Journal of Hazardous Materials Letters 2 (2021) 100026

Contents lists available at ScienceDirect

Journal of Hazardous Materials Letters

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

The distribution of persistent, mobile and toxic (PMT) pharmaceuticals and personal care products monitored across Chinese water resources

Chen Huang [a,b,c], Biao Jin [a,b,c,*], Min Han [a,b,c], Yang Yu [d], Gan Zhang [a,b], Hans Peter H. Arp [e,f]

[a] State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, 510640, China
[b] CAS Center for Excellence in Deep Earth Science, Guangzhou, 510640, China
[c] University of Chinese Academy of Sciences, Beijing, 10069, China
[d] Solid Waste and Chemicals Management Center, Ministry of Ecology and Environment (MEE), Beijing, 100029, China
[e] Norwegian Geotechnical Institute (NGI), P.O. Box 3930, Ullevaal Stadion, N-0806, Oslo, Norway
[f] Norwegian University of Science and Technology (NTNU), NO-7491, Trondheim, Norway

A R T I C L E I N F O

Keywords:
Drinking water
Groundwater
Surface water
vPvM
PPCP

A B S T R A C T

Hazard classifications have recently been introduced for persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances, which are those that negatively impact water resources if substantially emitted into the environment. Many pharmaceuticals and personal care products (PPCPs) may meet this classification. Our study focused on 169 detected PPCPs in surface water, groundwater and drinking water in China among a total of 432 PPCPs that were monitored for across 75 studies. We assessed if these could be classified as PMT/vPvM substances based on the recent European criteria for industrial substances. For most PPCPs, persistency half-life data were lacking; therefore, definitive classifications could not be made. In surface water, 52 (37.7 %) of the detected PPCPs met, or were strongly suspected to meet, the PMT/vPvM criteria. Over half of these were antibiotic compounds. The industrialized Yangtze, Haihe and Pearl river basins were the most impacted. We hypothesized the proportion of PPCPs monitored meeting the PMT/vPvM criteria in drinking water and groundwater would be larger than surface water. This was supported as 44.3 % of PPCPs in these media met, or based on weight-of-evidence likely meet, the PMT/vPvM criteria; though, a definitive comparison was hindered by a lack of persistence data.

1. Introduction

Increasing contamination of water resources by synthetic chemicals is a global concern (De Baat et al., 2020). Synthetic chemicals such as pharmaceuticals and personal care products (PPCPs) can enter natural aquatic environments via wastewater discharge (Petrie et al., 2015; Tran et al., 2018). Recent studies have detected different PPCPs in diverse water resources, including rivers (Dong et al., 2016; Li et al., 2019; Peng et al., 2017; Yao et al., 2018; Zhou et al., 2016a), lakes (Wang et al., 2019, 2017; Zhou et al., 2016b), groundwater (Peng et al., 2014; Yang et al., 2017; Yao et al., 2017), coastal water (Cheng et al., 2016; Du et al., 2017; Yang et al., 2020) and drinking water (Ben et al., 2020; Feng et al., 2020; Lin et al., 2016; Lv et al., 2019). In order to protect drinking water resources, chemicals with high persistency (P) and sub-surface mobility (M) have been prioritized as pollutants with drinking water concerns, particularly within Europe as part of the Chemicals Strategy for Sustainability (EU, 2020). These prioritized substances are named as persistent, mobile and toxic (PMT) and very persistent, very mobile (vPvM) substances, and the corresponding draft criteria are currently being evaluated by the European Commission (EU, 2020; Hale et al., 2020a; Reemtsma et al., 2016). Once these substances are released into the aqueous environment, they may potentially pass natural and artificial barriers, and finally occur in groundwater and drinking water over long time scales, depending on the emission volume and location (Arp and Hale, 2019; Hale et al., 2020b). Removal of these substances can become technically difficult and expensive (Arp et al., 2017; Goldenman et al., 2019; Reemtsma et al., 2016).

The chemical industry in China has grown sharply during the last decades (Wang et al., 2020; Zhang et al., 2020). PPCPs are widely detected in China's freshwater environment (Liu et al., 2020; Su et al., 2020). In 2018 China initiated a national plan to prevent and remediate the contamination of drinking water sources (MEE and MWR, 2018). Herein, we present a screening study to assess how many PPCPs in general meet the recently introduced European PMT/vPvM criteria, based on chemical property data and weight-of-evidence (Neumann and Schliebner, 2019). The specific goal of this study is to identify (high potential) PMT/vPvM substances among the detected PPCPs in China's surface water, groundwater and drinking water, and to assess their abundance. As

* Corresponding author at: State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, 510640, China.

E-mail address: jinbiao@gig.ac.cn (B. Jin).

http://doi.org/10.1016/j.hazl.2021.100026
Received 23 February 2021; Received in revised form 4 May 2021; Accepted 5 May 2021
Available online 9 May 2021

the substance properties of P and M collectively enable PMT/vPvM substances to be transported over long distances from the point of emission, remain for long time intervals in subsurface waters, and also potentially penetrate through drinking water treatment facilities (Arp and Hale, 2019; Hale et al., 2020b), we also test the hypothesis that the percentage of PPCPs detected in groundwater and drinking water meeting the PMT/vPvM criteria (i.e., number of PPCP-PMT/vPvM in water divided by total number of PPCP in water) will be larger than the corresponding percentage in surface water.

