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What's in the water? – Target and suspect screening of contaminants of emerging concern in raw water and drinking water from Europe and Asia

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ABSTRACT

There is growing worry that drinking water can be affected by contaminants of emerging concern (CECs), potentially threatening human health. In this study, a wide range of CECs (n = 177), including pharmaceuticals, pesticides, perfluoroalkyl substances (PFASs) and other compounds, were analysed in raw water and in drinking water collected from drinking water treatment plants (DWTPs) in Europe and Asia (n = 13). The impact of human activities was reflected in large numbers of compounds detected (n = 115) and high variation in concentrations in the raw water (range 15-7995 ng L^{-1} for Σ_{177}CECs). The variation was less pronounced in drinking water, with total concentration ranging from 35 to 919 ng L^{-1}. Treatment efficiency was on average 65 ± 28%, with wide variation between different DWTPs. The DWTP with the highest ΣCEC concentrations in raw water had the most efficient treatment procedure (average treatment efficiency 89%), whereas the DWTP with the lowest Σ_{177}CEC concentration in the raw water had the lowest average treatment efficiency (2.3%). Suspect screening was performed for 500 compounds ranked high as chemicals of concern for drinking water, using a prioritisation tool (SusTool). Overall, 208 features of interest were discovered and three were confirmed with reference standards. There was co-variation between removal efficiency in DWTPs for the target compounds and the suspected features detected using suspect screening, implying that removal of known contaminants can be used to predict overall removal of potential CECs for drinking water production. Our results can be of high value for DWTPs around the

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globe in their planning for future treatment strategies to meet the increasing concern about human exposure to unknown CECs present in their drinking water.

1. Introduction

Large amounts of synthetic organic chemicals are used worldwide in products, goods and daily life (Richardson and Ternes 2014; Benotti et al. 2009a; Geissen et al. 2015; Ruff et al. 2015; Schwarzenbach et al. 2006; Stuart et al. 2012; Padhye et al. 2014b; Sörengård et al. 2019). These chemicals can potentially reach water bodies used for production of drinking water and compromise raw water quality (Tröger et al., 2018, 2020). Major point sources of chemicals include wastewater treatment plants (WWTPs), industries and hospitals (Gago-Ferrero et al. 2017; Sörengård et al. 2019; Loos et al. 2013). Insufficient removal of contaminants of emerging concern (CECs) during drinking water treatment could pose a risk to human exposure (Falconer et al. 2006), e.g. to pesticides (Petrovic, Gonzalez, and Barcelo 2003; Badach, Nazimek, and Kaminska 2007; Mekonen et al. 2016; Fava et al. 2010), pharmaceuticals and personal care products (PPCPs) (Stackelberg et al. 2007; Webb et al. 2003) and flame retardants (Garcia-Lopez, Rodriguez, and Cela 2010; Wang, Liu, and Yin 2011). Another pressing matter is potential human exposure to per- and polyfluoroalkyl substances (PFASs) via drinking water (Hu et al. 2016; Sharma et al. 2016; Zafeiraki et al. 2015), due to the occasional high concentrations, high persistence, bioaccumulation and potential toxic characteristics of these substances (Gebbink, Glynn, and Berger 2015; Gyllenhammar et al. 2015).

Conventional drinking water treatment processes (e.g. sand filtration and flocculation) are usually efficient in removing pathogens, but inefficient in removing CECs (Margot et al. 2013; Stackelberg et al. 2007; Ternes et al. 2002; Tröger et al. 2018; Sörengård et al. 2019). There is therefore a need to complement existing treatment efficiency studies with investigations specifically focusing on CECs. Treatment through sorption materials, such as granular activated carbon (GAC), has been shown to remove CECs (Margot et al. 2013; Stackelberg et al. 2007; Ternes et al. 2002; Tröger et al., 2020), but complete removal is commonly not achieved (McCleaf et al. 2017; Tröger et al. 2018) because of weak binding of some CECs (McCleaf et al. 2017), decreasing removal efficiency for CECs with increasing operating time of the GAC material (Kennedy et al. 2015; McCleaf et al. 2017; Tröger et al., 2020) and co-sorption of dissolved organic matter (Lavonen et al. 2015; McCleaf et al. 2017; Golovko et al. 2020; Ullberg et al. 2021). Most CEC removal efficiency studies to date have been conducted with a selected number of CECs and little is known about the removal of a broad range of CECs in current full-scale drinking water treatment plants (DWTPs).

The most common approach when screening for CECs in environmental samples is target screening using reference standards for quantification and confirmation (Benotti et al. 2009b; Gago-Ferrero et al. 2017; Padhye et al. 2014a; Ren et al. 2020; Togola and Budzinski 2008; Tröger et al. 2018). A complementary approach is suspect screening, where features detected using high resolution mass spectrometry (HRMS) are compared against a list of suspects containing the compounds of interest (Andres-Costa, Andreu, and Pico 2016; Bade, Bijlsma, et al. 2015; Gago-Ferrero et al. 2018; Gago-Ferrero et al. 2015; Hug et al. 2014; Schymanski et al. 2015). A suspect list relevant for drinking water can be created by prioritising compounds based on their physicochemical properties (Dürig et al., 2019) and/or exposure indices and usage quantities derived from regulatory databases (Gago-Ferrero et al. 2018). To build confidence in the identification, mass accuracy, fragmentation and isotopic profiles can be considered, leading to different levels of confidence (Schymanski et al. 2014). Suspect screening approaches have been applied to search for CECs in surface water and groundwater (Andres-Costa, Andreu, and Pico 2016; Gago-Ferrero et al. 2015), but there is a lack of suspect screening studies focusing on drinking water quality.

This study addressed the lack of international studies on CECs and their behaviour in full-scale DWTPs. A wide-scope screening of CECs in raw and drinking water samples from 13 different DWTPs in 11 countries across Europe and Asia was performed, to better understand the presence and behaviour of CECs during different drinking water treatment processes. The aim was to investigate the relationship between treatment efficiency of target analytes and the presence of unknown CECs in water in a screening study. Specific objectives were I) to investigate the occurrence of a large variety of CECs (n = 177) including pharmaceuticals, PFASs, pesticides (including metabolites) and other compounds in raw water and drinking water, II) to assess their removal efficiency in a number of case studies, III) to perform a suspect screening of 500 compounds prioritised using SusTool (Dürig et al., 2019) and compare their removal with target compounds, and IV) to identify a selected number of unknown CECs using reference standards.

2. Materials and methods

2.1. Sampling sites and sample collection

In total, 13 DWTPs located in 11 different European (n = 8) and Asian (n = 3) countries were selected for the study (Table 1). The selected case study objects only comprised DWTPs that use surface water as raw water, as previous studies have indicated that surface water is more strongly impacted by CECs than groundwater (Stuart et al. 2012; Cahill et al. 2004). The 13 DWTPs employed different treatment according to their needs, while some DWTPs did not implement advanced treatments at all. Reverse osmosis was incorporated as a treatment step in one of the DWTPs investigated. All DWTPs except two employed GAC filtration and eight employed advanced oxidation through ozonation (Table 1). Several of the DWTPs studied used some type of chlorination as a final disinfection step. Quenching of the residual chlorine in those samples was not performed, in order to keep sample pre-treatment consistent and not alter the sample nature, since reducing agents may also interfere with other chemicals present in the water. Exact locations of the DWTPs are not given, to maintain confidentiality. Instead, the sites are referred to by the country name and an index where more than one plant was studied (Table 1). It should be noted throughout the paper that the selected DWTPs are representative of one type of treatment standard in their respective country, not an average standard for that country.

Grab samples of raw water and finished drinking water were collected at each DWTP using 1-L polypropylene (PP) bottles that were filled directly from available taps. Triplicate samples of each matrix were collected at the same time at each location, by sequentially filling up three 1-L bottles (i.e. six bottles in total from each plant). The samples were sent by express shipment in cooling

Table 1
Information about the 13 different drinking water treatment plants (DWTPs) from which samples were collected

Location	Source water	Intake depth	Daily production (x 1000 m^3)	Number of consumers	Artificial infiltration	Pre-chlorination	Coagulation	Flocculation	Sedimentation	Rapid sand filtration	Slow sand filtration	GAC	Ultraviolet radiation	Chlorination	Ozonation	Ultrafiltration	Reverse osmosis	Other treatment Techniques
Belgium	Surface water	N/A	150	750 K	N	N	Y	Y	Y	Y	N	Y	Y	Y	N	N	N	Flotation
China #1	Qing Reservoir - Yangtze River	N/A	40	100 K	N	N	N	Y	Y	Y	N	Y	N	Y	Y	N	N	
China #2	Jin Reservoir - Huangpu River	N/A	30	35 K	N	N	N	Y	Y	Y	N	Y	N	Y	Y	N	N	Ozone pre-treatment
Czech Republic	River Úhlava	0 -1.5 m	37	210 K	N	N	Y	N	Y	Y	N	Y	Y	Y	Y*	N	N	
Germany	Reservoir water	50-60 m	86	190 K	N	N	Y	Y	N	N	Y	N	N	Y	N	N	N	Hardening Auto catalytic filtration
Italy #1	Lake water	40 m	35	N/A	N	N	N	Y	N	Y	N	Y	N	N	Y	N	N	pH adjustment
Italy #2	Po River water	5 m	86	250 K	N	N	N	Y	Y	N	N	Y	N	Y	Y	N	N	
Japan	Surface water	0-1 m	60	190 K	N	N	Y	Y	Y	N	N	Y	N	Y	Y	N	N	
Spain	Surface water NE Spain	River bed	270	N/A	N	Y	Y	N	Y	Y	N	Y	N	Y	Y	Y	Y	
Sweden	Lake Mälaren	4-28 m	140	700 K	N	N	Y	Y	Y	Y	N	Y	Y	Y	N	N	N	
Switzerland	Lake Zurich	30 m	78	500 K	N	N	N	N	N	Y	Y	Y	N	N	Y	N	N	
The Netherlands	River bank filtrate	14-45 m	36	200 K	River Bank	N	N	N	N	Y	N	Y	Y	N	N	N	N	Carry-over filter
Vietnam	Saigon River	4 m	300	240 K	N	Y	Y	Y	Y	Y	N	N	N	Y	N	N	N	pH adjustment

GAC = granular activated carbon; Y = Yes; N = No; N/A = not available;
*shut down on the day of sampling due to technical problems

boxes to our laboratory at the Swedish University of Agricultural Sciences (SLU), where they were stored at 4°C until extraction.

2.2. Chemicals and reference standards

The target method included 177 CECs from a wide range of compound categories, comprising pesticides (n = 74), pharmaceuticals (n = 66), PFASs (n = 14), phthalates (n = 3), food additives (n = 2), flame retardants (n = 4), hormones (n = 6), industrial chemicals (n = 6), drug (n = 1) and siloxane (n = 1) (Table A1 in the Appendix). The CECs were selected based on previous detection in drinking water (Petrovic, Gonzalez, and Barcelo 2003; Xindi C. Hu 2016; Ivancev-Tumbas 2014; Westerhoff et al. 2005; Webb et al. 2003; Mekonen et al. 2016; Benotti et al. 2009a; Kumar and Xagoraraki 2010; Segura et al. 2011; Padhye et al. 2014a) and on availability of reference standards. In total, 37 isotopically labelled internal standards (ISs) were used, representing most compound groups included in the method. The IS mixture was prepared in methanol at a concentration of 500 ng mL^{-1} of each IS per compound. The native compounds were assigned to their corresponding IS if available, or otherwise assigned to an IS based on expert judgment considering retention time, molecular structure and ionisation characteristics (Table A1 in the Appendix).

All PFAS standards were purchased from Wellington Laboratories (Guelph, Canada) and all pesticide standards were purchased from Teknolab Sorbent (Kungsbacka, Sweden). Remaining standards were purchased from Sigma Aldrich (Buchs, Switzerland). All buffers, acids and bases were of LC-MS grade purity and purchased from Sigma Aldrich (Buchs, Switzerland). The solvents acetonitrile (LC-MS grade) and methanol (LC-MS grade) were purchased from Merck (Darmstadt, Germany), and ethanol (AnalaR purity) from VWR International (Fontenay-sous-Bois, France). Ultrapure water (Milli-Q) was generated in-house by a water purification system (Millipore; Bedford, USA).

2.3. Extraction of water samples

All triplicate samples were extracted separately using a SPE-DEX semi-automated extraction system (4790 SPE-DEX®; Horizon Technology, Salem, New Hampshire, USA) previously used by (Tröger et al., 2020). Instead of conventional solid phase extraction (SPE) cartridges, this device uses HLB SPE disks (47 mm, Atlantic HLB-M, Horizon Technology). In brief, 1 L from each PP bottle was transferred to a glass bottle and 40 µL of IS mixture (20 ng of each IS) were added to each sample. An in-line 1-µm glass fibre filter (1 Micron - Fine, Fast Flow Sediment Pre-Filters Horizon Technology) was placed before the SPE disk, to protect it from clogging. The system, including the sorbent and the filter, was pre-conditioned using 25 mL Milli-Q water, followed by 25 mL methanol twice and twice with 25 mL Milli-Q water. After pre-conditioning, the sample was applied through the filter and onto the SPE disk and the system was washed twice using 25 mL Milli-Q water with 5% methanol. The system was then air-dried at room temperature for 10 min before elution using 25 mL methanol followed by 25 mL of acetonitrile (for details, see Table A2 in the Appendix). The eluate was stored at -20°C and later reduced to ~1 mL using a TurboVap Classic II (Biotage, USA). The extract was then transferred to a 12 mL glass tube, followed by two rinsings of the TurboVap tube using ethanol (4 mL), where the rinse portions were combined with the sample extract. The extract was reduced to ~0.5 mL and transferred to an amber glass LC-MS vial. The glass tube was rinsed twice with 0.5 mL of ethanol, which was added to the vial. The extract in the vial was reduced further to <0.5 mL and finally diluted to 1 mL with Milli-Q water. The extracts were stored at -20°C until instrumental analysis.

2.4. Instrumental analysis and software

All analyses were performed using a quadrupole-time-of-flight (QToF) mass spectrometer (Xevo G2-S, Waters, Manchester, UK) coupled to a ultra-performance liquid chromatography (UPLC) system (Acquity H-Class with FTN injector, Waters, Milford, USA). The columns used were an Acquity UPLC BEH-C18 (Waters, 2.1 × 100 mm, 1.7 µm particle size) for the negative ionisation mode and a Acquity UPLC HSS T3-C18 (Waters, 2.1 × 100 mm, 1.8 µm particle size) for the positive mode analysis. The liquid chromatography (LC) flow consisted of a linear gradient of Milli-Q water and acetonitrile. The mobile phases used in negative mode were Milli-Q water with 5 mM ammonium acetate and 0.01% of ammonium hydroxide added to both the water and acetonitrile. In positive mode, 0.01% of formic acid was added to both the water and acetonitrile phases and 5 mM of ammonium formate were added to the water phase. The same linear gradient was used in both ionisation modes, with a flow rate of 0.5 mL min^{-1}. The gradient started at 5% acetonitrile and increased to 99% acetonitrile with a total run time of 21 min. The injection volume was set to 10 µL. The main instrument settings were: 350V capillary voltage in positive mode, 400 V in negative mode, 4 V low collision energy and 10 to 45 eV for high collision energy (ramping). Data were collected using MS^E-mode and the resolution was ~30 000 at 556.28 m/z, with leucine enkephalin used as lock spray (for lock mass correction). The software used for both data collection and evaluation was UNIFI v1.8.2. More details of the instrumental analysis are given in Tröger et al. (Tröger et al. 2018).

