
23. Brack W, Ait-Aissa S, Burgess RM, Busch W, Creusot N, Di Paolo C, Escher BI, Hewitt LM, Hilscherova K, Hollender J, Hollert H, Jonker W, Kool J, Lamoree M, Muschket M, Neumann S, Rostkowski P, Ruttkies C, Schollee J, Schymanski EL, Schulze T, Seiler TB, Tindall AJ, Umbuzeiro GD, Vrana B, Krauss M (2016) Effect-directed analysis supporting monitoring of aquatic environments—an in-depth overview. Sci Total Environ 544:1073–1118
24. Kuzmanovic M, Ginebreda A, Petrovic M, Barcelo D (2015) Risk assessment based prioritization of 200 organic micropollutants in 4 Iberian rivers. Sci Total Environ 503:289–299
25. Network of Reference Laboratories, Research Centres and Related Organisations for monitoring of emerging environmental substances. https://www.norman-network.net/. Accessed 20 May 2023.
26. Regulations of the Ministry of Ecology and Environment: List of Key Controlled Emerging Contaminants; 2023. https://www.gov.cn/zhengce/2022-12/30/content_5734728.htm. Accessed 20 May 2023.
27. Zhao ZH, Gong XH, Ding QQ, Jin M, Wang ZD, Lu SY, Zhang L (2021) Environmental implications from the priority pollutants screening in impoundment reservoir along the eastern route of China's South-to-North Water Diversion Project. Sci Total Environ 794:11
28. Gaston L, Lapworth DJ, Stuart M, Arnscheidt J (2019) Prioritization approaches for substances of emerging concern in groundwater: a critical review. Environ Sci Technol 53:6107–6122
29. Zhou SB, Di Paolo C, Wu X, Shao Y, Seiler TB, Hollert H (2019) Optimization of screening-level risk assessment and priority selection of emerging pollutants—the case of pharmaceuticals in European surface waters. Environ Int 128:1–10
30. Zhong MM, Wang TL, Zhao WX, Huang J, Wang B, Blaney L, Bu QW, Yu G (2022) Emerging organic contaminants in Chinese surface water: identification of priority pollutants. Engineering 11:111–125

31. Arnot JA, Mackay D (2008) Policies for chemical hazard and risk priority setting: can persistence, bioaccumulation, toxicity, and quantity information be combined? Environ Sci Technol 42:4648–4654
32. Kumar A, Xagoraraki I (2010) Pharmaceuticals, personal care products and endocrine-disrupting chemicals in U.S. surface and finished drinking waters: a proposed ranking system. Sci Total Environ 408:5972–5989
33. Publications Office of the European Union. https://op.europa.eu/en/publication-detail/-/publication/f4bc0323-77eb-4f63-be65-abbbad27aa9a/language-en. Accessed 20 May 2023.
34. Li Y, Zhang LY, Liu XS, Ding J (2019) Ranking and prioritizing pharmaceuticals in the aquatic environment of China. Sci Total Environ 658:333–342
35. Bu QW, Cao YB, Yu G, He XF, Zhang HD, Sun JY, Yun MQ, Cao ZG (2020) Identifying targets of potential concern by a screening level ecological risk assessment of human use pharmaceuticals in China. Chemosphere 246:8
36. Sui Q, Wang B, Zhao WT, Huang J, Yu G, Deng SB, Qiu ZF, Lu SG (2012) Identification of priority pharmaceuticals in the water environment of China. Chemosphere 89:280–286
37. Guo QR, Wei DB, Wang FP, Chen M, Du YG (2021) A novel risk score-based prioritization method for pollutants in reclaimed water. Sci Total Environ 795:9
38. Kang Y, Chen YQ, Zhou MJ, Xu YF, Feng HJ, Chen RY (2022) Identification of regional industrial priority pollutants in surface water: a field study in Taihu Lake Basin. Front Environ Sci 10:11
39. Chen YL, Jiang CX, Wang YL, Song RR, Tan Y, Yang YY, Zhang ZL (2022) Sources, environmental fate, and ecological risks of antibiotics in sediments of Asia's longest river: a whole-basin investigation. Environ Sci Technol 56:14439–14451
40. Cui XA, Dong J, Huang ZF, Liu CY, Qiao XC, Wang X, Zhao XR, Zheng BH, Shen JS (2020) Polychlorinated biphenyls in the drinking water source of the Yangtze River: characteristics and risk assessment. Environ Sci Eur 32:9
41. Johnson AC, Jurgens MD, Su C, Zhang M, Zhang YQ, Shi YJ, Sweetman A, Jin XW, Lu YL (2018) Which commonly monitored chemical contaminant in the Bohai Region and the Yangtze and pearl rivers of china poses the greatest threat to aquatic wildlife? Environ Toxicol Chem 37:1115–1121
42. Leng YF, Xiao HL, Li Z, Liu Y, Huang K, Wang J (2021) Occurrence and ecotoxicological risk assessment of perfluoroalkyl substances in water of lakes along the middle reach of Yangtze River, China. Sci Total Environ 788:11
43. Tang ZW, Huang QF, Yang YF, Zhu XH, Fu HH (2013) Organochlorine pesticides in the lower reaches of Yangtze River: occurrence, ecological risk and temporal trends. Ecotox Environ Safe 87:89–97
44. Xu H, Liu Y, Xu X, Lan HC, Qi WX, Wang DH, Liu HJ, Qu JH (2022) Spatiotemporal variation and risk assessment of phthalate acid esters (PAEs) in surface water of the Yangtze River Basin, China. Sci Total Environ 836:8
45. Estimation Programs Interface SuiteTM for MicrosoftÒ Windows, v 4.11. https://eur-lex.europa.eu/legal-content/EN/ALL/?uri=CELEX:32013L0039. Accessed 10 May 2023.