2. Material and methods

2.1. Literature survey

Over 75 relevant publications of freshwater PPCP monitoring data in China were considered, including 69 for surface water, 7 for groundwater and 4 for drinking water (see Table S1 in the supplementary material). Specifically, substance information including their names, reported concentrations, sampling location and CAS numbers, were obtained. In total, 432 PPCPs have been monitored within these 75 studies (Table S2); and of this, only 138 of these PPCPs have been detected in surface water (see Table S4), and 106 PPCPs in groundwater and/or drinking water (see Table S8). It is important to mention that the monitoring methods, target analytes and analytical approaches applied in different studies did vary, therefore introducing uncertainties to our interpretation of the data, particularly when testing the hypothesis by comparing surface water data to ground- and drinking water data.

2.2. P, M and T assessment

First an existing list of PMT substances registered under REACH in 2017 (Arp and Hale, 2019) was consulted to see which of the 432 target compounds were previously evaluated. Though the REACH regulation does not explicitly apply to PPCPs but only industrial substances, REACH does contain some PPCPs if they also have an industrial use (Arp and Hale, 2019). For substances not evaluated, persistency, mobility and toxicity were assessed sequentially following the recently developed guidelines for REACH registered substances (Arp and Hale, 2019), as summarized below.

2.2.1. Persistency assessment

The persistency (P) criteria are adopted from Annex VIII of REACH, which is based on the exceedance of measured half-lives in specified environmental media. Substances already on the REACH candidate list of substances of very high concern (SVHC) for being PBT/vPvB substances or on the Stockholm Convention's POP list would automatically receive a P or vP evaluation. A conclusion of not persistent, "not P", can be based on standardised tests to show the substances are readily or inherently biodegradable (European Chemicals Agency, 2017). The primary source for the experimentally determined degradation half-lives as well as inherent/readily biodegradable screening tests were from the PubChem database (NIH, 2021), which were extracted manually by doing individual queries. In case P assessments were not conclusive for a substance, a further screening test was carried out either by using the PBT-BIOWIN Screening approach mentioned in the REACH PBT guideline (European Chemicals Agency, 2017) or by using the QSAR Toolbox "P" predictor (OECD, 2021). When P assessments using the above two screening tools were conflicting, the Arnot-BIOWIN approach (Arnot et al., 2005) was utilized to help to draw the final P conclusions. If the target compounds were not assessable by using BIOWIN, the CompTox Chemicals Dashboard (US EPA, 2021) provided by US EPA was utilized for the P assessment. It should be noted that these methods to estimate P have a large uncertainty range (Li et al., 2020). From a comparison with experimental data it was observed that BIOWIN can predict OECD screening tests for ready biodegradability with 72 % overall efficiency (n = 1714), and that comparisons with measured half-life values indicate geometric standard deviations of a factor 10–20 (Arp et al., 2017). When there was no experimental half-life evidence of a substance being "not P", "P" or "vP", two categories were made based on weight-of-evidence using the above methods: "potential P/vP" and "potential P/vP + + ", with the latter having the most weight-of-evidence. Justifications for individual decisions for each PPCP are provided in the supplementary material, Table S2, based on the PMT/vPvM guideline (Arp and Hale, 2019).

2.2.2. Mobility assessment

Mobility is a unique criterion for the PMT/vPvM assessment (Neumann and Schliebner, 2019). Experimental log K_{oc} values (between pH 4–9) are the basis of the M criteria, with values under 4.0 being the cut off for mobile (M) and 3.0 for very mobile (vM) (Neumann and Schliebner, 2019). If no such data was available, screening parameters can be used as part of a weight-of-evidence assessment. These parameters include the octanol-water partitioning coefficient, log $K_{ow,}$ for neutral compounds or the pH dependent octanol-water distribution coefficient, log D_{ow}, for ionizable substances, where a cut-off value of < 4.5 (between pH 4–9) is an indicator for mobility, depending on the ionic charge (Arp and Hale, 2019). Experimental log K_{oc} and log K_{ow} values were obtained from the PubChem database, log D_{ow} values at different pH were queried from Chemaxon software (ChemAxon, 2021). For borderline M cases based on log K_{ow}/D_{ow} a category "potential M/vM" was utilized, and the suggested screening cutoffs were shifted based on the uncertainty of correlations between log K_{ow}/D_{ow} and log K_{oc} (Arp and Hale, 2019). As an example, for neutral compounds, anions or ionizable compounds with experimentally determined log $K_{ow}/D_{ow,}$ between 4.5 and 3.5 are considered "Potential M/vM", between 3.5 and 2.5 as M and less than 2.5 as vM. Further criteria for zwitterions, ionizable substances with no experimental pKa values were also implemented (Arp and Hale, 2019).

2.2.3. Toxicity assessment

The criterion for toxicity (T) is based on Annex VIII for PBT assessment with additional considerations specific for drinking water, including carcinogenic category 2, cell mutagenic category 2, and endocrine disrupting properties (Neumann and Schliebner, 2019). Data for the hazard categories were acquired from the public C&L registry in ECHA website (ECHA, 2020). No observed effect concentrations (NOEC) were obtained from the EnviroTox database (HESI, 2020). If a substance satisfies any above-mentioned criterion it is considered "T". When the criteria are not met, a Cramer Class assessment was performed using QSAR Toolbox (Arp and Hale, 2019), with Cramer Class III being considered "Potential T". In case a Cramer Class III did not occur, the substance was assumed to be "not T".