The samples were analysed using a target method with the compounds described in section 2.2 (Table A1 in the Appendix) and by suspect screening for a list of 500 compounds created using SusTool (Dürig et al., 2019) (see section 2.5).

2.5. Suspect list creation

The suspect list created using SusTool (Dürig et al., 2019) included in total 500 compounds. SusTool uses a database comprising of >30 000 compounds, which are relevant for human and/or environmental exposure, and a scoring system to prioritise suspects based on physicochemical properties, environmental fate characteristics, endocrine disruption potential, usage quantity and exposure indices. Although SusTool includes a large database, it is not exhaustive and could be complemented with even more compounds (e.g. CEC transformation products and disinfection by-products) as well as more toxicological parameters. The parameters used to prioritise the compounds were log D (pH adjusted octanol/water partition coefficient), log K_{oc} (organic carbon/water partition coefficient), log S_w (water solubility), log BCF (bioconcentration factor), biodegradation, QI (quantity index), EI (exposure index) for water, EI for sewage treatment and EI for consumers. Each parameter was assigned a weight between 1-5 according to its relevance for a suspect list focused on surface water and drinking water (see Table 2). A high final score means high ranking on the suspect list. The database was sorted based on the total score, and only compounds deemed to be LC compatible (log K_{ow}<5 (octanol/water partition coefficient)) were selected for further consideration. The top 500 compounds were selected for suspect screening. The full list is given in Table A6 in the Appendix and the full SusTool Excel file, with all details, can be downloaded from the supporting information in (Dürig et al., 2019).

2.6. Quality assurance and method performance

All compounds were identified using accurate mass screening with a 10 ppm mass error data extraction window and retention

Table 2
Weighting factors used to create the suspect list for screening of contaminants of emerging concern (CECs).

Parameter	Weight
log *D*	4
log K_{oc}	2
log S_w	5
Log BCF	1
Biodegradation	1
log K_{oa}	0
ED potential for ER	5
ED potential for AR	5
ED potential for TTR	5
EI_{Air}	0
EI_{Water}	4
EI_{Soil}	0
$EI_{Sewage\ treatment}$	2
$EI_{Consumer}$	3
QI	3

ED: Endocrine disruption, ER: oestrogen receptor, AR: androgen receptor, TTR: transthyretin transport protein, for other abbreviations see section 2.5

time using a one-minute time window. Isotope patterns and fragmentation spectra were also considered for the identification. The software (UNIFI) performs an *in silico* fragmentation of all compounds and searches for matching fragments in the high-collision energy spectra for each identified peak. If a matching fragment is found, it increases the identification certainty. The ±H adduct was used for quantification in all cases, and all target compounds were quantified using an external 8-point calibration curve, in 50:50 methanol:Milli-Q, with concentrations ranging from 0 to 120 ng L^{-1}.

The method detection limit (MDL, ng L^{-1}) for the 177 target compounds was calculated from the detection limit (DL) as:

$$MDL = DL + \left(3 * RSD_{spiked} * DL\right)$$

$$DL = C_{spiked} * R_{cutoff} / \left(R_{spiked} - R_{blank}\right)$$

C_{spiked}: nominal concentration in the spiked sample (50 ng L^{-1})
R_{cutoff}: minimum detector counts (100) used to not discard a peak
R_{spiked}: average detector counts in spiked sample
R_{blank}: average detector counts (if detected) in blank sample
RSD_{spiked}: relative standard deviation in the spiked sample

A cut-off value of 100 counts for discarding a peak was applied, based on expert judgment in accordance with normal noise conditions during a typical analytical run. For quality control, a triplicate of 1 L drinking water (tap water from the laboratory, SLU, Uppsala, Sweden) was spiked with 50 ng of each target compound (n = 177), and a triplicate of the same drinking water was analysed unspiked as a blank for blank subtraction. The average MDL was 2.6 ng L^{-1}, with a median of 0.24 ng L^{-1}. For more details, see Table A1 in the Appendix. The MDL was also used as the quantification limit. The recovery from SPE extraction was calculated by dividing the average response (peak area) in three spiked control samples (drinking water spiked with 50 ng) by the average response in another set of three control samples spiked after extraction (drinking water spiked with 50 ng). Any response in the three unspiked blank control sample was subtracted from all spiked samples. The average recovery was 82%, with a median of 90% (for details, see Table A1 in the Appendix). Matrix effects during the analysis were calculated by comparing the average response from the three control samples spiked after extraction with the response for two calibration points (from the external calibration curve) at a similar concentration (but without matrix). Any response observed for the unspiked control sample was subtracted from the spiked triplicate. The average matrix effect was -22%, with a median of -30% (for details, see Table A1 in the Appendix).

To compensate for any deviation in accuracy when determining the final concentration of the samples, a correction factor (CF) was calculated for each compound by dividing 100 by the accuracy. The accuracy was calculated by dividing the average measured concentration in the three spiked control samples by the nominal added concentration (50 ng L^{-1}) and then multiplying by 100.

The final concentration in the sample was calculated as:

$$C_{Final} = C_{Sample} * CF$$

C_{Final}: corrected concentration
C_{Sample}: measured concentration in the sample
CF: correction factor calculated from the control samples

Ideally, *CF* should be 1.00 for all compounds, but there are two main circumstances that can cause deviation from the ideal value: a difference in recovery between the selected IS and the native compound being quantified, or a difference in ion suppression/enhancement between the IS and the measured compound. The average *CF* was 1.24, with a median of 1.08. For more details, see Table A1 in the Appendix.

All reported concentrations of individual compounds are given as the average concentration for the triplicate samples. If a compound was only detected in one or two of the triplicate samples, the concentration was considered zero in any replicate with concentration <MDL in calculation of the average concentration. Principal component analysis (PCA) was conducted using SIMCA V16.0.1, and the analyses were performed with the default settings in the software (i.e. unit variance and mean centring).

2.7. Removal efficiency

The removal efficiency of each target CEC was calculated for each DWTP by dividing the drinking water concentration by the raw water concentration, subtracting this ratio from 1 and multiplying by 100 to get the removal percentage. This was done for all compounds detected in the raw water at concentrations above the MDL. If the concentration in the corresponding drinking water was below MDL, MDL/2 was used for the calculation of removal efficiency. Any negative removal efficiencies was considered zero for the calculation of the averages removal.

3. Results and discussion

3.1. CECs in raw water

In total, 115 out of the 177 target compounds were detected in at least one water sample (Table A3 in the Appendix). The average (± standard deviation) number of detected compounds for all 13 different DWTPs was 44 (±16). The number of detected compounds varied substantially between the different case study sites and reflected local CEC contamination profiles. It should again be highlighted that the study objects are named after country origin, but should not be considered typical representatives of DWTPs for that country, but rather as examples of DWTPs located in various European and Asian countries. Samples from Germany had the lowest number of detected compounds (6), while samples from Spain had significantly higher numbers of detected compounds (71). The high number of detected compounds in samples from the Spanish DWTP can be explained by their source water being highly impacted by wastewater discharges (Bade et al., 2015; Gago-Ferrero et al. 2017).

For further discussion and visualisation, the compounds were divided into four categories: pesticides (n = 45), pharmaceuticals

(n = 47), PFASs (n = 11) and other CECs (n = 11), with the exception of sucralose, which was clearly the dominant compound at all sites (except in Germany) and was therefore considered separately (Fig. 1). In addition to sucralose, on average 15 (±6) pesticides, 6 (±2) PFASs, 17 (±10) pharmaceuticals and 4 (±3) other CECs were detected at the 13 different sites. In raw water samples from China #1, China #2, The Netherlands, Germany and Vietnam, pesticides was the most frequently detected compound group. In samples from Japan, equal numbers of pesticide (n = 19) and pharmaceutical (n = 19) compounds were detected. At the remaining DWTPs, pharmaceuticals was the most frequently detected compound group (n = 8 to n = 39) (for details, see Table A3 in the Appendix).

There was large variation in the raw water concentrations of CECs between the different sites (range 15-7995 ng L^{-1}) (Fig. 1a, Table A3 in the Appendix). Samples from Spain generally showed the highest sum concentrations of each compound category, except for PFASs, where samples from China #2 showed the highest total concentration (143 ng L^{-1}). Samples from Sweden, Germany, Italy #1 and Switzerland had relatively low total CEC concentrations (15-247 ng L^{-1}) in comparison with those from Spain, China #2 and Japan (2466-7995 ng L^{-1}). The CEC concentrations in raw water are highly influenced by the population impacting the source water (Nguyen et al. 2017; Gago-Ferrero et al. 2017), land uses in the catchment area (Ren et al. 2020; You et al. 2015), treatment standards for wastewater and industrial wastewater discharges, chemical/pharmaceutical usage patterns (Kot-Wasik, Jakimska, and Sliwka-Kaszynska 2016) and untreated wastewater discharges to receiving waters. Pharmaceuticals are commonly discharged with municipal and hospital wastewater effluent, due to insufficient removal in WWTPs (Bade et al., 2015; Gago-Ferrero et al. 2017; Kot-Wasik, Jakimska, and Sliwka-Kaszynska 2016; Loos et al. 2013; Sörengård et al. 2019). The level of pesticide pollution is strongly linked to the fraction of agricultural land, the intensity of agricultural activities and pesticide use patterns by farmers and the surface runoff in the catchment area (Reichenberger et al. 2007; Vereecken 2005; Zalidis et al. 2002). PFASs have a relatively diffuse dispersal pattern in surface waters (Gago-Ferrero et al. 2017; Tröger et al., 2020), but show elevated concentrations near point sources, such as fire-fighting fields and airports that formerly used aqueous film-forming foams (Ahrens et al. 2015; Backe, Day, and Field 2013; Hu et al. 2016) or water bodies affected by manufacturing of fluorinated chemicals (Hu et al. 2016; Wang et al. 2018).

To further elucidate differences in raw water quality between sites, PCA was employed using the CEC concentration data from all DWTPs (n = 13) (Fig. A1 in the Appendix). For improved site separation and a better possibility to interpret relations between DWTPs, Spain was excluded from the PCA plot (Fig. 1). The first two principal components (PCs) jointly explained 49% (PC1: 29%, PC2: 20%) of the total variation (Fig. 1b). In the biplot with all DWTPs included (Fig. A1 in the Appendix), Spain was the site that contributed most to the variation along PC1, while China #2 was plotted far from the other DWTPs along PC2. These separations were driven by higher levels of pharmaceuticals in the Spanish DWTP samples and higher levels of pesticides and PFASs in the Chinese #2 DWTP samples. With Spain removed (Fig. 1b), most DWTPs were still clustered around origo, but China #2 separated from the rest along PC1, driven by higher levels of pesticides and PFASs. Japan and Czech Republic were separated from the other DWTPs along PC2, due to their higher levels of pharmaceuticals.

3.2. CECs in drinking water

In total, 58 out of the 177 target compounds were detected in at least one drinking water sample, compared with 115 in the raw water (Table A4 in the Appendix). The number of detected compounds varied between 11 CECs in sample Italy #2 and 35 CECs in China #2. The average number of detected compounds was 19 (±8) for the 13 different sites, compared with 44 (±16) in the raw water.

There was large variation in the CEC concentrations in drinking water (range 35-919 ng L^{-1}) between sites (Table A4 in the Appendix). The sample from China #2 had the highest overall concentration (919 ng L^{-1}), with sucralose concentration remaining high after treatment in China #1, China #2, Spain and Japan (302-497 ng L^{-1}). Although found at high concentrations, sucralose is an approved food additive. Assuming a per capita drinking water consumption of 2 L per day and a body weight of 60 kg, the intake dose of sucralose from drinking water (~0.02 µg/day//kg body weight) would be orders of magnitude below the safe daily intake (5000 µg/day/kg body weight) (Soh et al. 2011). Apart from sucralose, samples from Spain had low concentrations of CECs in the finished drinking water (79 ng L^{-1}) considering the high concentration of CECs measured in the raw water (4573 ng L^{-1}). This can be explained by the use of reverse osmosis as an advanced treatment method at the Spanish DWTP, which has previously been shown to have high performance for CEC removal (Radjenovic et al. 2008).

The relationship between DWTPs and their respective CEC concentrations was evaluated by PCA (Fig. A2 in the Appendix). For improved site separation, China #2 was excluded in a subsequent PCA (Fig. 2b), where the two first PCs jointly explained 46% (PC1: 24%, PC2: 22%) of the total variation. In the biplot including all DWTPs (Fig. A2 in the Appendix), China #2 was separated from the rest of the DWTPs along PC1, driven by high levels of most CECs, while Vietnam stood out along PC2 due to its higher levels of pesticides. With China #2 removed (Fig. 2b), China #1 and Vietnam were separated from the other DWTPs, with Vietnam still due to higher pesticide levels and China #1 due to high levels of sucralose and PFASs.