46. Ecotox Knowledgebase. https://cfpub.epa.gov/ecotox/. Accessed 20 May 2023.
47. Agriculture Research Service Pesticide Properties Database. https://sitem.herts.ac.uk/aeru/ppdb/en/index.htm. Accessed 10 May 2023.
48. Tang JF, Sun J, Ke ZY, Yin HL, Yang L, Yen H, Li XH, Xu YY (2021) Organophosphate esters in surface soils from a heavily urbanized region of Eastern China: occurrence, distribution, and ecological risk assessment. Environ Pollut 291:9
49. Wu JY, Zhu T, Chen ZM, Guo JS, Hou XY, Wang DR, Zhang LX, Gao JM (2022) Occurrence, seasonal variation, potential sources, and risks of organophosphate esters in a cold rural area in Northeast China. Sci Total Environ 834:11
50. You J, Chen ZM, Hou XY, Guo JS, Wang CC, Gao JM (2022) Occurrence, potential sources and risks of organophosphate esters in the high-elevation region, Tibet, China. Sci Total Environ 806:9
51. Ren JH, Shi HC, Liu JC, Zheng CY, Lu GH, Hao SF, Jin Y, He C (2023) Occurrence, source apportionment and ecological risk assessment of thirty antibiotics in farmland system. J Environ Manage 335:11
52. Yang YY, Owino AA, Gao Y, Yan X, Xu C, Wang J (2016) Occurrence, composition and risk assessment of antibiotics in soils from Kenya, Africa. Ecotoxicology 25:1194–1201
53. Li C, Chen JY, Wang JH, Ma ZH, Han P, Luan YX, Lu AX (2015) Occurrence of antibiotics in soils and manures from greenhouse vegetable production bases of Beijing China and an associated risk assessment. Sci Total Environ 521:101–107
54. Zhang HB, Luo YM, Wu LH, Huang YJ, Christie P (2015) Residues and potential ecological risks of veterinary antibiotics in manures and composts associated with protected vegetable farming. Environ Sci Pollut Res 22:5908–5918
55. Wang L, Liu YY, Zhang YW, Chen SW, Zhang NN, Wang ZF, Liu HF (2023) Estimation and potential ecological risk assessment of multiphase PAEs in mangrove wetlands in Dongzhai Harbor, Hainan. Sci Total Environ 870:11
56. Shan GQ, Wang Z, Zhou LQ, Du P, Luo XX, Wu QN, Zhu LY (2016) Impacts of daily intakes on the isomeric profiles of perfluoroalkyl substances (PFASs) in human serum. Environ Int 89–90:62–70
57. Ray S, McLeese DW, Zitko V (1980) Sediment sorption and toxicity of organochlorine pesticides to marine-invertebrates. Abstr Pap Am Chem Soc 180:180-ENVR
58. GB 2763–2021 Maximum residue limits of pesticides in food. http://2763.foodmate.net/. Accessed 14 May 2023.
59. GB 31650–2019 Query of residues of veterinary drugs in animal food. http://31650.foodmate.net/?#/. Accessed 10 May 2023.
60. Ossai CJ, Iwegbue CMA, Tesi GO, Olisah C, Egobueze FE, Nwajei GE, Martincigh BS (2023) Spatial characteristics, sources and exposure risk of polychlorinated biphenyls in dusts and soils from an urban environment in the Niger Delta of Nigeria. Sci Total Environ 883:163513
61. Sun HW, Qi YL, Zhang D, Li QX, Wang J (2016) Concentrations, distribution, sources and risk assessment of organohalogenated contaminants in soils from Kenya, Eastern Africa. Environ Pollut 209:177–185
62. Agency for Toxic Substances and Disease Registry. https://www.atsdr.cdc.gov/. Accessed 20 May 2023.
63. Gramatica, P. (2010) Chemometric methods and theoretical molecular descriptors in predictive QSAR modeling of the environmental behavior of organic pollutants. Recent advances in QSAR studies: methods and applications. p. 327–366.