2.2.4. PMT/vPvM assessment

The final categories were as follows: 1) *vPvM* – both vP and vM criteria were fulfilled; 2) *PMT* – the P, M and T criteria were fulfilled (a substance can be both PMT and vPvM); 3) *Potential PMT/vPvM + +* – the Potential P/vP + + category was fulfilled along with either vM or both M and T (here " + + " indicates there is a high likelihood criteria are met based on weight-of-evidence, even thoughdefinitive experimental data are lacking). Alternatively, the P or vP and were fulfilled along with Potential M/vM and T; 4) *Potential PMT/vPvM* – the Potential P/vP criteria were fulfilled along with either M/vM, or Potential M/vM and/or T; 5) *PM* – a combination of either PM, vPM or PvM was concluded for a "not T" or "Potential T" substance; 6) *Not PMT/vPvM* – either "not P" or "not M" was fulfilled; 7) *No conclusions possible* – data was either missing (e.g. chemical structures) or too uncertain to make conclusions.

3. Results and discussion

3.1. Availability of data

Detailed information of the 432 PPCPs monitored for in Chinese surface water studies are provided in Table S3. It was only possible to make definitive "not P", P and vP conclusions for 68 substances, due to the lack of experimental half-lives. Persistence evaluations were mainly assessed based on weight-of-evidence categories. Persistency being a data bottle neck is typically observed for such screening studies (Arp et al., 2017; Strempel et al., 2012). For mobility, by contrast, conclusions of "not M", M, and vM could be made for 334 substances. For toxicity, there were 144 definitive T and "not T" conclusions (Table S2). Therefore, amongst the 432 substances, for only 84 could definitive conclusions be made, with categories being vPvM & PMT (3 substances), PMT (6 substances), PM (3 substances) and not PMT (72 substances). For 343 substances a weight-of-evidence conclusion of either "Potential PMT/vPvM" and "Potential PMT/vPvM+ +" assessments were made, for 203 substances and 140 substances, respectively. "No conclusions possible" occurred for 5 substances, due to a lack of structural information.

3.2. Occurrence of PMT/vPvM substances in surface water

Among the 432 PPCPs, 138 were detected in surface water (Table S4). The distribution of PMT categories amongst them is presented in Fig. 1a. Specifically, 3 surface water PPCPs (2.2 %) were assessed as “PMT”, 49 (35.5 %) were assessed as “potential PMT/vPvM+ +”, 1 as “PM”, and 65 (47.1 %) as “Potential PMT/vPvM”s. Only 19 (13.8 %) of the PPCPs were identified as “not PMT/vPvM”, with 12 having experimentally determined short half-lives or deemed ready/inherently biodegradable, and the other 7 not meeting the “M” criteria. The three substances that definitively met the PMT criteria are carbamazepine, diazepam, amantadine (Table S4).

3.2.1. Surface water concentrations

Concentration data of the identified PMT and potential PMT/vPvM+ + substances in surface water were obtained from different studies and are summarized in Table S5. The number of monitoring data points where these substances were detected ranged from 1 to 84, depending on the substance (see Table S6). This was due in part to the different analytes and methods used across the different studies. Based on the monitoring data, the median concentrations of the most abundant PMT and potential PMT/vPvM+ + substances were ranked and plotted in Fig. 1b. Among these substances the median concentrations ranged from 1 ng/L to 100 ng/L. The three most abundant ones based on the median concentrations were triclosan, florfenicol and erythromycin.

3.2.2. Types of PPCPs in surface water

Over 59.6 % of the PMT and Potential PMT/vPvM+ + substances detected in Chinese surface water were antibiotic compounds (Fig. 2a). It has been previously reported that antibiotic substances were able to break through Chinese waste water treatment processes (Ben et al., 2020), in addition to them being increasingly synthesized and consumed in China in the last decade (Liu et al., 2020; Zhang et al., 2015). According to a nation-wide monitoring study of PPCPs in surface water in China, about 75 % of the detected pharmaceuticals were antibiotics (Bu et al., 2013).