Although sucralose was by far the largest contributor (mainly due to high concentrations in raw water) to the total CEC concentration in drinking water (average 160 ± 170 ng L^{-1}) at all DWTPs except Germany, Italy #2 and Vietnam, it only made up, on average, 54% (±30%) of the total CEC concentration in samples from the 13 DWTPs. This demonstrates that there also are other substances which might be of concern for human exposure. PFASs showed the highest number of detected compounds out of all categories in eight of the DWTPs, with an average of six compounds per plant detected when considering all DWTPs. In Sweden, the drinking water guideline value is 90 ng L^{-1} for Σ_{11}PFASs (Gobelius et al. 2018). This limit was only exceeded in the drinking water from China #2, where a total of 150 ng L^{-1} of PFASs was detected. The second highest concentration was in China #1 (27 ng L^{-1}). At least three individual PFASs (e.g. PFOA and PFHpA) were detected in all drinking water samples, and thus removal of PFASs from the raw water is shown to be problematic for all DWTPs studied. In Sweden, pharmaceuticals was the compound category with the highest number of detected compounds, but due to the low concentrations in the raw water, the total detected concentration was only 36 ng L^{-1}. In China #1, China #2, Czech Republic (temporarily suspended ozonation could be the cause in this case) and Vietnam, pesticides was the category with the highest number of detected compounds. The Swedish drinking water guideline (and the parametric value in the "Proposal for a Directive of the European Parliament and of the Council on the quality of water intended for human consumption" (Livsmedelsverket 2014)) allows a total concentration of pesticides of 500 ng L^{-1}, or 100 ng L^{-1} for an individual pesticide compound. No sample exceeded the Swedish total pesticide concentration limit, although Vietnam came close (336 ng L^{-1}). However, the individual concentration of 2,4-dichlorophenoxyacetic acid in the sample from Vietnam (302

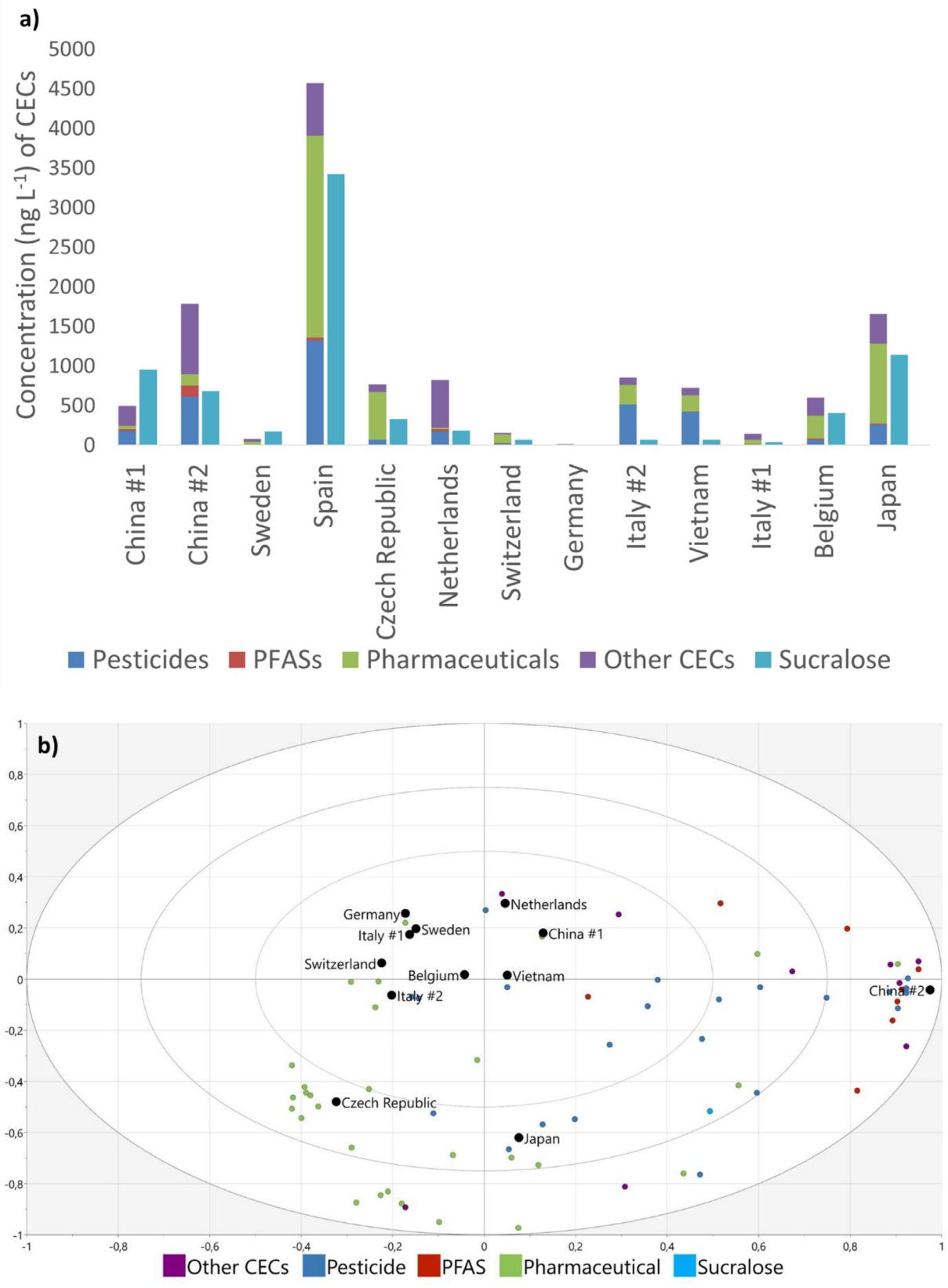

Fig. 1. a) Concentrations of contaminants of emerging concern (CECs) detected in raw water used by the 13 drinking water treatment plants (DWTPs), divided by compound category. b) Principal component analysis (PCA) biplot for raw water concentrations of individual CECs at all DWTPs except Spain. The first two principal components (PCs) jointly explained 49% of the total variation (PC1: 29%, PC2: 20%).

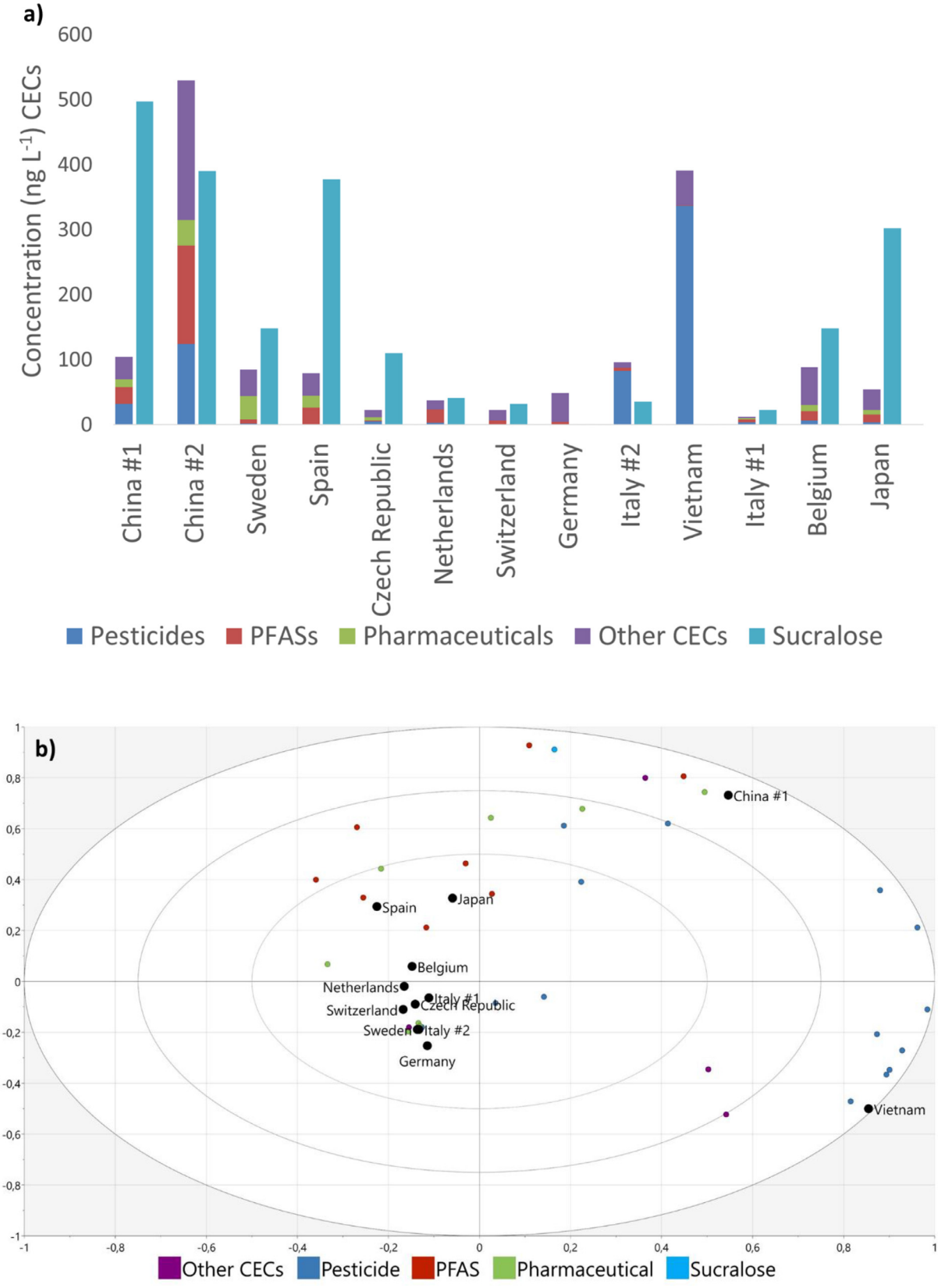

Fig. 2. a) Concentrations of contaminants of emerging concern (CECs) detected in drinking water at the 13 drinking water treatment plants (DWTPs), shown per compound category. b) Principal component analysis (PCA) biplot for drinking water levels of individual CECs at all DWTPs except China #2. The first two principal components (PCs) jointly explained 46% of the total variation (PC1: 24%, PC2: 22%).

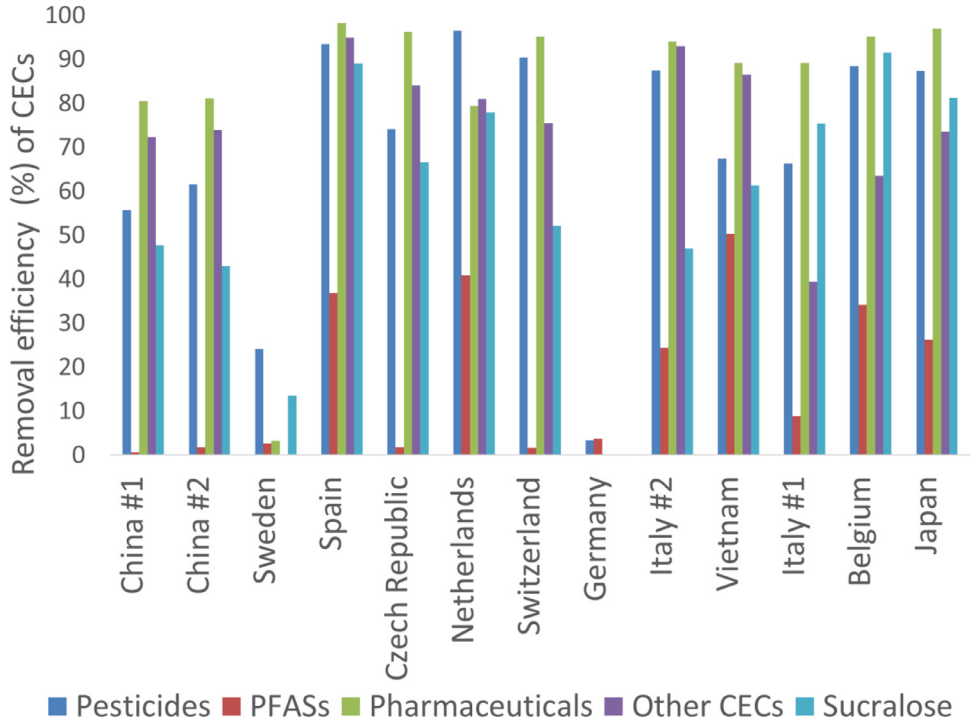

Fig. 3. Average removal efficiency (%) in the 13 drinking water treatment plants (DWTPs) for each compound category of contaminants of emerging concern (CECs).

ng L^{-1}) exceeded the guideline value for individual pesticides by threefold. Pesticide pollution is thus another compound group of concern for DWTPs, especially in countries heavily influenced by agricultural activities, as shown in previous studies (Badach, Nazimek, and Kaminska 2007; Fava et al. 2010).

3.3. Overall removal efficiency of micropollutants

DWTPs have many parameters to consider in regards to maintaining a high standard for their drinking water, where the removal of CECs is only one of them. Other parameters to consider in the overall treatment process include the removal of dissolved organic carbon (DOC), metals and pathogens. All parameters need to be considered together and affects decisions on which barriers (microbial and chemical) to use. Our case study on removal efficiencies of CECs showed that the average efficiency across all detected compounds and all DWTPs was 65% (±28%) with the value ranging from 2.3% (Germany) to 89% (Spain) (Fig. 3a). The German DWTP showed low removal efficiency; however, likely sufficient treatment as only a few (n = 6) compounds at low levels were detected in the raw water. The DWTP in Germany, with treatment based only on coagulation-flocculation, rapid sand filtration and final chlorine disinfection, is able to use powdered activated carbon (PAC) as a treatment step in cases where it is considered necessary (but was not applied before the sampling in this study). The second lowest removal efficiency was shown by the Swedish DWTP, with an average removal efficiency of 9.1% for 22 detected compounds, demonstrating that GAC filtration is not guaranteed to achieve good CEC removal. The high removal efficiency of CEC in the Spanish DWTP can be attributed to the use of reverse osmosis, which has previously been shown to work well for removing CECs (Boleda, Galceran, and Ventura 2011). All removal efficiency data are given in Table A5 in the Appendix.

It should be noted that the removal efficiencies are based on the detected target compounds analysed (Table A5 in the Appendix), representing a wide-scope screening approach. Still, it is not an exhaustive list of all potential CECs in the analysed water samples. Potentially present CECs representing more hydrophobic compounds and compounds with other functional groups than those included in our target list may react differently to the treatment steps employed by the DWTPs. Additionally, applying chlorination, ozonation or ultraviolet disinfection can transform natural organic matter (NOM) or other organic compounds into hazardous disinfection by-products potentially also classified as CECs (Postigo et al. 2021; Zhang et al. 2020), but not targeted in this study. Moreover, it cannot be excluded that differences in the treatment efficiencies between DWTPs (Fig. 3) to some extent might be due to differing levels of NOM in the raw water. High levels of NOM is known to pose a challenge for several drinking water technologies (Sillanpää et al. 2018).

Of all compound groups, PFASs showed the lowest removal efficiency, of on average 18 ±18% in the 13 different DWTPs, indicating that PFASs is a problematic compound group for drinking water producers, as reported previously (Belkouteb et al. 2020). Pharmaceuticals were removed most efficiently during the drinking water treatment, with an average removal of 83 ±26%, whereas the other groups had an average removal efficiency of 62-69%. Previous studies have also observed lower removal of PFASs compared with other CECs (Tröger et al., 2020). Even the Spanish DWTP, with the highest overall removal efficiency, only achieved an average removal of 37% for PFASs. However, despite the overall low removal efficiencies for PFASs, the sum of concentrations of PFASs was generally low in finished drinking water (0.8-27 ng L^{-1}), except for China #2 (151 ng L^{-1}).