64. Gramatica P, Pilutti P, Papa E (2004) A tool for the assessment of VOC degradability by tropospheric oxidants starting from chemical structure. Atmos Environ 38:6167–6175
65. Sangion A, Gramatica P (2016) PBT assessment and prioritization of contaminants of emerging concern: pharmaceuticals. Environ Res 147:297–306
66. Gramatica P, Cassani S, Sangion A (2016) Aquatic ecotoxicity of personal care products: QSAR models and ranking for prioritization and safer alternatives' design. Green Chem 18:4393–4406
67. Sangion A, Gramatica P (2016) Hazard of pharmaceuticals for aquatic environment: Prioritization by structural approaches and prediction of ecotoxicity. Environ Int 95:131–143
68. Zhao XG, Jin HY, Ji ZQ, Li DH, Kaw HY, Chen JF, Xie ZY, Zhang TZ (2020) PAES and PAHs in the surface sediments of the East China Sea: occurrence, distribution and influence factors. Sci Total Environ 703:8
69. Tang ZW, Yang ZF, Shen ZY, Niu JF, Liao RF (2007) Distribution and sources of organochlorine pesticides in sediments from typical catchment of the Yangtze River, China. Arch Environ Contam Toxicol 53:303–312
70. Deng FC, Sun JT, Dou RN, Yu XL, Wei Z, Yang CP, Zeng XF, Zhu LZ (2020) Contamination of pyrethroids in agricultural soils from the Yangtze River Delta, China. Sci Total Environ 731:7
71. Li P, Yu R, Hou F, Zhao Y (2023) Legacy and emerging poly- and perfluoroalkyl substances in wastewater treatment plant and receiving water: abundance, removal, and potential ecological risk. Environ Sci Pollut Res 30:29929–29941
72. Tong XE, You LH, Zhang JJ, Chen HT, Nguyen VT, He YL, Gin KYH (2021) A comprehensive modelling approach to understanding the fate, transport and potential risks of emerging contaminants in a tropical reservoir. Water Res 200:9
73. Zhou YR, Zhou ZY, Lian YJ, Sun X, Wu YN, Qiao LQ, Wang ML (2021) Source, transportation, bioaccumulation, distribution and food risk assessment of perfluorinated alkyl substances in vegetables: a review. Food Chem 349:13
74. Han LR, Chang C, Yan SW, Qu CK, Tian YL, Guo JP, Guo JH (2023) Distribution, Sources and risk assessment of polychlorinated biphenyls in sediments from Beiluo River. Toxics 11:12

75. Xiao SK, Wu Q, Pan CG, Yin C, Wang YH, Yu KF (2021) Distribution, partitioning behavior and potential source of legacy and alternative per- and polyfluoroalkyl substances (PFASs) in water and sediments from a subtropical Gulf, South China Sea. Environ Res 201:10
76. Zhang QQ, Xia ZH, Wu MM, Wang LP, Yang H (2017) Human health risk assessment of DDTs and HCHs through dietary exposure in Nanjing, China. Chemosphere 177:211–216
77. Dong LY, Wang ST, Qu JZ, You H, Liu DM (2021) New understanding of novel brominated flame retardants (NBFRs): neuro (endocrine) toxicity. Ecotox Environ Safe 208:14
78. Ling SY, Zhou SQ, Tan JQ, Lu C, Fu MR, Peng C, Zhang W, Hu SQ, Lin KF, Zhou BS (2022) Brominated flame retardants (BFRs) in sediment from a typical e-waste dismantling region in Southern China: occurrence, spatial distribution, composition profiles, and ecological risks. Sci Total Environ 824:8
79. Chua EM, Shimeta J, Nugegoda D, Morrison PD, Clarke BO (2014) Assimilation of polybrominated diphenyl ethers from microplastics by the marine amphipod. Allorchestes Compressa, Environ Sci Technol 48:8127–8134
80. Xu C, Niu LL, Zou DL, Zhu SY, Liu WP (2019) Congener-specific composition of polychlorinated biphenyls (PCBs) in soil-air partitioning and the associated health risks. Sci Total Environ 684:486–495
81. European Chemicals Agency. https://echa.europa.eu/hot-topics/perfluoroalkyl-chemicals-pfas. Accessed 20 May 2023.
82. P.R.C (2023) China's List of Key Emerging Contaminants under Control (2023). https://www.mee.gov.cn/xxgk2018/xxgk/xxgk02/202212/t20221230_1009167.html. Accessed 20 May 2023.
83. List of substances subject to POPs Regulation. https://www.echa.europa.eu/list-of-substances-subject-to-pops-regulation. Accessed 20 May 2023.
84. Huang K, Li YL, Bu D, Fu J, Wang ML, Zhou W, Gu LY, Fu YL, Cong ZY, Hu BY, Fu JJ, Zhang AQ, Jiang GB (2022) Trophic magnification of short-chain per- and polyfluoroalkyl substances in a terrestrial food chain from the Tibetan Plateau. Environ Sci Technol Lett 9:147–152
85. Li XH, Yin PH, Zhao L (2016) Phthalate esters in water and surface sediments of the Pearl River Estuary: distribution, ecological, and human health risks. Environ Sci Pollut Res 23:19341–19349

Publisher's Note