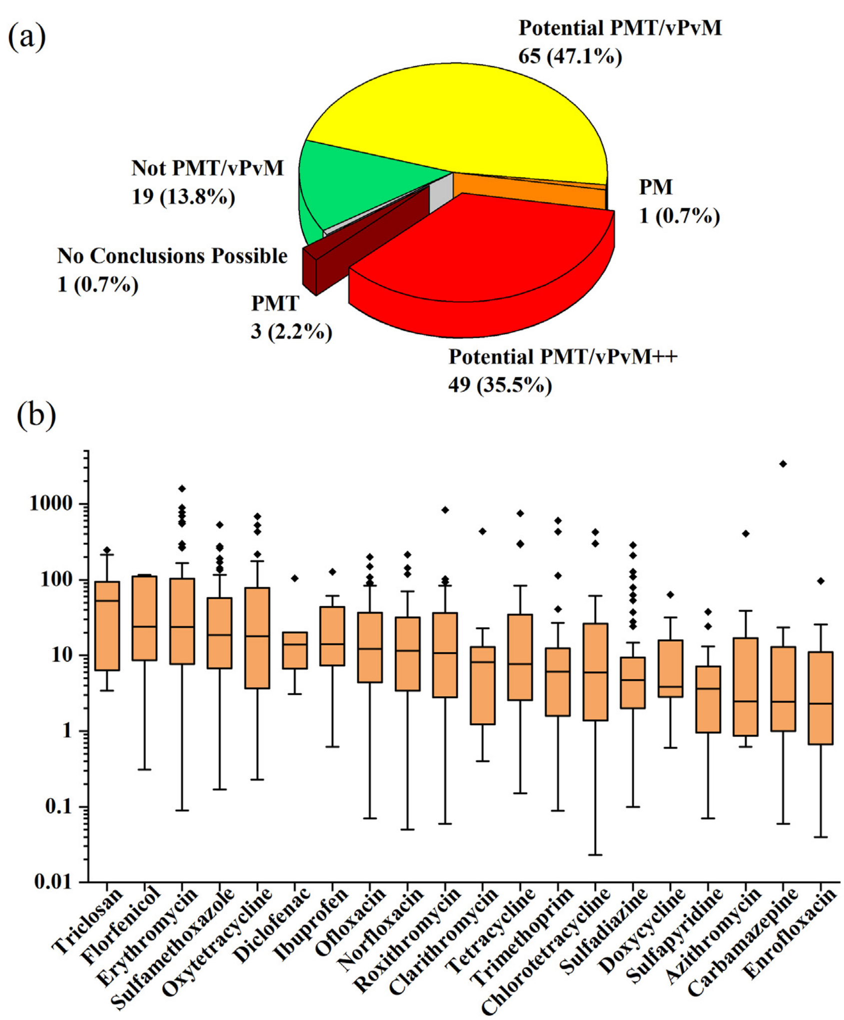

Fig. 1. PMT/vPvM assessment of PPCPs detected in Chinese surface water (panel a) and box plot of the median concentration for the most abundant PMT and potential PMT/vPvM+ + substances (panel b).

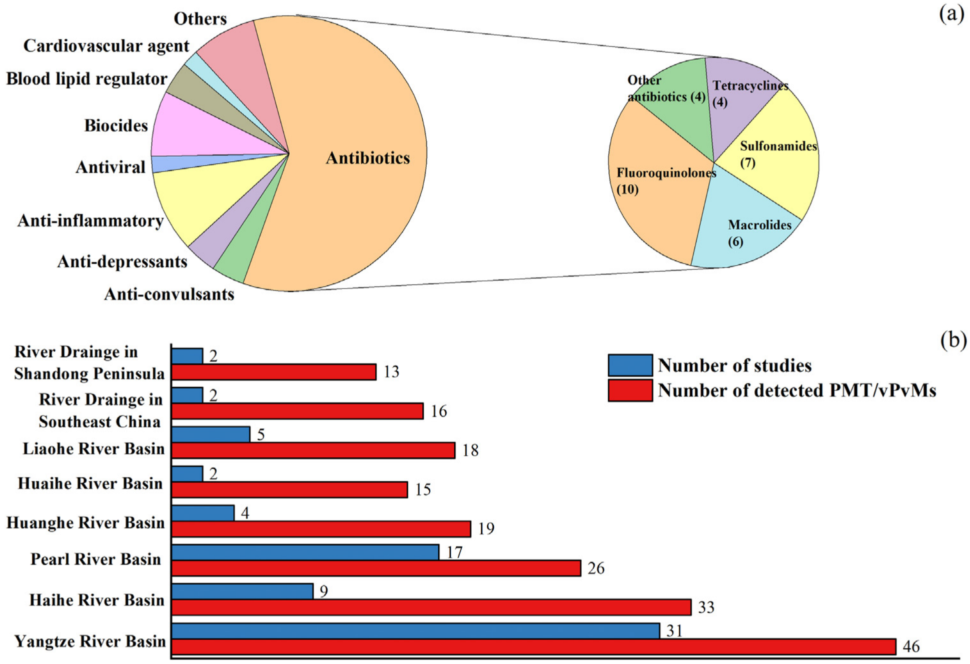

Fig. 2. Use type of the 52 detected PMT/vPvM PPCPs in surface water (panel a) and their distribution in Chinese surface water basins. along with the number of the studies per basin (panel b).

Moreover, fluoroquinolone-antibiotics and sulfonamide-antibiotics contributed 32.3 % and 22.6 % of the detected substances meeting the PMT/Potential PMT/vPvM++ criteria, respectively. According to our literature study, sulfonamides are one of the most frequently detected PPCPs in Chinese surface water, with 88 % of the studies having detected them.

3.2.3. Spatial distribution

The monitoring studies have mainly been conducted in Yangtze River Basin, Pearl River Basin and Haihe River Basin. The three river basins are the most populated and industrialized areas in China, and they are impacted heavily by domestic wastewaters. This could be the main reason for the occurrence of more prioritized substances detected in these three river basins (Fig. 2). For instance, over 30 PMT and potential PMT/vPvM ++ substances were found in Yangtze river basin and Haihe river basin. The fact that less PMT and potential PMT/vPvM++ substances were identified in other river basins also could be due to insufficient monitoring data, as indicated by the number of studies in Fig. 2b. Erythromycin, norfloxacin, ofloxacin, oxytetracycline, roxithromycin, sulfamethazine, sulfamethoxazole, tetracycline, were found in all the eight river basins