Environmental mobility of individual CECs is mainly governed by their sorption to hydrophobic materials (Reemtsma et al. 2016). Theoretically, partition coefficients could be expected to predict the removal behaviour of individual CECs in a DWTP, with sorption to GAC as one major retention mechanism. The relationship between two physicochemical properties (log K_{oc} and log D) of the individual CECs and their removal efficiencies (found in this study) (Table A5 in the Appendix) was investigated through linear regres-

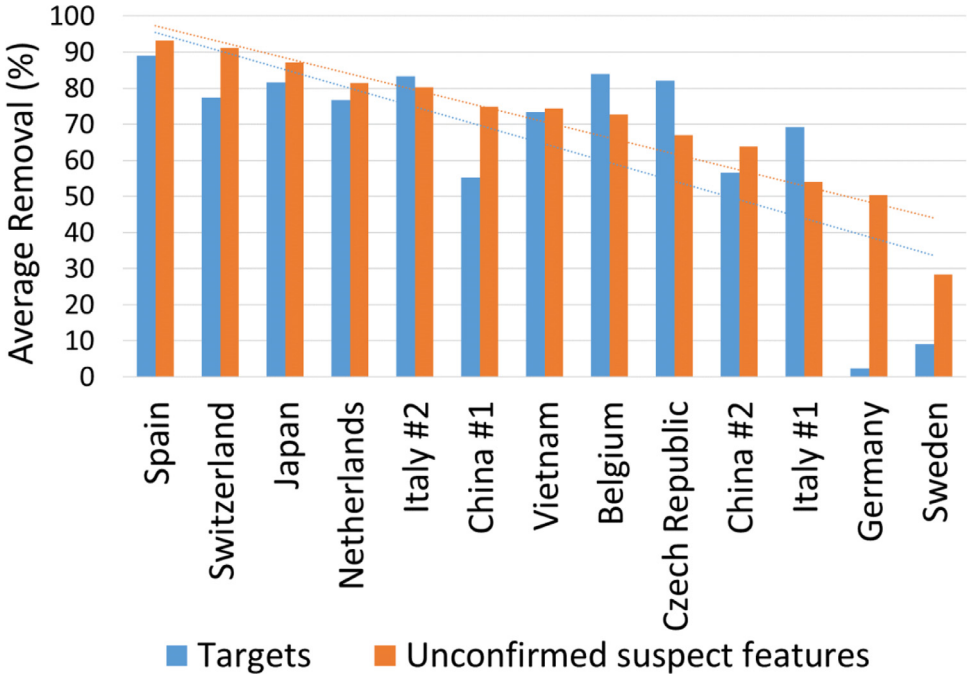

Fig. 4. Overall removal (%) of suspect features (n = 15-65) and the detected target compounds (n = 6-71) in the 13 DWTPs.

sion analyses. No relevant predictive relationships, where an increase in log K_{oc} or log D corresponded to an increase in removal efficiency, were found (Figs. A3 and A4 in the Appendix). The possibility of detecting significant relationships would likely be higher in controlled pilot- or laboratory-scale experiments.

3.4. Suspect screening

To investigate a broader set of compounds, suspect screening was performed by searching for 500 suspects in both positive and negative ionisation mode in all raw and drinking water triplicate samples. A database was created in UNIFI with the molecular structures for all 500 compounds prioritised by SusTool (see section 2.5). This database was later used to perform *in silico* fragmentation of the compounds. To be considered a detected feature to match a suspect, a maximum ±2 mDa mass error was required. To increase confidence in the assigned suspects, only features that had at least one detected *in silico* fragment with a maximum mass error of ±4 mDa were considered. The next step was to manually check all suggested candidates and judge their peak shapes, in order to classify them as real peak or noise integration. A subset of the suspects, only containing peaks (and their retention times) that passed the quality criteria, was then created and these suspects were re-analysed as if target compounds. To readily compile the data from the 26 different triplicate samples analysed with the new semi-target list, a custom R-script was applied to determine the number of detections for each feature in each triplicate samples (0-3 detections). The output was compiled (Table A7 in the Appendix), together with some basic mass spectrometry (MS) parameters for all detected features. In total, 208 features were detected in all triplicates of at least one sample, with some detected both in positive and negative ion mode and/or at different retention times, resulting in a number of 175 unique detected suspects.

To examine the behaviour of the detected features in the DWTP processes, the removal was calculated in a similar way as for the target compounds, with the exception that peak response (area) for each feature was used instead of concentration. Non-detects in the drinking water were substituted with the response cut-off (100) for peak rejection in the data processing method instead of MDL/2 (Table A8 in the Appendix). It should be noted that this approach assumes the same response in raw water and drinking water for the same amount of a compound. The number of features detected in samples from each DWTP varied from 15 (Switzerland) to 65 (Spain). The average removal estimate for each individual feature in each DWTP was then compared against the removal of the target compounds (Fig. 4). To check for common trends, the DWTPs were sorted according to declining average removal of the suspects and trend lines were added for targets and suspects. These trend lines for targets and suspects agreed relatively well. The average removal of suspects differed by between -15% and +48% from the average removal of target compounds, with the largest differences observed for samples from Germany (48%) and Sweden (19%). Spain, with the highest average removal of target compounds, also had the highest removal of suspect features, while Sweden, which had the second worst removal of targets (after Germany), had the worst removal of suspect features. Germany showed a relatively large discrepancy between removal of the targets and the suspects. This can potentially be explained by high uncertainty in the calculated target removal efficiency of Germany, because of the availability of only six data points, compared with 32 for suspect features. Given most DWTPs followed a common trend, removal of a broad range of known compounds can be used as an indication of removal of unknown compounds. This observation may be of high value for DWTPs around the globe in their planning for future treatment strategies to meet the increasing concern about human exposure to unknown CECs present in their drinking water. Still, the findings in this study also highlight the potential for unknown, potentially hazardous compounds to slip through the treatment processes at DWTPs if their attributes are similar to those of target compounds known to slip through.

3.5. Identification of suspects

To identify the most relevant CECs for the DWTPs out of the 208 suspect features detected, further prioritisation was needed. In this process, only suspects detected in the finished drinking wa-

ter, since humans are unavoidably exposed to these features were selected. This prioritisation decreased the number of suspect features to 86. Next, features present in only one DWTP were removed, to increase relevance for the drinking water sector in general rather than information for an individual DWTP. The remaining 39 features were then evaluated manually from an analytical chemistry point of view, by judging whether the suspect feature had a realistic retention time (as judged from the molecular structure) and whether it was detected in an appropriate ion mode (as judged from the molecular structure). This manual deselection reduced the list down to 27 potential detected suspects. Of those, 19 were available to purchase as reference standards from our main supplier, with two (sucralose and triisopropanolamine) already analysed using the target method and considered confirmed suspects. Consequently, a total of 17 reference compounds were purchased: D-(−)-salicin, 4-hydroxyphenylpyruvic acid, serotonin, salidroside, ginkgolide A, ginkgolide J, ginkgolide C, helicin, chlorogenic acid, 5-amino-2-hydroxy-3-sulfobenzoic acid, 7H-dodecafluoroheptanoic acid, DL-vanillactic acid lithium salt hydrate, dimidium bromide, dhurrin, asperuloside, γ-glu-cys and 4,4′-disulfanediylbis(2-aminobutanoic acid).

Of these 17 compounds, dhurrin did not ionise and could not be analysed, while 14 showed good ionisation and chromatography but their retention times did not match those of the corresponding features in the samples. Of the two remaining compounds, vanillactic acid eluted at the same retention time as the suspect feature, but its fragmentation pattern did not closely match that of the sample feature. In the end, only 7H-dodecafluoroheptanoic acid was fully confirmed with matching retention time and fragmentation pattern. This compound is very similar to perfluoroheptanoic acid (PFHpA), which was found in the raw water samples from all 13 DWTPs. The only difference between the two molecules is that 7H-dodecafluoroheptanoic acid has one F-atom substituted with an H-atom. In the samples, 7H-dodecafluoroheptanoic acid occurred in both raw water and drinking water from China #1, China #2 and Italy #1, while it was only present in drinking water from Spain, Czech Republic, Germany and Italy #2. Occurrence of a CEC in drinking water, but not in the raw water, indicates that it could be a transformation product created from a parent PFAS (Merino et al. 2016) during one or several treatment steps in the DWTP. The occurrence of this compound has previously been tentatively confirmed using suspect screening in samples of heavily contaminated wastewater from a fluorochemical manufacturing plant in China (Wang et al. 2018).

4. Conclusions

Concentrations of CECs in raw water and drinking water were screened using comparative data on samples obtained from 13 full-scale DWTPs located in different countries and continents. The analyses clearly showed that many known and unknown mobile CECs pass through artificial barriers (DWTP treatment) around the world and are found in treated drinking water, although in generally low concentrations (mostly below statutory threshold levels). This emphasizes the value of employing good analytical methods and extensive detection workflows to detect and identify CECs in DWTPs and to evaluate the efficiency of treatment techniques.

The raw water used by the different DWTPs contained a wide range of CECs, including PFASs, pharmaceuticals, pesticides and other compounds. In total, 115 different CECs out of 177 analysed were detected in at least one water sample. Detection of PFASs in drinking water samples gives cause for concern, due to their possible adverse effects on humans. The Swedish drinking water guideline value of 90 ng L^{-1} for Σ_{11}PFASs was exceeded in drinking water at one DWTP in China. Another problematic group is pesticides, which can have adverse effects on human health. The Swedish drinking water guideline value of 500 ng L^{-1} for total pesticides was not exceeded at any site, but the limit for an individual pesticide (100 ng L^{-1}) was exceeded threefold at one DWTP (Vietnam). Apart from this, none of the measured concentrations exceeded national guideline values for drinking water.

The 13 DWTPs studied applied different combinations of treatment strategies to remove CECs from the raw water, with varying removal efficiency for the target compounds analysed in this study. Five of the treatment plants had average removal efficiency >80%, which can be considered very good. Spain had the most advanced treatment, using reverse osmosis, which resulted in the highest removal efficiency (89%) of all 13 DWTPs. DWTPs in Sweden and Germany had the lowest removal of target compounds (<10%), but also had the lowest concentrations of CECs in raw water, so the finished drinking water still had similar concentrations to the other DWTPs, showing that poor removal does not necessarily result in poor drinking water quality. Although, low removal could be an issue with unknown CECs, since Sweden and Germany also had the lowest removal efficiency of the suspect compounds. Overall, there was relatively good agreement between removal of the target compounds and the suspect features. Thus, a selected number of target CECs can potentially be used to estimate the removal efficiency of CECs during drinking water treatment processes and potential exposure via drinking water in humans, although a more extensive study is needed to confirm our findings. Three compounds detected using suspect screening were confirmed using reference standards (triisopropanolamine, sucralose and 7H-dodecafluoroheptanoic acid), showing that SusTool can be used to suggest CECs in raw and drinking water to screen for. To further increase the scope in future studies, disinfection by-products formed during chlorination, UV-radiation or ozonation treatment could be included in the suspect screening.

Declaration of Competing Interest

All author hereby declares no conflict of interest.

Acknowledgements

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Appendix

Tables A1–A8 and Figs. A1–A4

Table A1
List of all target compounds analysed, along with their descriptors and method parameters for the instrumental analysis. Method parameters include recovery (%, calculated on response), matrix effect (%, calculated on response), relative standard deviation (RSD; %, calculated on concentration), concentration correction factor (unitless), blank concentration (ng L^{-1}), and MDLs (ng L^{-1}). N/D = not detected, MDL = Method detection limit

Compound	CAS#	Compound Category	Ion Mode	Neutral Mass (DA)	Retention Time (min)	Internal Standard	Recovery (%) (response)	Matrix effect (%) (response)	RSD (%) (conc)	Correction Factor	Blank (ng L^{-1})	MDL (ng/L)
10,11-Dihydro-10-hydroxycarbamazepine	29331-92-8	Pharmaceutical	+H	254.1055	4.9	IS - Oxazepam -d5	95.9	27.8	6.3	1.37	N/D	0.97
10,11-Dihydrocarbamazepine	3564-73-6	Pharmaceutical	+H	238.1106	6.7	IS - Methadone - d3	99.1	-84.0	14.6	3.08	N/D	0.24
2,4-Dichlorophenoxyacetic acid	94-75-7	Pesticide	-H	219.9694	3.8	IS - Perfluorohexanoic acid (PFHxA)-13C2	85.1	-6.0	11.7	1.13	N/D	20.07
2,6-Dichlorbenzamid (BAM)	2008-58-4	Pesticide	+H	188.9748	3.5	IS - DEET-d10	110.1	-32.5	6.8	0.98	N/D	2.97
4-(Trifluoromethyl)benzenesulfonamide	830-43-3	Industrial Chemical	-H	225.0071	5.3	IS - Irbesartan-d7	95.4	-19.6	2.9	0.81	N/D	1.00
4-Amino-6-(trifluoromethyl)benzene-1,3-disulfonamide	654-62-6	Industrial Chemical	-H	318.9908	2.5	IS - Furosemide-d5	66.2	-50.6	13.3	1.14	N/D	2.82
4-Chloro-4′-fluorobutyrophenone	3874-54-2	Industrial Chemical	+H	200.0404	7.0	IS - TCEP-d12	89.4	-12.9	4.9	1.13	N/D	0.45
5-Amino-2-chlorotoluene-4-sulfonic acid	88-53-9	Industrial Chemical	-H	220.9913	2.9	IS - Furosemide-d5	59.2	-50.3	12.9	1.15	N/D	6.50
Acetaminophen	103-90-2	Pharmaceutical	+H	151.0633	2.0	IS - Codeine-d3	76.5	-60.0	13.6	1.70	N/D	1.83
Acetamiprid	135410-20-7	Pesticide	+H	222.0672	4.8	IS - TCEP-d12	102.3	-4.3	4.7	0.90	N/D	0.10
Alachlor	15972-60-8	Pesticide	+H	269.1183	10.2	IS - DEET-d10	100.4	-44.8	3.6	1.31	N/D	0.56
Amidosulfuron	120923-37-7	Pesticide	+H	369.0413	6.3	IS - DEET-d10	46.0	46.1	19.2	1.07	N/D	0.50
Amitryptiline	50-48-6	Pharmaceutical	+H	277.1830	7.4	IS - Methadone - d3	52.5	-64.8	10.3	2.57	N/D	0.11
Atenolol	29122-68-7	Pharmaceutical	+H	266.1630	2.1	IS - Atenolol-d7	63.3	-6.0	11.1	1.26	N/D	0.22
Atrazine	1912-24-9	Pesticide	+H	215.0938	7.3	IS - DEET-d10	102.7	-39.1	2.3	1.04	N/D	0.07
Atrazine-desethyl	6190-65-4	Pesticide	+H	187.0625	4.4	IS - Citalopram-d4	101.1	-58.7	12.6	1.33	N/D	0.24
Atrazine-desisopropyl	1007-28-9	Pesticide	+H	173.0468	3.3	IS - Citalopram-d4	108.8	-54.5	16.6	1.12	N/D	0.38
Azithromycin	83905-01-5	Pharmaceutical	+H	748.5085	5.1	IS - Citalopram-d4	66.9	-13.7	6.8	1.11	N/D	0.13
Azoxystrobin	131860-33-8	Pesticide	+H	403.1168	9.5	IS - DEET-d10	90.0	-17.5	1.7	0.94	0.03	0.04
Bentazon	25057-89-0	Pesticide	-H	240.0569	2.7	IS - Irbesartan-d7	87.8	-22.8	1.9	0.90	N/D	1.38
Benzyl butyl phthalate	85-68-7	Phthalate	+H	312.1362	12.2	IS - Progesterone - 13C3	65.6	-39.4	25.9	1.50	N/D	10.67
Bezafibrate	41859-67-0	Pharmaceutical	+H	361.1081	7.8	IS - Bezafibrate-d4	96.1	25.2	1.8	1.16	N/D	0.16
Bicalutamide	90357-06-5	Pharmaceutical	-H	430.0610	8.1	IS - Oxazepam -d5	94.3	-23.2	8.2	0.91	N/D	0.08
Bifenox-acid	53774-07-5	Pesticide	-H	326.9701	5.7	IS - Oxazepam -d5	102.6	-30.2	11.4	0.92	N/D	10.02
Bis(2-ethylhexyl) phosphate	298-07-7	Industrial Chemical	-H	322.2273	8.4	IS - Irbesartan-d7	93.0	-34.2	3.7	1.08	1.03	0.48
Bisoprolol	66722-44-9	Pharmaceutical	+H	325.2253	5.4	IS - Citalopram-d4	53.9	-13.8	7.0	1.23	N/D	0.05
Bitertanol	55179-31-2	Pesticide	+H	337.1790	10.2	IS - TCEP-d12	94.5	-7.3	8.5	0.90	N/D	4.09
Boscalid	188425-85-6	Pesticide	+H	342.0327	9.6	IS - DEET-d10	92.2	-24.1	2.3	0.95	N/D	0.97
Caffeine	58-08-2	Food Additive	+H	194.0804	2.9	IS - Caffeine-13C3	94.6	-21.6	1.5	0.97	1.64	0.66
Carbendazim	10605-21-7	Pesticide	+H	191.0695	3.8	IS - Citalopram-d4	56.8	-19.4	12.8	1.25	N/D	0.16
Cetirizine	83881-51-0	Pharmaceutical	+H	388.1554	7.0	IS - Citalopram-d4	88.4	-38.2	11.6	1.09	N/D	0.07
Chloramphenicol	56-75-7	Pharmaceutical	-H	322.0123	4.6	IS - Irbesartan-d7	97.8	-40.5	8.1	1.03	N/D	0.61
Chlorfenvinphos	470-90-6	Pesticide	+H	357.9695	10.7	IS - DEET-d10	92.4	-33.8	1.5	1.20	N/D	0.10
Chloridazon	1698-60-8	Pesticide	+H	221.0356	4.4	IS - DEET-d10	99.7	-24.6	2.9	0.92	N/D	0.06
Chlorzoxazone	95-25-0	Pharmaceutical	-H	168.9931	4.4	IS - Irbesartan-d7	88.5	-14.8	4.7	0.82	N/D	2.10
Citalopram	59729-33-8	Pharmaceutical	+H	324.1638	6.2	IS - Citalopram-d4	73.6	-15.2	2.3	0.94	0.86	0.05
Clarithromycin	81103-11-9	Pharmaceutical	+H	747.4769	7.8	IS - Citalopram-d4	76.7	-36.0	7.8	1.22	0.08	0.02
Climbazole	38083-17-9	Pharmaceutical	+H	292.0979	9.0	IS - Diazepam-d5	91.4	-27.0	3.1	1.12	0.02	0.03
Clomazone	81777-89-1	Pesticide	+H	239.0713	8.4	IS - Citalopram-d4	101.0	-50.7	10.7	1.17	N/D	0.77
Clopidogrel	113665-84-2	Pharmaceutical	+H	321.0590	11.7	IS - Methadone - d3	72.2	-51.8	6.1	1.42	0.25	0.05
Clothianidin	210880-92-5	Pesticide	+H	249.0087	4.1	IS - DEET-d10	108.9	-36.3	9.2	1.04	N/D	2.97
Codeine	76-57-3	Pharmaceutical	+H	299.1521	2.7	IS - Codeine-d3	76.3	-30.4	1.1	1.05	N/D	0.08
Cyanazine	21725-46-2	Pesticide	+H	240.0890	6.3	IS - Oxazepam -d5	113.2	-5.4	27.1	1.42	N/D	0.39
Cyazofamid	120116-88-3	Pesticide	+H	324.0448	10.8	IS - DEET-d10	94.4	-18.6	4.5	1.03	N/D	4.60

(*continued on next page*)

Table A1 (*continued*)

Compound	CAS#	Compound Category	Ion Mode	Neutral Mass (DA)	Retention Time (min)	Internal Standard	Recovery (%) (response)	Matrix effect (%) (response)	RSD (%) (conc)	Correction Factor	Blank (ng L^{-1})	MDL (ng/L)
Cybutryne	28159-98-0	Pesticide	+H	253.1361	9.6	IS - DEET-d10	84.8	-27.9	2.0	1.05	N/D	0.03
Cyflufenamid	180409-60-3	Pesticide	+H	412.1210	12.1	IS - TPP-d21	81.4	-63.6	14.5	1.06	N/D	0.73
Cyprodinil	121552-61-2	Pesticide	+H	225.1266	10.3	IS - TPP-d21	46.5	-51.1	1.5	1.24	N/D	0.08
DEET (N,N-Diethyl-3-methylbenzamide)	134-62-3	Pesticide	+H	191.1310	7.5	IS - DEET-d10	103.9	-32.0	0.7	0.89	0.64	0.03
Diazepam	439-14-5	Pharmaceutical	+H	284.0716	8.7	IS - Diazepam-d5	87.5	-6.9	0.7	0.92	0.02	0.03
Dibutyl phosphate	107-66-4	Industrial Chemical	-H	210.1021	3.7	IS - Furosemide-d5	27.3	-33.1	9.4	2.12	N/D	6.16
Dichlorprop	120-36-5	Pesticide	-H	233.9850	4.2	IS - Irbesartan-d7	82.9	-20.7	4.7	0.92	N/D	27.26
Diclofenac	15307-86-5	Pharmaceutical	-H	295.0167	5.7	IS - Diclofenac -13C6	70.3	10.3	4.0	0.73	N/D	10.99
Dienogest	65928-58-7	Hormone	+H	311.1885	7.2	IS - Venlafaxine-d6	84.7	-30.2	4.6	1.18	N/D	0.09
Difenoconazole	119446-68-3	Pesticide	+H	405.0647	11.0	IS - Methadone - d3	82.7	-44.7	6.2	1.08	N/D	0.10
Diflufenican	83164-33-4	Pesticide	-H	394.0741	11.1	IS - Perfluoroundecanoic acid (PFUnDA)-13C2	70.1	-62.5	23.4	1.04	N/D	2.63
Dimethoate	60-51-5	Pesticide	+H	228.9996	4.5	IS - TEP-d15	59.0	-53.2	1.7	1.12	N/D	0.81
Diuron	330-54-1	Pesticide	+H	232.0170	7.6	IS - Oxazepam -d5	106.9	-13.0	4.7	1.66	N/D	0.19
Enalapril	75847-73-3	Pharmaceutical	+H	376.1998	5.5	IS - Oxazepam -d5	90.8	30.5	5.1	1.29	N/D	0.07
Fenofibrate	49562-28-9	Pharmaceutical	+H	360.1128	13.1	IS - TPP-d21	52.9	-73.6	29.9	2.40	N/D	6.07
Fenpiclonil	74738-17-3	Pesticide	-H	235.9908	8.0	IS - Furosemide-d5	64.5	-39.3	8.1	0.95	N/D	0.40
Fexofenadine	83799-24-0	Pharmaceutical	+H	501.2879	7.3	IS - Oxazepam -d5	93.8	32.2	1.5	1.34	0.03	0.02
Fluazinam	79622-59-6	Pesticide	-H	463.9514	10.4	IS - Perfluoroundecanoic acid (PFUnDA)-13C2	74.7	-75.7	23.2	1.54	N/D	0.34
Fluconazole	86386-73-4	Pharmaceutical	+H	306.1041	4.1	IS - TCEP-d12	96.2	2.6	6.1	0.87	N/D	0.30
Fludioxonil	131341-86-1	Pesticide	-H	248.0397	8.3	IS - Perfluorooctane Sulfonamide (FOSA)-13C8	53.9	-47.3	19.2	1.00	N/D	0.25
Flufenacet	142459-58-3	Pesticide	+H	363.0665	10.3	IS - Isoproturon-d3	101.6	-27.6	6.5	1.32	N/D	0.70
Fluopicolide	239110-15-7	Pesticide	+H	381.9654	9.8	IS - Isoproturon-d3	93.9	-25.8	3.7	1.51	N/D	0.11
Flusilazole	85509-19-9	Pesticide	+H	315.1003	9.9	IS - Citalopram-d4	92.3	-36.3	6.2	0.98	N/D	0.07
Flutriafol	76674-21-0	Pesticide	+H	301.1027	7.4	IS - Isoproturon-d3	102.4	-12.7	0.3	1.08	N/D	0.12
Foramsulfuron	173159-57-4	Pesticide	+H	452.1114	6.3	IS - Citalopram-d4	30.0	81.2	16.1	1.17	N/D	0.54
Fuberidazole	3878-19-1	Pesticide	+H	184.0637	4.5	IS - DEET-d10	96.7	-30.9	1.5	1.00	N/D	0.05
Furosemide	54-31-9	Pharmaceutical	-H	330.0077	3.9	IS - Furosemide-d5	63.5	-45.2	12.7	1.02	N/D	6.98
Gestodene	60282-87-3	Hormone	+H	310.1933	8.8	IS - Isoproturon-d3	95.3	-26.5	1.3	1.38	N/D	0.53
Glibenclamide	10238-21-8	Pharmaceutical	+H	493.1438	9.8	IS - DEET-d10	88.8	-20.0	6.9	1.16	N/D	0.19
Glimepiride	93479-97-1	Pharmaceutical	+H	490.2250	10.2	IS - Isoproturon-d3	88.1	-5.4	16.2	1.32	N/D	0.34
Hexamethylcyclotrisiloxane	541-05-9	Siloxane	+H	222.0564	5.0	IS - TCEP-d12	93.9	-13.0	2.5	1.11	N/D	0.70
Hexazinone	51235-04-2	Pesticide	+H	252.1586	5.8	IS - Isoproturon-d3	100.9	-3.3	2.3	1.07	N/D	0.05
Hydrochlorothiazide	58-93-5	Pharmaceutical	-H	296.9645	1.9	IS - Furosemide-d5	75.1	-41.9	8.3	0.83	N/D	12.44
Ifosfamide	3778-73-2	Pharmaceutical	+H	260.0248	4.9	IS - Oxazepam -d5	96.4	14.3	4.3	1.53	N/D	0.05
Imidacloprid	138261-41-3	Pesticide	+H	255.0523	4.4	IS - Oxazepam -d5	101.0	110.1	3.5	0.77	N/D	0.27
Irbesartan	138402-11-6	Pharmaceutical	+H	428.2325	8.4	IS - DEET-d10	94.9	-33.8	7.8	1.07	N/D	0.05
Isoproturon	34123-59-6	Pesticide	+H	206.1419	7.6	IS - Isoproturon-d3	105.6	3.8	0.8	0.81	N/D	0.05
Ivermectin	70288-86-7	Pharmaceutical	-H	874.5079	14.7	IS - Perfluoroundecanoic acid (PFUnDA)-13C2	61.0	-56.8	30.8	0.99	N/D	30.51
Ketoprofen	22071-15-4	Pharmaceutical	+H	254.0943	7.9	IS - Bezafibrate-d4	96.3	46.8	5.1	1.11	N/D	0.89
Lamotrigine	84057-84-1	Pharmaceutical	+H	255.0079	4.1	IS - Lidocaine -d10	102.4	-49.4	11.0	1.03	N/D	0.06
Levamisole	14769-73-4	Pharmaceutical	+H	204.0721	2.9	IS - Codeine-d3	88.7	-46.9	5.0	1.21	N/D	0.11
Levonorgestrel	17489-40-6	Hormone	+H	312.2089	9.4	IS - DEET-d10	96.2	-36.2	6.0	1.17	N/D	0.42
Linuron	330-55-2	Pesticide	+H	248.0119	8.9	IS - Citalopram-d4	98.9	-41.8	10.6	1.03	N/D	3.29
Loperamide	53179-11-6	Pharmaceutical	+H	476.2231	8.6	IS - Methadone - d3	66.9	-37.9	5.8	1.19	0.07	0.03
Loratadine	79794-75-5	Pharmaceutical	+H	382.1448	10.6	IS - DEET-d10	77.9	-30.8	12.7	1.28	0.15	0.03
Losartan	114798-26-4	Pharmaceutical	+H	422.1622	7.4	IS - Isoproturon-d3	104.2	-8.1	4.2	0.89	N/D	0.11
Mandipropamid	374726-62-2	Pesticide	+H	411.1237	9.7	IS - DEET-d10	94.3	-24.9	3.2	1.04	N/D	0.06

(*continued on next page*)

Table A1 (*continued*)