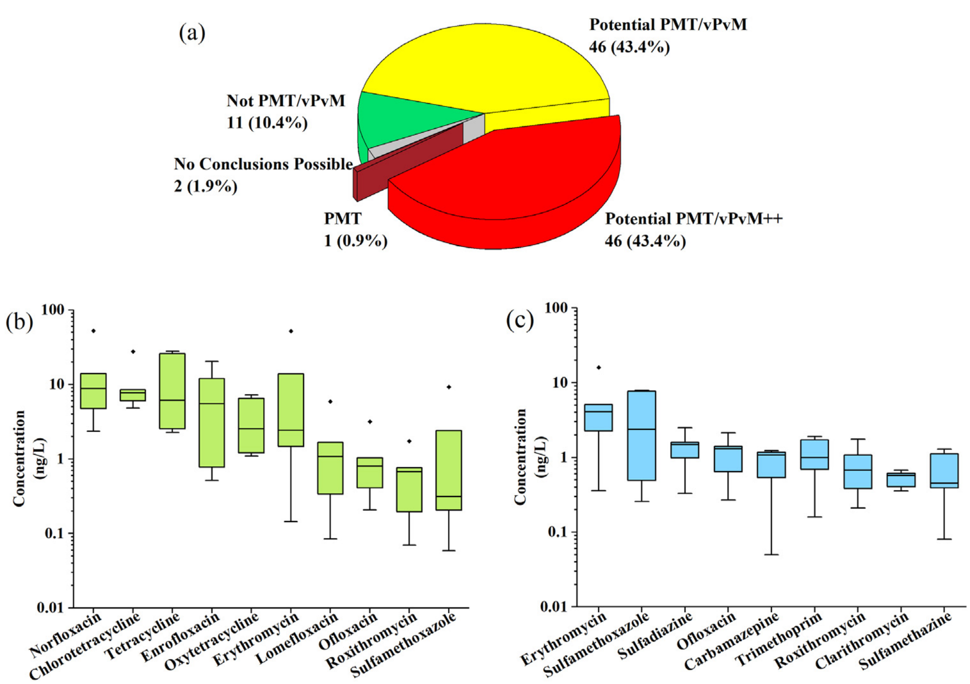

Fig. 3. PMT/vPvM assessment of PPCPs detected in drinking water and groundwater in China (panel a), and the concentration of the most abundant PPCP-PMT/vPvM substances detected in groundwater (panel b) and drinking water (panel c).

(see table S7), indicating extensive consumption of these substances in China.

3.3. Occurrence of PMT/vPvM substances in groundwater and drinking water

In total 106 PPCPs were detected in the drinking water and groundwater monitoring studies, 75 of which were also detected in the surface water studies, and 31 were not detected in the surface water studies. The reason for the 31 substances in drinking water and groundwater not being detected in surface water is attributed to the varying target substances included and limits of detection across the monitoring studies. As presented in Fig. 3a, 47 substances were identified as the PMT and potential PMT/ vPvM + + accounting for over 44.3 % of the detected PPCPs. This fraction is higher than that obtained for the surface water (i.e. 37.7 %) as shown in Fig. 1a. Only one substance detected in drinking water/groundwater had a measured half-life (carbamazepine, see Table S8). Fig. 3 b and c present the PMT and potential PMT/vPvM + + substances that are detected in groundwater and/or drinking water, and that they were, again, dominated by antibiotic compounds.

A similarly conducted assessment of 3859 REACH industrial substances with an organic substituent (and European volumes of greater than 10 tonnes per year) concluded that 58 % were not PMT/ vPvM, 19 % were "Potential PMT/vPvM", 14 % had no conclusion possible, and only 4% either met or were strongly suspected to meet the PM, PMT, and/or vPvM criteria. The much larger fraction of PPCPs meeting or suspected to meet the PMT/vPvM criteria in this study could be due to PPCPs in general being more persistent and mobile than industrial substances. One hypothesis that could account for this is that a combination of long product shelf lives and rapid depuration rates could be attractive properties for the design of many PPCPs, and these properties could, respectively, be correlated with environmental persistency and mobility. It would be of interest to pursue this hypothesis in follow-up studies. Similarly, it would be of interest to investigate if PPCPs tend to be more persistent and mobile than other commercial or regulatory groups of chemicals.

The corresponding median concentration of the substances detected in groundwater and drinking water varied from sub ng/L to 10 ng/L. In order to exemplify the PMT and potential PMT/vPvM + + detected in both groundwater and drinking water, the corresponding maximum mean concentration were presented in Table 1. Over half of these substances occurred at higher concentrations in groundwater compared with the detected counterparts in drinking water.

This data supports hypothesis that the percentage of PPCPs detected in groundwater and drinking water that meet the PMT/vPvM criteria is somewhat larger than the fraction of substances detected in surface water. However, the discrepancy in target analytes, locations and detection limits across the studies questions the statistical robustness of testing this hypothesis; follow-up studies should pursue this hypothesis using a consistent analytical approach.

Table 1
The PPCPs detected in both groundwater and drinking water in China that meet or are strongly expected to meet the PMT/vPvM criteria.