Compound	CAS#	Compound Category	Ion Mode	Neutral Mass (DA)	Retention Time (min)	Internal Standard	Recovery (%) (response)	Matrix effect (%) (response)	RSD (%) (conc)	Correction Factor	Blank (ng L^{-1})	MDL (ng/L)
MCPA	94-74-6	Pesticide	-H	200.0240	3.7	IS - Perfluorohexanoic acid (PFHxA)-13C2	93.8	-4.8	12.9	1.02	N/D	22.13
Mebendazole	31431-39-7	Pharmaceutical	+H	295.0957	6.8	IS - Methadone - d3	48.7	-33.1	5.8	1.44	N/D	0.23
Meclofenamic acid	644-62-2	Pharmaceutical	-H	295.0167	6.3	IS - Furosemide-d5	43.3	-11.0	8.7	1.08	N/D	22.67
Mecoprop	7085-19-0	Pesticide	-H	214.0397	4.1	IS - Perfluorohexanoic acid (PFHxA)-13C2	97.9	-8.6	15.6	1.04	N/D	31.71
Memantine	19982-08-2	Pharmaceutical	+H	179.1674	5.3	IS - TEP-d15	70.2	-72.9	18.4	1.52	N/D	4.63
Metalaxyl	57837-19-1	Pesticide	+H	279.1471	7.7	IS - Isoproturon-d3	101.4	-15.3	2.0	1.19	N/D	0.05
Metazachlor	67129-08-2	Pesticide	+H	277.0982	8.1	IS - Isoproturon-d3	99.8	-15.5	2.4	1.09	N/D	0.13
Methabenzthiazuron	18691-97-9	Pesticide	+H	221.0623	6.9	IS - DEET-d10	95.7	-27.1	2.8	1.01	N/D	0.11
Methadone	76-99-3	Pharmaceutical	+H	309.2093	7.6	IS - Methadone - d3	65.6	-32.3	0.5	1.06	N/D	0.07
Metolachlor	51218-45-2	Pesticide	+H	283.1339	10.2	IS - DEET-d10	96.4	-35.0	1.0	1.16	N/D	0.07
Metoprolol	51384-51-1	Pharmaceutical	+H	267.1834	4.3	IS - Lidocaine -d10	52.7	-13.8	4.2	1.18	N/D	0.08
Metribuzin	21087-64-9	Pesticide	+H	214.0888	6.3	IS - TEP-d15	40.2	-31.9	71.2	1.09	N/D	0.55
Metronidazole	443-48-1	Pharmaceutical	+H	171.0644	2.3	IS - Ofloxacin-d3	63.4	-46.5	18.3	1.20	N/D	0.85
Metsulfuron methyl	74223-64-6	Pesticide	+H	381.0743	6.2	IS - Oxazepam -d5	94.0	173.5	6.5	0.67	N/D	0.11
Mirtazapine	61337-67-5	Pharmaceutical	+H	265.1579	4.8	IS - Venlafaxine-d6	78.6	-25.9	2.1	1.24	N/D	0.07
Monobenzyl Phthalate	2528-16-7	Phthalate	-H	256.0736	4.0	IS - Irbesartan-d7	95.0	-35.3	1.0	0.98	N/D	3.39
Monobutyl Phthalate	131-70-4	Phthalate	-H	222.0892	3.5	IS - Furosemide-d5	57.8	-28.1	10.8	0.90	N/D	14.04
N-Desmethylcitalopram	62498-67-3	Pharmaceutical	+H	310.1481	6.1	IS - Methadone - d3	73.2	-61.3	27.1	1.65	0.33	0.09
Nicotine	54-11-5	Drug	+H	162.1157	1.2	IS - Nicotine - d4	94.2	-66.9	3.8	0.99	N/D	0.74
Niflumic acid	4394-00-7	Pharmaceutical	-H	282.0616	5.9	IS - Irbesartan-d7	95.5	-26.8	2.5	0.89	N/D	0.15
Norethindrone	68-22-4	Hormone	+H	298.1933	8.4	IS - Isoproturon-d3	97.1	-27.6	1.3	1.37	N/D	0.21
Norfloxacin	70458-96-7	Pharmaceutical	+H	319.1332	3.5	IS - Sulfamethoxazole-d4	11.3	-37.9	28.4	4.77	N/D	6.64
Ofloxacin	82419-36-1	Pharmaceutical	+H	361.1438	3.6	IS - Sulfamethoxazole-d4	48.8	-6.4	18.8	0.75	N/D	0.17
Omeprazole	73590-58-6	Pharmaceutical	+H	345.1147	6.0	IS - Sulfamethoxazole-d4	30.8	-65.4	44.2	2.95	N/D	2.96
Oxazepam	604-75-1	Pharmaceutical	+H	286.0509	6.9	IS - Oxazepam -d5	89.7	78.9	2.1	0.97	N/D	0.27
Oxycodone	76-42-6	Pharmaceutical	+H	315.1471	3.0	IS - Lidocaine -d10	72.7	-27.3	4.1	1.09	N/D	0.11
Penconazole	66246-88-6	Pesticide	+H	283.0643	10.0	IS - DEET-d10	93.8	-35.0	1.8	1.16	N/D	0.12
Perfluoro-2-propoxypropanoic acid (GenX)	13252-13-6	PFAS	-H	329.9750	5.8	IS - Perfluorohexanoic acid (PFHxA)-13C2	87.3	-15.4	2.3	1.12	N/D	15.39
Perfluorobutane sulfonic acid (PFBS)	375-73-5	PFAS	-H	299.9503	5.4	IS - Perfluorohexane sulfonic acid (PFHxS)-18O2	103.1	-15.5	5.5	0.98	4.84	0.06
Perfluorodecanoic acid (PFDA)	335-76-2	PFAS	-H	513.9673	8.6	IS - Perfluorodecanoic acid (PFDA)-13C2	92.9	-44.4	0.7	1.00	0.14	0.14
Perfluorododecanoic acid (PFDoDA)	307-55-1	PFAS	-H	613.9609	9.9	IS - Perfluorododecanoic acid (PFDoDA)-13C2	85.0	-87.9	15.0	0.98	0.08	0.98
Perfluoroheptanoic acid (PFHpA)	375-85-9	PFAS	-H	363.9769	6.4	IS - Perfluorooctanoic acid (PFOA)-13C4	97.7	-12.5	3.4	0.87	N/D	0.16
Perfluorohexane sulfonic acid (PFHxS)	355-46-4	PFAS	-H	399.9439	7.3	IS - Perfluorohexane sulfonic acid (PFHxS)-18O2	100.5	-20.9	1.3	1.05	0.11	0.05
Perfluorohexanoic acid (PFHxA)	307-24-4	PFAS	-H	313.9801	5.5	IS - Perfluorohexanoic acid (PFHxA)-13C2	98.9	-11.0	3.0	0.96	N/D	0.35
Perfluorononanoic acid (PFNA)	375-95-1	PFAS	-H	463.9705	7.9	IS - Perfluorononanoic acid (PFNA)-13C5	97.4	-32.5	1.9	1.06	N/D	0.11
Perfluorooctane sulfonamide (FOSA)	754-91-6	PFAS	-H	498.9535	8.6	IS - Perfluorooctane Sulfonamide (FOSA)-13C8	102.0	-72.9	3.0	1.08	N/D	0.55
Perfluorooctane sulfonic acid (PFOS)	1763-23-1	PFAS	-H	499.9375	8.8	IS - Perfluorooctane sulfonic acid (PFOS)-13C4	92.6	-38.1	2.8	1.08	0.13	0.06
Perfluorooctanoic acid (PFOA)	335-67-1	PFAS	-H	413.9737	7.2	IS - Perfluorooctanoic acid (PFOA)-13C4	100.8	-26.0	4.8	1.03	0.31	0.14
Perfluoropentanoic acid (PFPeA)	2706-90-3	PFAS	-H	263.9833	4.3	IS - Perfluorodecanoic acid (PFDA)-13C2	46.9	3.4	10.4	1.06	N/D	1.53
Perfluorotetradecanoic acid (PFTeDA)	376-06-7	PFAS	-H	713.9545	11.1	IS - perfluorotetradecanoic acid (PFTeDA)-13C2	101.2	-89.4	3.1	1.08	N/D	1.13
Perfluoroundecanoic acid (PFUnDA)	2058-94-8	PFAS	-H	563.9641	9.3	IS - Perfluoroundecanoic acid (PFUnDA)-13C2	82.5	-66.9	1.9	1.06	0.07	0.34
Picoxystrobin	117428-22-5	Pesticide	+H	367.1031	11.0	IS - DEET-d10	92.2	-40.8	5.9	1.17	N/D	0.47
Pirimicarb	23103-98-2	Pesticide	+H	238.1430	6.8	IS - Methadone - d3	61.4	-36.0	11.0	1.21	N/D	0.06
Prochloraz	67747-09-5	Pesticide	+H	375.0308	10.5	IS - Progesterone - 13C3	88.9	-37.6	0.9	1.07	N/D	0.11

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Table A1 (*continued*)

Compound	CAS#	Compound Category	Ion Mode	Neutral Mass (DA)	Retention Time (min)	Internal Standard	Recovery (%) (response)	Matrix effect (%) (response)	RSD (%) (conc)	Correction Factor	Blank (ng L^{-1})	MDL (ng/L)
Progesterone	57-83-0	Hormone	+H	314.2246	10.7	IS - Progesterone - 13C3	87.7	-30.9	1.2	1.03	N/D	0.66
Propamocarb	24579-73-5	Pesticide	+H	188.1525	2.3	IS - Codeine-d3	81.6	-46.7	5.3	1.28	N/D	0.21
Propiconazole	60207-90-1	Pesticide	+H	341.0698	10.4	IS - Citalopram-d4	92.8	-36.1	12.4	1.01	N/D	0.08
Propoxycarbazone	145026-81-9	Pesticide	+H	398.0896	5.4	IS - Oxazepam -d5	105.3	200.4	8.1	0.52	N/D	0.30
Propranolol	525-66-6	Pharmaceutical	+H	259.1572	5.7	IS - Sulfamethoxazole-d4	56.1	-25.6	18.1	0.72	N/D	0.08
Propyzamide	23950-58-5	Pesticide	+H	255.0218	9.5	IS - DEET-d10	105.5	-37.3	5.7	0.97	N/D	5.10
Prothioconazole-desthio	120983-64-4	Pesticide	+H	311.0592	9.3	IS - DEET-d10	93.9	-32.1	1.4	1.08	N/D	0.10
Pyraclostrobin	175013-18-0	Pesticide	+H	387.0986	11.4	IS - TPHP-d15	72.4	-49.1	3.2	0.89	0.07	0.09
Pyrimethamine	58-14-0	Pharmaceutical	+H	248.0829	5.1	IS - TEP-d15	31.9	-32.7	7.9	1.40	N/D	0.08
Pyroxsulam	422556-08-9	Pesticide	+H	434.0620	6.8	IS - Oxazepam -d5	97.3	176.2	6.3	0.60	N/D	0.03
Quinmerac	90717-03-6	Pesticide	+H	221.0244	3.5	IS - Metronidazole-d4	4.0	15.4	30.3	7.93	N/D	5.13
Quinoxyfen	124495-18-7	Pesticide	+H	306.9967	12.3	IS - TPHP-d15	52.9	-78.7	14.8	2.82	0.26	0.23
Ramipril	87333-19-5	Pharmaceutical	+H	416.2311	7.1	IS - Isoproturon-d3	87.8	-6.0	4.2	1.27	N/D	0.05
Roxithromycin	80214-83-1	Pharmaceutical	+H	836.5246	7.9	IS - Citalopram-d4	68.7	-39.0	9.8	1.46	N/D	0.04
Silthiofam	175217-20-6	Pesticide	+H	267.1113	10.6	IS - Citalopram-d4	91.9	-42.5	12.0	1.12	N/D	0.19
Sotalol	3930-20-9	Pharmaceutical	+H	272.1195	2.1	IS - Ofloxacin-d3	48.2	-32.2	15.5	1.36	N/D	0.79
Sucralose	56038-13-2	Food Additive	-H	396.0146	3.0	IS - Losartan -d4	93.6	-33.5	3.7	0.65	N/D	18.15
Sulfaclozine	102-65-8	Pharmaceutical	-H	284.0135	2.1	IS - Furosemide-d5	46.6	-42.5	14.3	1.32	N/D	16.85
Sulfamethoxazole	723-46-6	Pharmaceutical	+H	253.0521	4.6	IS - Sulfamethoxazole-d4	29.9	37.8	2.2	0.78	N/D	0.69
Sulfosulfuron	141776-32-1	Pesticide	+H	470.0678	7.4	IS - DEET-d10	41.6	89.9	5.4	0.92	N/D	0.30
Sulindac	38194-50-2	Pharmaceutical	+H	356.0882	7.3	IS - Isoproturon-d3	94.6	-25.5	3.5	1.44	N/D	0.44
TCEP (Tris(2-chloroethyl) phosphate)	115-96-8	Flame Retardant	+H	283.9539	6.9	IS - TCEP-d12	105.0	-13.5	6.9	0.98	N/D	1.65
Telmisartan	144701-48-4	Pharmaceutical	+H	514.2369	9.5	IS - Isoproturon-d3	90.8	-15.4	5.7	1.24	0.03	0.01
Terbuthylazine	5915-41-3	Pesticide	+H	229.1094	8.8	IS - Citalopram-d4	96.9	-34.0	10.4	0.88	N/D	0.08
Terbutryn	886-50-0	Pesticide	+H	241.1361	9.5	IS - DEET-d10	83.6	-34.5	2.5	1.20	0.02	0.04
Testosterone	58-22-0	Hormone	+H	288.2089	8.3	IS - Isoproturon-d3	100.8	-32.5	3.6	1.51	N/D	0.47
Theobromine	83-67-0	Pharmaceutical	+H	180.0647	2.3	IS - Metronidazole-d4	47.6	-32.0	5.2	1.10	N/D	4.32
Thiabendazole	148-79-8	Pharmaceutical	+H	201.0361	4.3	IS - Metronidazole-d4	16.8	-54.6	31.6	4.58	N/D	0.54
Thiacloprid	111988-49-9	Pesticide	+H	252.0236	5.5	IS - TCEP-d12	105.7	-3.0	3.0	0.88	N/D	0.08
Thiamethoxam	153719-23-4	Pesticide	+H	291.0193	3.6	IS - TCEP-d12	100.4	-2.1	12.0	0.94	N/D	0.32
Thifensulfuron methyl	79277-27-3	Pesticide	+H	387.0307	6.1	IS - Oxazepam -d5	83.4	120.3	13.1	0.94	N/D	0.19
Tramadol	27203-92-5	Pharmaceutical	+H	263.1885	4.4	IS - TCEP-d12	87.5	-19.6	6.4	1.24	0.28	0.09
Triadimefon	43121-43-3	Pesticide	+H	293.0931	9.5	IS - Isoproturon-d3	93.0	-25.1	2.3	1.39	N/D	0.30
Triflusulfuron-methyl	126535-15-7	Pesticide	+H	492.1039	9.7	IS - Bezafibrate-d4	96.4	25.6	5.1	1.30	N/D	0.11
Triisopropanolamine	122-20-3	Pharmaceutical	+H	191.1521	0.7	IS - Codeine-d3	78.9	-41.1	13.4	1.14	N/D	0.32
Triticonazole	131983-72-7	Pesticide	+H	317.1295	9.0	IS - Isoproturon-d3	107.5	-15.8	1.4	1.02	N/D	0.18
Valsartan	137862-53-4	Pharmaceutical	-H	435.2270	4.3	IS - Irbesartan-d7	90.8	-34.4	3.5	1.05	N/D	0.78
Venlafaxine	93413-69-5	Pharmaceutical	+H	277.2042	5.3	IS - Venlafaxine-d6	84.3	-21.8	1.7	1.05	N/D	0.07
Verapamil	52-53-9	Pharmaceutical	+H	454.2832	7.4	IS - Citalopram-d4	56.3	-25.5	3.2	1.35	0.67	0.03
α-HBCD	134237-50-6	Flame Retardant	-H	641.6447	13.1	IS - perfluorohexadecanoic acid (PFHxDA)-13C2	48.3	-83.2	22.5	1.87	N/D	43.81
β-HBCD	134237-51-7	Flame Retardant	-H	641.6447	13.3	IS - perfluorohexadecanoic acid (PFHxDA)-13C2	50.8	-81.6	9.9	1.55	N/D	10.72
γ-HBCD	134237-52-8	Flame Retardant	-H	641.6447	13.9	IS - perfluorohexadecanoic acid (PFHxDA)-13C2	46.2	-81.9	15.1	1.65	N/D	14.03
						Average	**81.5**	**-22.2**	**8.4**	**1.24**	**0.07**	**2.58**
						Median	**90.0**	**-30.2**	**5.7**	**1.08**	**0.00**	**0.24**

Table A2
Details of the SPE-DEX 4790 extraction programme.

PreWet cycle (conditioning)				
Solvent	Soak time		AirDry time	
	minutes	*seconds*	*minutes*	*seconds*
Prewet5 MilliQ	0	30	0	10
Prewet1 MeOH	0	30	0	10
Prewet2 MeOH	0	30	0	10
Prewet3 MilliQ	0	30	0	10
Prewet4 MilliQ	0	30	0	10
Sample cycle (sample application)				
Fixed step				
Wash cycle (washing step)				
Solvent	**Soak time**		**AirDry time**	
	minutes	*seconds*	*minutes*	*seconds*
Rinse1 5% MeOH	0	10	0	10
Rinse1 5% MeOH	0	10	0	10
Sample AirDry cycle (dry time)				
			AirDry time	
			minutes	*seconds*
			10	0
Rinse cycle (elution steps)				
Solvent	**Soak time**		**AirDry time**	
	minutes	*seconds*	*minutes*	*seconds*
Rinse2 MeOH	1	0	0	30
Rinse3 ACN	1	0	0	45

Table A3
Average CEC concentrations (ng L^{-1}) obtained from analysis of triplicate raw water samples from the 13 selected DWTPs.

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
10,11-Dihydro-10-hydroxycarbamazepine	<MDL	<MDL	<MDL	107.45	<MDL	<MDL	<MDL	<MDL	11.27	<MDL	<MDL	<MDL	<MDL
2,4-Dichlorophenoxyacetic acid	51.53	<MDL	<MDL	33.83	27.52	<MDL	<MDL	<MDL	<MDL	178.01	<MDL	<MDL	20.62
4-Chloro-4′-fluorobutyrophenone	<MDL	<MDL	<MDL	182.93	21.91	<MDL	<MDL	<MDL	<MDL	9.00	<MDL	9.11	21.41
5-Amino-2-chlorotoluene-4-sulfonic acid	<MDL	106.29	<MDL	64.08	<MDL	395.66	<MDL	<MDL	<MDL	38.25	<MDL	<MDL	41.12
Acetaminophen	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	17.01	<MDL	<MDL	<MDL	<MDL
Acetamiprid	1.86	8.21	<MDL	8.10	<MDL	<MDL	<MDL	<MDL	2.09	7.59	<MDL	<MDL	1.08
Alachlor	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	7.83	<MDL	<MDL	<MDL
Amitryptiline	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.55	<MDL	<MDL
Atenolol	<MDL	<MDL	<MDL	10.96	3.64	<MDL	1.02	<MDL	7.16	<MDL	0.92	<MDL	4.82
Atrazine	8.66	73.96	<MDL	<MDL	2.62	<MDL	0.51	<MDL	5.81	6.63	0.41	2.96	1.04
Atrazine-desethyl	3.50	8.06	<MDL	<MDL	5.96	<MDL	<MDL	<MDL	11.46	2.44	0.89	4.14	<MDL
Atrazine-desisopropyl	<MDL	2.39	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Azithromycin	<MDL	<MDL	<MDL	49.04	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.59	<MDL	<MDL
Azoxystrobin	6.85	10.55	0.12	0.68	0.16	<MDL	<MDL	<MDL	2.12	30.05	0.10	3.01	1.95
Bentazon	14.87	221.35	1.49	4.34	9.98	106.28	<MDL	<MDL	11.96	16.96	<MDL	8.08	70.71
Benzyl butyl phthalate (BBP)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Bezafibrate	<MDL	<MDL	<MDL	6.65	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	5.44
Bicalutamide	<MDL	0.42	8.44	5.29	4.39	<MDL	0.47	<MDL	0.91	<MDL	1.64	2.97	19.65
Bis(2-ethylhexyl) phosphate	3.15	37.37	<MDL	45.69	3.75	9.85	<MDL	1.14	5.31	13.94	1.00	4.98	1.81
Bisoprolol	<MDL	<MDL	<MDL	13.95	1.70	<MDL	0.91	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Boscalid	<MDL	<MDL	<MDL	7.85	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Caffeine	36.52	107.76	31.13	277.90	67.28	10.11	17.78	12.90	89.64	32.26	52.38	69.17	217.48
Carbendazim	61.62	45.36	<MDL	1141.09	1.20	6.57	6.21	<MDL	6.83	97.41	0.92	3.81	58.76
Cetirizine	<MDL	<MDL	<MDL	23.38	20.06	<MDL	<MDL	<MDL	2.08	12.62	1.54	8.96	15.74
Chloramphenicol	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.81	<MDL	<MDL	<MDL
Chloridazon (Pyrazon)	<MDL	<MDL	<MDL	<MDL	0.24	20.66	<MDL	<MDL	0.25	<MDL	<MDL	17.92	<MDL
Citalopram	<MDL	<MDL	<MDL	26.98	2.07	<MDL	1.23	<MDL	0.09	<MDL	<MDL	<MDL	<MDL
Clarithromycin	<MDL	<MDL	<MDL	24.06	27.75	<MDL	1.73	<MDL	3.87	<MDL	3.13	0.66	18.48
Climbazole	0.23	0.58	<MDL	3.90	2.17	<MDL	0.48	<MDL	2.00	0.64	0.61	0.21	<MDL
Clomazone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	7.59	<MDL	<MDL	<MDL	<MDL
Clopidogrel	<MDL	<MDL	<MDL	0.61	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Codeine	<MDL	<MDL	<MDL	92.78	1.25	<MDL	<MDL	<MDL	1.13	<MDL	0.87	<MDL	<MDL
Cyanazine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	10.72
Cybutryne	<MDL	<MDL	0.21	<MDL	<MDL	0.11	0.11	<MDL	<MDL	<MDL	<MDL	<MDL	2.49
Cyprodinil	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.64	<MDL	<MDL	1.49	<MDL
DEET	1.91	6.68	0.59	5.70	1.42	2.59	2.62	<MDL	0.30	8.09	0.96	1.61	7.68
Diazepam	3.13	6.17	<MDL	18.86	<MDL	0.19	<MDL	<MDL	<MDL	<MDL	<MDL	0.11	<MDL
Dibutyl phosphate	13.47	74.25	<MDL	72.14	<MDL	11.09	<MDL	<MDL	<MDL	<MDL	<MDL	74.24	<MDL
Diclofenac	<MDL	<MDL	<MDL	36.77	28.26	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Difenoconazole I	<MDL	0.23	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	2.85	<MDL	<MDL	<MDL
Diuron	2.44	2.73	<MDL	70.75	<MDL	9.62	7.05	<MDL	<MDL	15.29	1.02	1.38	37.47
Fexofenadine	<MDL	<MDL	2.70	17.64	6.94	<MDL	3.94	<MDL	2.34	7.08	9.25	3.56	437.31

(*continued on next page*)

Table A3 (*continued*)

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
Fluconazole	11.93	17.39	<MDL	204.48	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	3.25	20.86	<MDL
Fludioxonil	<MDL	<MDL	<MDL	1.04	<MDL	<MDL	0.36	<MDL	5.09	<MDL	<MDL	<MDL	4.35
Flufenacet	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	3.99	<MDL	<MDL	<MDL	<MDL
Flusilazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.48	<MDL	<MDL	<MDL
Flutriafol	0.63	19.14	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
FOSA (perfluorooctane sulfonamide)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Fuberidazole	<MDL	<MDL	<MDL	<MDL	<MDL	0.29	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Furosemide	<MDL	<MDL	<MDL	28.49	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Hexamethylcyclotrisiloxane	62.80	91.10	<MDL	<MDL	<MDL	21.93	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	14.22
Hexazinone	0.89	3.73	<MDL	<MDL	1.90	0.33	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	6.69
Imidacloprid	2.48	6.32	<MDL	19.86	11.53	<MDL	<MDL	<MDL	1.98	5.18	<MDL	<MDL	1.29
Irbesartan	2.02	33.61	<MDL	51.38	26.82	<MDL	2.20	<MDL	21.23	<MDL	1.62	1.94	26.03
Isoproturon	4.18	93.62	<MDL	3.73	<MDL	11.61	0.53	0.26	<MDL	<MDL	<MDL	0.62	<MDL
Ketoprofen	<MDL	<MDL	<MDL	15.34	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Lamotrigine	0.34	0.45	12.02	56.65	15.52	0.59	14.73	<MDL	4.67	<MDL	2.90	22.92	14.91
Levamisole	2.51	<MDL	<MDL	14.47	<MDL	<MDL	<MDL	<MDL	<MDL	2.37	<MDL	<MDL	<MDL
Loratadine	<MDL	<MDL	<MDL	0.40	<MDL	<MDL	<MDL	<MDL	<MDL	0.04	<MDL	<MDL	<MDL
Losartan	<MDL	5.23	<MDL	148.28	9.21	<MDL	3.41	<MDL	4.99	4.06	1.06	3.71	9.98
Mandipropamid	<MDL	0.87	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.32	<MDL
MCPA	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	27.39
Mebendazole	<MDL	<MDL	<MDL	1.86	<MDL	<MDL	<MDL	<MDL	<MDL	1.10	<MDL	<MDL	<MDL
Mecoprop	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metalaxyl	1.97	2.63	<MDL	1.72	0.24	<MDL	<MDL	<MDL	0.30	8.36	0.16	<MDL	1.74
Methabenzthiazuron	<MDL	<MDL	<MDL	<MDL	<MDL	4.68	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Methadone	<MDL	<MDL	<MDL	2.61	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metolachlor	2.99	12.53	<MDL	<MDL	0.25	<MDL	<MDL	<MDL	245.92	3.83	0.72	6.86	1.81
Metoprolol	0.64	<MDL	<MDL	1.94	14.25	<MDL	2.15	<MDL	4.84	<MDL	0.75	0.72	0.37
Metribuzin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metronidazole	6.68	<MDL	<MDL	13.32	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metsulfuron methyl	0.38	11.44	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.39	<MDL
Mirtazapine	<MDL	<MDL	<MDL	7.18	1.17	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Monobutyl Phthalate (MBP)	114.56	362.17	<MDL	<MDL	<MDL	94.84	<MDL	<MDL	<MDL	<MDL	15.40	68.82	24.46
N-Desmethylcitalopram	<MDL	<MDL	<MDL	3.74	1.25	<MDL	0.49	<MDL	0.42	<MDL	<MDL	<MDL	<MDL
Nicotine	<MDL	<MDL	<MDL	14.88	<MDL	36.30	<MDL	<MDL	<MDL	<MDL	<MDL	4.45	<MDL
Niflumic acid	<MDL	<MDL	<MDL	<MDL	<MDL	1.47	<MDL	<MDL	1.68	0.47	1.28	2.45	<MDL
Ofloxacin	<MDL	<MDL	<MDL	23.33	<MDL	<MDL	<MDL	<MDL	0.82	<MDL	0.31	<MDL	<MDL
Oxazepam	<MDL	<MDL	2.00	50.17	2.87	<MDL	1.82	<MDL	<MDL	<MDL	<MDL	7.10	<MDL
Oxycodone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	3.01	<MDL	<MDL
PFBS (perfluorobutane sulfonic acid)	1.47	7.65	<MDL	2.79	<MDL	13.65	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
PFDA (perfluorodecanoic acid)	<MDL	0.85	<MDL	0.29	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
PFHpA (perfluoroheptanoic acid)	1.05	3.94	0.79	3.28	0.30	1.24	0.37	0.24	0.26	0.45	0.54	2.12	1.87
PFHxA (perfluorohexanoic acid)	6.89	10.30	1.60	5.89	0.68	2.85	0.87	<MDL	0.68	0.91	0.75	3.42	4.44
PFHxS (perfluorohexane sulfonic acid)	0.77	82.47	1.14	0.73	<MDL	1.28	0.27	<MDL	0.06	<MDL	0.24	0.63	0.36

(*continued on next page*)

Table A3 (*continued*)