Chemical Name	CAS Number	Use Type	Maximum C_{mean} (ng/L)*	
			Groundwater	Drinking water
Norfloxacin	70458−96-7	Antibiotic	52.6	12.0
Erythromycin	114−07-8	Antibiotic	52.2	16.0
Tetracycline	60−54-8	Antibiotic	28.0	2.87
Chlorotetracycline	57−62-5	Antibiotic	27.8	2.10
Enrofloxacin	93106−60-6	Antibiotic	20.3	16.23
Doxycycline	564−25-0	Antibiotic	18.1	4.60
Sulfamethoxazole	723−46-6	Antibiotic	9.28	7.90
Oxytetracycline	79−57-2	Antibiotic	7.24	23.0
Lomefloxacin	98079−51-7	Antibiotic	5.90	0.150
Ofloxacin	82419−36-1	Antibiotic	3.18	2.14
Roxithromycin	80214−83-1	Antibiotic	1.74	1.75
Sulfadiazine	68−35-9	Antibiotic	1.47	2.48
Sulfapyridine	144−83-2	Antibiotic	0.950	18.1
Sulfamethazine	57−68-1	Antibiotic	0.620	1.29
Trimethoprim	738−70-5	Antibiotic	0.530	1.90
Clarithromycin	81103−11-9	Antibiotic	0.400	0.670
Sulfathiazole	72−14-0	Antibiotic	0.360	0.180
Azithromycin	83905−01-5	Antibiotic	0.360	1.65

* The references are provided in table S9 in the supplementary material.

4. Implications

These results indicate that a large portion of PPCPs detected in Chinese surface water, groundwater and drinking water are or potentially are PMT/vPvM substances. The identified PMT and potential PMT/vPvM + + substances are a concern for drinking water and groundwater quality, since the concentration of these substances may potentially increase with increasing emissions (Hale et al., 2020b). Collectively, these results support the need to adopt a national PMT chemical strategy for the protection of water resources in China (Jin et al., 2020), which can include better safeguards for lower use or emissions of PPCPs meeting the PMT/vPvM criteria, and enhanced water treatment strategies. The study also emphasizes that there is a need for better half-life (persistency) characterization of the PPCPs detected in surface water, groundwater, and drinking water, as well as novel, biodegradable PPCPs, to better safeguard water resources.

Declaration of Competing Interest

The authors report no declarations of interest.

Acknowledgements

B.J. acknowledges support from Guangdong Foundation for Science and Technology Research (2020B1212060053; 2019A1515011035), and a grant from State Key Laboratory of Organic Geochemistry, Chinese Academy of Sciences (SKLOG2020-4). G.Z. acknowledges funding from Guangdong Science and Technology Projects (2018B030324002). H.P.H. A. acknowledges German Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety (FKZ3719654080).

Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.hazl.2021.100026.

References

Arnot, J., Gouin, T., Mackay, D., 2005. Practical Methods for Estimating Environmental Biodegradation Rates (No. CEMN Report No. 200503). Canadian Environmental Modelling Network, Trent University.
Arp, H.P.H., Hale, S.E., 2019. Improvement of Guidance and Methods for the Identification and Assessment of PM/PMT Substances; FKZ 3716 67 416 0. ISSN: 1862-4804. German Environmental Agency (UBA), Dessau-Rosslau, Germany.
Arp, H.P.H., Brown, T.N., Berger, U., Hale, S.E., 2017. Ranking REACH registered neutral, ionizable and ionic organic chemicals based on their aquatic persistency and mobility. Environ. Sci. Process. Impacts 19, 939–955. https://doi.org/10.1039/C7EM00158D.
Ben, Y., Hu, M., Zhang, X., Wu, S., Wong, M.H., Wang, M., Andrews, C.B., Zheng, C., 2020. Efficient detection and assessment of human exposure to trace antibiotic residues in drinking water. Water Res. 175115699 https://doi.org/10.1016/j.watres.2020.115699.

Bu, Q., Wang, B., Huang, J., Deng, S., Yu, G., 2013. Pharmaceuticals and personal care products in the aquatic environment in China: a review. J. Hazard. Mater. 262, 189–211. https://doi.org/10.1016/j.jhazmat.2013.08.040.
ChemAxon; ChemAxon: https://chemaxon.com. (http://chemaxon.com, retrieved on November, 2020).
Cheng, D., Xie, Y., Yu, Y., Liu, X., Zhao, S., Cui, B., Bai, J., 2016. Occurrence and partitioning of antibiotics in the water column and bottom sediments from the intertidal zone in the Bohai Bay, China. Wetlands 36, 167–179. https://doi.org/10.1007/s13157-014-0561-y.
De Baat, M.L., Van der Oost, R., Van der Lee, G.H., Wieringa, N., Hamers, T., Verdonschot, P.F.M., De Voogt, P., Kraak, M.H.S., 2020. Advancements in effect-based surface water quality assessment. Water Res. 183116017 https://doi.org/10.1016/j.watres.2020.116017.
Dong, D., Zhang, L., Liu, S., Guo, Z., Hua, X., 2016. Antibiotics in water and sediments from Liao River in Jilin Province, China: occurrence, distribution, and risk assessment. Environ. Earth Sci. 75, 1202. https://doi.org/10.1007/s12665-016-6008-4.
Du, J., Zhao, H., Liu, S., Xie, H., Wang, Y., Chen, J., 2017. Antibiotics in the coastal water of the South Yellow Sea in China: occurrence, distribution and ecological risks. Sci. Total Environ. 595, 521–527. https://doi.org/10.1016/j.scitotenv.2017.03.281.
ECHA. C&L Inventory. https://echa.europa.eu/information-on-chemicals/cl-inventory-database (retrieved September, 2020).
EU, 2020. Chemicals Strategy for Sustainability Towards a Toxic-free Environment; COM (2020) 667 Final. European Commission.
European Chemicals Agency, 2017. Guidance on Information Requirements and Chemical Safety Assessment Chapter R.11: PBT/VPvB Assessment Version 3.0; ED-01-17-294-EN-N. European Chemicals Agency.
Feng, Li, Cheng, Y., Zhang, Y., Li, Z., Yu, Y., Feng, Lei, Zhang, S., Xu, L., 2020. Distribution and human health risk assessment of antibiotic residues in large-scale drinking water sources in Chongqing area of the Yangtze River. Environ. Res. 185109386 https://doi.org/10.1016/j.envres.2020.109386.
Goldenman, G., Fernandes, M., Holland, M., Tugran, T., Nordin, A., Schoumacher, C., McNeill, A., 2019. The Cost of Inaction : A Socioeconomic Analysis of Environmental and Health Impacts Linked to Exposure to PFAS, TemaNord. Nordisk Ministerråd, Copenhagen https://doi.org/10.6027/TN2019-516.
Hale, S.E., Arp, H.P.H., Schliebner, I., Neumann, M., 2020a. What's in a name: Persistent, Mobile, and Toxic (PMT) and Very Persistent and Very Mobile (vPvM) substances. Environ. Sci. Technol. https://doi.org/10.1021/acs.est.0c05257 acs.est.0c05257.
Hale, S.E., Arp, H.P.H., Schliebner, I., Neumann, M., 2020b. Persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances pose an equivalent level of concern to persistent, bioaccumulative and toxic (PBT) and very persistent and very bioaccumulative (vPvB) substances under REACH. Environ. Sci. Eur. 32, 155. https://doi.org/10.1186/s12302-020-00440-4.
HESI, 2020. EnviroTox - Tools for Calculating Ecotoxicological Thresholds of Concern. (Accessed on September 7, 2020) https://envirotoxdatabase.org/.
Jin, B., Huang, C., Yu, Y., Zhang, G., Arp, H.P.H., 2020. The need to adopt an international PMT strategy to protect drinking water resources. Environ. Sci. Technol. https://doi.org/10.1021/acs.est.0c04281.
Li, Y., Ding, J., Zhang, L., Liu, X., Wang, G., 2019. Occurrence and ranking of pharmaceuticals in the major rivers of China. Sci. Total Environ. 696133991 https://doi.org/10.1016/j.scitotenv.2019.133991.
Li, Y., Zhang, L., Ding, J., Liu, X., 2020. Prioritization of pharmaceuticals in water environment in China based on environmental criteria and risk analysis of top-priority pharmaceuticals. J. Environ. Manage. 253109732 https://doi.org/10.1016/j.jenvman.2019.109732.
Lin, T., Yu, S., Chen, W., 2016. Occurrence, removal and risk assessment of pharmaceutical and personal care products (PPCPs) in an advanced drinking water treatment plant (ADWTP) around Taihu Lake in China. Chemosphere 152, 1–9. https://doi.org/10.1016/j.chemosphere.2016.02.109.
Liu, N., Jin, X., Feng, C., Wang, Z., Wu, F., Johnson, A.C., Xiao, H., Hollert, H., Giesy, J.P., 2020. Ecological risk assessment of fifty pharmaceuticals and personal care products (PPCPs) in Chinese surface waters: a proposed multiple-level system. Environ. Int. 136105454 https://doi.org/10.1016/j.envint.2019.105454.
Lv, J., Zhang, L., Chen, Y., Ye, B., Han, J., Jin, N., 2019. Occurrence and distribution of pharmaceuticals in raw, finished, and drinking water from seven large river basins in China. J. Water Health 17, 477–489. https://doi.org/10.2166/wh.2019.250.
MEE, MWR, 2018. National Action Plan for Environmental Protection of Centralized Drinking Water Sources; 000014672/2018-00402. Ministry of Ecology and Environment of People's Republic of China.
Neumann, M., Schliebner, I., 2019. Protecting the Sources of Our Drinking Water: the Criteria for Identifying Persistent, Mobile and Toxic (PMT) Substances and Very Persistent and Very Mobile (VPvM) Substances Under EU Regulation REACH (EC) No 1907/2006; Texte 127/2019. ISSN: 1862-4804. German Environmental Agency (UBA), Dessau-Rosslau, Germany.
NIH. PubChem; National Institute of Health. https://pubchem.ncbi.nlm.nih.gov/. (retrieved on May to August, 2020).
OECD; QSAR Toolbox, Version 4.4.1; Organisation for Economic Co-operation and Development. http://www.qsartoolbox.org (retrieved on May to August, 2020).
Peng, X., Ou, W., Wang, C., Wang, Z., Huang, Q., Jin, J., Tan, J., 2014. Occurrence and ecological potential of pharmaceuticals and personal care products in groundwater and reservoirs in the vicinity of municipal landfills in China. Sci. Total Environ. 490, 889–898. https://doi.org/10.1016/j.scitotenv.2014.05.068.
Peng, F.-J., Pan, C.-G., Zhang, M., Zhang, N.-S., Windfeld, R., Salvito, D., Selck, H., Van den Brink, P.J., Ying, G.-G., 2017. Occurrence and ecological risk assessment of emerging organic chemicals in urban rivers: Guangzhou as a case study in China. Sci. Total Environ. 589, 46–55. https://doi.org/10.1016/j.scitotenv.2017.02.200.
Petrie, B., Barden, R., Kasprzyk-Hordern, B., 2015. A review on emerging contaminants in wastewaters and the environment: current knowledge, understudied areas and recommendations for future monitoring. Water Res. 72, 3–27. https://doi.org/10.1016/j.watres.2014.08.053.
Reemtsma, T., Berger, U., Arp, H.P.H., Gallard, H., Knepper, T.P., Neumann, M., Quintana, J.B., Voogt, Pde, 2016. Mind the gap: persistent and mobile organic compounds—water contaminants that slip through. Environ. Sci. Technol. 50, 10308–10315. https://doi.org/10.1021/acs.est.6b03338.
Strempel, S., Scheringer, M., Ng, C.A., Hungerbühler, K., 2012. Screening for PBT chemicals among the “Existing” and “New” chemicals of the EU. Environ. Sci. Technol. 46, 5680–5687. https://doi.org/10.1021/es3002713.
Su, C., Cui, Y., Liu, D., Zhang, H., Baninla, Y., 2020. Endocrine disrupting compounds, pharmaceuticals and personal care products in the aquatic environment of China: which chemicals are the prioritized ones? Sci. Total Environ. 720137652 https://doi.org/10.1016/j.scitotenv.2020.137652.
Tran, N.H., Reinhard, M., Gin, K.Y.-H., 2018. Occurrence and fate of emerging contaminants in municipal wastewater treatment plants from different geographical regions-a review. Water Res. 133, 182–207. https://doi.org/10.1016/j.watres.2017.12.029.
US EPA. CompTox Chemistry Dashboard. The United States Environmental Protection Agency. https://comptox.epa.gov/dashboard. (retrieved on March, 2021).
Wang, Z., Du, Y., Yang, C., Liu, X., Zhang, J., Li, E., Zhang, Q., Wang, X., 2017. Occurrence and ecological hazard assessment of selected antibiotics in the surface waters in and around Lake Honghu, China. Sci. Total Environ. 609, 1423–1432. https://doi.org/10.1016/j.scitotenv.2017.08.009.
Wang, Y., Liu, Y., Lu, S., Liu, X., Meng, Y., Zhang, G., Zhang, Y., Wang, W., Guo, X., 2019. Occurrence and ecological risk of pharmaceutical and personal care products in surface water of the Dongting Lake, China-during rainstorm period. Environ. Sci. Pollut. Res. 26, 28796–28807. https://doi.org/10.1007/s11356-019-06047-4.
Wang, Z., Walker, G.W., Muir, D.C.G., Nagatani-Yoshida, K., 2020. Toward a global understanding of chemical pollution: a first comprehensive analysis of national and regional chemical inventories. Environ. Sci. Technol. 54, 2575–2584. https://doi.org/10.1021/acs.est.9b06379.
Yang, L., He, J.-T., Su, S.-H., Cui, Y.-F., Huang, D.-L., Wang, G.-C., 2017. Occurrence, distribution, and attenuation of pharmaceuticals and personal care products in the riverside groundwater of the Beiyun River of Beijing, China. Environ. Sci. Pollut. Res. 24, 15838–15851. https://doi.org/10.1007/s11356-017-8999-0.
Yang, L., Zhou, Y., Shi, B., Meng, J., He, B., Yang, H., Yoon, S.J., Kim, T., Kwon, B.-O., Khim, J.S., Wang, T., 2020. Anthropogenic impacts on the contamination of pharmaceuticals and personal care products (PPCPs) in the coastal environments of the Yellow and Bohai seas. Environ. Int. 135105306 https://doi.org/10.1016/j.envint.2019.105306.
Yao, L., Wang, Y., Tong, L., Deng, Y., Li, Y., Gan, Y., Guo, W., Dong, C., Duan, Y., Zhao, K., 2017. Occurrence and risk assessment of antibiotics in surface water and groundwater from different depths of aquifers: a case study at Jianghan Plain, central China. Ecotoxicol. Environ. Saf. 135, 236–242. https://doi.org/10.1016/j.ecoenv.2016.10.006.
Yao, B., Yan, S., Lian, L., Yang, X., Wan, C., Dong, H., Song, W., 2018. Occurrence and indicators of pharmaceuticals in Chinese streams: a nationwide study. Environ. Pollut. 236, 889–898. https://doi.org/10.1016/j.envpol.2017.10.032.
Zhang, Q.-Q., Ying, G.-G., Pan, C.-G., Liu, Y.-S., Zhao, J.-L., 2015. Comprehensive evaluation of antibiotics emission and fate in the river basins of China: source analysis, multimedia modeling, and linkage to bacterial resistance. Environ. Sci. Technol. 49, 6772–6782. https://doi.org/10.1021/acs.est.5b00729.
Zhang, X., Sun, X., Jiang, R., Zeng, E.Y., Sunderland, E.M., Muir, D.C.G., 2020. Screening new persistent and bioaccumulative organics in China's inventory of industrial chemicals. Environ. Sci. Technol. 54, 7398–7408. https://doi.org/10.1021/acs.est.0c01898.
Zhou, H., Ying, T., Wang, X., Liu, J., 2016a. Occurrence and preliminarily environmental risk assessment of selected pharmaceuticals in the urban rivers. China. Sci. Rep. 6, 34928. https://doi.org/10.1038/srep34928.
Zhou, L., Wu, Q.L., Zhang, B., Zhao, Y., Zhao, B., 2016b. Occurrence, spatiotemporal distribution, mass balance and ecological risks of antibiotics in subtropical shallow Lake Taihu, China. Environ. Sci. Process. Impacts 18, 500–513. https://doi.org/10.1039/C6EM00062B.