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
PFNA (perfluorononanoic acid)	0.31	2.03	0.24	0.52	<MDL	0.26	0.15	<MDL	0.12	0.16	0.30	0.27	1.66
PFOA (perfluorooctanoic acid)	11.98	29.55	0.79	3.49	0.17	3.74	0.46	<MDL	0.19	1.08	0.79	2.70	2.12
PFOS (perfluorooctane sulfonic acid)	0.69	4.15	1.45	18.58	<MDL	2.79	0.96	0.12	0.13	<MDL	0.90	1.33	0.90
PFPeA (perfluoropentanoic acid)	<MDL	1.91	<MDL	3.11	<MDL	3.23	<MDL	<MDL	<MDL	<MDL	2.00	4.33	2.73
PFUnDA (perfluoroundecanoic acid)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Prochloraz	0.48	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Progesterone	<MDL	<MDL	<MDL	8.20	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Propamocarb	<MDL	6.85	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.87	<MDL	<MDL	1.37	<MDL
Propiconazole I	2.18	11.69	0.77	4.95	0.73	<MDL	1.15	<MDL	0.45	16.09	<MDL	4.22	1.02
Propranolol	<MDL	<MDL	<MDL	3.19	<MDL	<MDL	0.12	<MDL	0.14	<MDL	<MDL	<MDL	<MDL
Prothioconazole-desthio	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	2.53	<MDL
Pyraclostrobin	<MDL	<MDL	<MDL	0.21	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Pyroxsulam	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.14	<MDL	<MDL	0.32	<MDL
Roxithromycin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	2.82
Sotalol	<MDL	<MDL	<MDL	<MDL	10.55	<MDL	<MDL	<MDL	2.67	<MDL	<MDL	<MDL	<MDL
Sucralose	949.71	682.82	171.30	3421.67	328.48	184.08	66.24	<MDL	66.06	67.19	37.71	404.79	1139.40
Sulfamethoxazole	<MDL	3.93	<MDL	53.18	13.76	<MDL	6.85	<MDL	3.16	5.77	2.38	6.88	16.69
TCEP	23.30	112.80	<MDL	<MDL	<MDL	23.89	1.87	<MDL	<MDL	<MDL	3.28	<MDL	56.45
Telmisartan	2.36	8.90	0.48	42.43	163.67	0.02	1.44	<MDL	14.52	1.03	4.73	11.12	85.63
Terbuthylazine	0.52	7.80	<MDL	<MDL	0.37	<MDL	0.82	0.39	202.85	<MDL	1.99	3.88	<MDL
Terbutryn	2.36	47.77	0.17	17.33	0.35	0.62	0.58	<MDL	0.60	3.14	0.12	0.51	0.05
Theobromine	<MDL	<MDL	<MDL	<MDL	167.64	<MDL	<MDL	<MDL	77.09	138.74	<MDL	52.81	194.96
Thiabendazole	<MDL	<MDL	<MDL	34.14	2.13	<MDL	<MDL	<MDL	1.24	<MDL	<MDL	63.64	31.73
Thiamethoxam	6.69	4.75	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	9.18	<MDL	<MDL	3.23
Tramadol	<MDL	<MDL	7.20	747.30	41.88	0.61	45.95	<MDL	2.26	4.32	2.41	37.04	14.28
Triadimefon	<MDL	<MDL	<MDL	<MDL	<MDL	6.52	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Triflusulfuron-methyl	<MDL	0.99	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.84	<MDL
Triisopropanolamine	4.47	11.67	0.86	118.44	11.01	13.93	12.95	<MDL	11.76	27.81	6.17	9.70	85.18
Valsartan	4.07	50.30	<MDL	386.72	13.69	2.21	6.35	<MDL	41.86	<MDL	3.96	23.55	22.31
Venlafaxine	<MDL	<MDL	1.57	100.51	11.85	<MDL	4.59	<MDL	2.31	1.02	1.38	9.06	1.27
Total concentration	***1444.1***	***2465.7***	***247.0***	***7995.2***	***1092.5***	***1005.7***	***221.7***	***15.1***	***917.2***	***791.5***	***177.9***	***1007.6***	***2798.1***
Pesticides	***179.0***	***609.6***	***3.3***	***1321.2***	***64.5***	***169.9***	***19.9***	***0.7***	***511.2***	***420.4***	***7.3***	***67.3***	***260.1***
PFASs	***23.2***	***142.9***	***6.0***	***38.7***	***1.2***	***29.0***	***3.1***	***0.4***	***1.4***	***2.6***	***5.5***	***14.8***	***14.1***
Pharmaceuticals	***38.4***	***138.7***	***35.3***	***2547.9***	***605.5***	***19.0***	***112.8***	***0.0***	***243.5***	***207.9***	***55.3***	***290.0***	***1007.6***
Other CECs	***253.8***	***891.7***	***31.1***	***665.8***	***92.9***	***603.7***	***19.6***	***14.0***	***95.0***	***93.4***	***72.1***	***230.8***	***376.9***
Sucralose	***949.7***	***682.8***	***171.3***	***3421.7***	***328.5***	***184.1***	***66.2***	***0.0***	***66.1***	***67.2***	***37.7***	***404.8***	***1139.4***
Number of detected compounds	***46***	***52***	***22***	***71***	***48***	***36***	***39***	***6***	***56***	***42***	***45***	***55***	***53***

Table A4
Average CEC concentrations (ng L^{-1}) obtained from analysis of triplicate drinking water samples from the 13 selected DWTPs

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
10,11-Dihydro-10-hydroxycarbamazepine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
2,4-Dichlorophenoxyacetic acid	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	301.59	<MDL	<MDL	<MDL
4-Chloro-4′-fluorobutyrophenone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
5-Amino-2-chlorotoluene-4-sulfonic acid	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Acetaminophen	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Acetamiprid	0.60	4.14	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	2.85	<MDL	<MDL	<MDL
Alachlor	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Amitryptiline	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Atenolol	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Atrazine	7.94	44.50	<MDL	<MDL	0.41	<MDL	<MDL	<MDL	1.33	4.85	0.39	0.29	0.24
Atrazine-desethyl	7.07	17.16	<MDL	<MDL	2.32	<MDL	<MDL	<MDL	23.24	4.41	0.82	3.72	<MDL
Atrazine-desisopropyl	2.14	7.59	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.27	<MDL	<MDL
Azithromycin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Azoxystrobin	0.07	0.14	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.98	<MDL	<MDL	<MDL
Bentazon	<MDL	<MDL	<MDL	<MDL	<MDL	2.78	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Benzyl butyl phthalate (BBP)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	14.82	<MDL	<MDL	<MDL	<MDL	42.61	<MDL
Bezafibrate	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Bicalutamide	<MDL	<MDL	8.49	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.20	<MDL	0.60
Bis(2-ethylhexyl) phosphate	<MDL	6.43	1.05	1.88	1.37	<MDL	<MDL	4.54	<MDL	6.14	<MDL	<MDL	0.96
Bisoprolol	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Boscalid	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Caffeine	10.71	<MDL	39.68	24.75	6.95	8.98	0.89	14.31	8.67	47.18	2.26	14.64	11.48
Carbendazim	0.97	1.16	<MDL	<MDL	1.21	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Cetirizine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Chloramphenicol	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Chloridazon (Pyrazon)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.57	<MDL
Citalopram	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Clarithromycin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Climbazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.22	<MDL	<MDL	<MDL
Clomazone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Clopidogrel	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Codeine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Cyanazine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.25
Cybutryne	<MDL	<MDL	0.21	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Cyprodinil	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
DEET	0.70	3.72	0.57	0.07	<MDL	<MDL	<MDL	0.12	<MDL	1.94	0.21	0.61	0.47
Diazepam	1.28	2.83	<MDL	0.13	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Dibutyl phosphate	<MDL	33.20	<MDL	8.10	<MDL	<MDL	<MDL	25.15	<MDL	<MDL	<MDL	<MDL	<MDL
Diclofenac	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Difenoconazole I	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.23	<MDL	<MDL	<MDL
Diuron	<MDL	<MDL	<MDL	0.90	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL

(*continued on next page*)

Table A4 (*continued*)

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
Fexofenadine	<MDL	<MDL	2.20	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Fluconazole	7.07	13.76	<MDL	10.17	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.23	7.33	<MDL
Fludioxonil	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Flufenacet	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Flusilazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Flutriafol	1.08	7.41	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
FOSA (perfluorooctane sulfonamide)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Fuberidazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Furosemide	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Hexamethylcyclotrisiloxane	<MDL	<MDL	<MDL	<MDL	3.37	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Hexazinone	0.64	1.97	<MDL	<MDL	0.60	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.82	
Imidacloprid	1.28	4.05	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	2.36	<MDL	<MDL	<MDL
Irbesartan	0.33	6.10	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.08	<MDL	0.51
Isoproturon	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.26	<MDL	<MDL	<MDL	<MDL	<MDL
Ketoprofen	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Lamotrigine	0.09	<MDL	11.91	<MDL	<MDL	<MDL	0.35	<MDL	<MDL	<MDL	0.25	0.42	<MDL
Levamisole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Loratadine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Losartan	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Mandipropamid	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
MCPA	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Mebendazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Mecoprop	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metalaxyl	0.86	1.18	<MDL	0.09	<MDL	<MDL	<MDL	<MDL	<MDL	3.06	<MDL	<MDL	0.15
Methabenzthiazuron	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Methadone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metolachlor	1.28	3.84	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	7.16	0.73	<MDL	0.30	0.48
Metoprolol	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metribuzin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metronidazole	2.83	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metsulfuron methyl	0.31	12.64	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Mirtazapine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Monobutyl Phthalate (MBP)	<MDL	63.21	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
N-Desmethylcitalopram	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Nicotine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Niflumic acid	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Ofloxacin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.46	<MDL	<MDL
Oxazepam	<MDL	<MDL	1.87	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Oxycodone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
PFBS (perfluorobutane sulfonic acid)	2.11	9.37	<MDL	3.19	<MDL	10.33	<MDL	<MDL	<MDL	<MDL	<MDL	0.22	<MDL
PFDA (perfluorodecanoic acid)	<MDL	0.78	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
PFHpA (perfluoroheptanoic acid)	1.08	4.17	0.75	2.55	0.30	1.02	0.53	0.41	0.47	0.26	0.58	1.83	1.36
PFHxA (perfluorohexanoic acid)	7.55	11.44	1.58	5.63	0.65	2.95	1.46	0.54	1.06	<MDL	0.80	3.65	3.61

(*continued on next page*)

Table A4 (*continued*)

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
PFHxS (perfluorohexane sulfonic acid)	0.88	85.20	1.27	0.23	<MDL	0.39	0.46	<MDL	<MDL	<MDL	0.28	0.27	0.24
PFNA (perfluorononanoic acid)	0.30	1.92	0.26	0.33	<MDL	<MDL	0.15	0.11	0.11	0.13	0.34	0.16	1.20
PFOA (perfluorooctanoic acid)	11.88	30.22	0.72	1.88	0.30	2.04	0.54	0.17	0.31	0.42	0.97	1.76	1.48
PFOS (perfluorooctane sulfonic acid)	0.70	4.07	1.63	4.14	<MDL	0.23	0.87	0.11	<MDL	<MDL	0.99	0.09	0.49
PFPeA (perfluoropentanoic acid)	2.07	3.98	<MDL	6.94	<MDL	3.42	2.04	2.23	3.07	<MDL	<MDL	6.43	3.48
PFUnDA (perfluoroundecanoic acid)	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Prochloraz	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Progesterone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Propamocarb	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Propiconazole I	1.50	5.75	0.81	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	7.31	<MDL	<MDL	<MDL
Propranolol	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Prothioconazole-desthio	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Pyraclostrobin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Pyroxsulam	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Roxithromycin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Sotalol	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Sucralose	497.05	389.80	148.19	377.06	109.83	40.75	31.70	<MDL	35.04	<MDL	22.86	148.17	301.85
Sulfamethoxazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
TCEP	24.06	112.36	<MDL	<MDL	<MDL	5.42	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	19.01
Telmisartan	0.02	0.16	0.61	<MDL	0.77	0.09	<MDL	<MDL	<MDL	0.07	<MDL	0.04	0.09
Terbuthylazine	0.56	5.08	<MDL	<MDL	0.49	<MDL	0.21	0.37	50.60	<MDL	1.14	0.65	<MDL
Terbutryn	<MDL	<MDL	0.16	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Theobromine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Thiabendazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.05	<MDL
Thiamethoxam	4.54	3.49	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	4.13	<MDL	<MDL	<MDL
Tramadol	<MDL	<MDL	8.02	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	0.09	0.30
Triadimefon	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Triflusulfuron-methyl	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Triisopropanolamine	<MDL	<MDL	1.20	2.03	2.51	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	1.17	<MDL
Valsartan	<MDL	16.58	<MDL	6.01	1.45	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	6.16
Venlafaxine	<MDL	<MDL	1.60	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Total concentration	***601.5***	***919.4***	***232.8***	***456.1***	***132.5***	***78.4***	***54.0***	***48.3***	***131.0***	***390.9***	***35.1***	***236.1***	***356.2***
Pesticides	*31.6*	*123.8*	*1.8*	*1.1*	*5.0*	*2.8*	*0.2*	*0.8*	*82.3*	*336.4*	*3.8*	*6.1*	*3.4*
PFASs	*26.6*	*151.2*	*6.2*	*24.9*	*1.2*	*20.4*	*6.1*	*3.6*	*5.0*	*0.8*	*4.0*	*14.4*	*11.8*
Pharmaceuticals	*11.6*	*39.4*	*35.9*	*18.3*	*4.7*	*0.1*	*0.3*	*0.0*	*0.0*	*0.3*	*2.2*	*10.1*	*7.7*
Other CECs	*34.8*	*215.2*	*40.7*	*34.7*	*11.7*	*14.4*	*15.7*	*44.0*	*8.7*	*53.3*	*2.3*	*57.2*	*31.4*
Sucralose	*497.0*	*389.8*	*148.2*	*377.1*	*109.8*	*40.8*	*31.7*	*0.0*	*35.0*	*0.0*	*22.9*	*148.2*	*301.9*
Number of detected compounds	***33***	***35***	***21***	***19***	***15***	***12***	***12***	***12***	***11***	***19***	***18***	***23***	***22***

Table A5
Removal efficiency (%) of all target compounds in the 13 selected DWTPs.

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
10,11-Dihydro-10-hydroxycarbamazepine	80.5	<MDL	<MDL	70.3	63.5	<MDL	<MDL	<MDL	<MDL	<0	<MDL	<MDL	51.3
2,4-Dichlorophenoxyacetic acid	67.7	49.5	<MDL	99.4	<MDL	<MDL	<MDL	<MDL	97.7	62.4	<MDL	<MDL	95.5
4-Chloro-4′-fluorobutyrophenone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	96.4	<MDL	<MDL	<MDL
5-Amino-2-chlorotoluene-4-sulfonic acid	8.3	39.8	<MDL	<MDL	84.5	<MDL	93.0	<MDL	77.0	27.0	5.4	90.1	76.9
Acetaminophen	<0	<0	<MDL	<MDL	61.1	<MDL	<MDL	<MDL	<0	<0	7.7	10.2	<MDL
Acetamiprid	<MDL	<0	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Alachlor	99.0	98.7	84.1	97.3	88.5	<MDL	<MDL	<MDL	99.1	93.4	81.0	99.4	99.0
Amitryptiline	95.4	99.7	53.6	84.1	93.1	97.4	<MDL	<MDL	94.2	95.9	<MDL	91.4	99.0
Atenolol	<MDL	<MDL	<MDL	93.8	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Atrazine	98.4	97.5	<MDL	100.0	<0	98.8	98.7	<MDL	98.9	99.9	91.6	98.0	99.9
Atrazine-desethyl	<MDL	<MDL	<MDL	<MDL	88.4	99.9	<MDL	<MDL	89.0	<MDL	<MDL	96.8	<MDL
Atrazine-desisopropyl	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	94.9	<MDL	<MDL	<MDL	<MDL
Azithromycin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	88.4
Azoxystrobin	<MDL	<MDL	0.2	<MDL	<MDL	84.6	84.7	<MDL	<MDL	<MDL	<MDL	<MDL	99.3
Bentazon	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	93.9	<MDL	<MDL	97.4	<MDL
Benzyl butyl phthalate	63.2	44.3	2.9	98.8	98.8	99.3	99.3	<MDL	94.2	76.0	78.3	62.4	93.9
Bezafibrate	<MDL	79.0	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	56.6	<MDL	<MDL	<MDL
Bicalutamide	96.1	96.5	<MDL	98.7	<MDL	99.0	98.7	<MDL	<MDL	99.4	90.7	93.1	99.7
Bis(2-ethylhexyl) phosphate	<MDL	<MDL	<MDL	88.1	<MDL	<MDL	65.2	<MDL	97.6	<MDL	<MDL	<MDL	97.2
Bisoprolol	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	91.2	<MDL	<MDL	<MDL	<MDL
Boscalid	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	97.7	<MDL	<MDL	<MDL
Caffeine	<0	61.3	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Carbendazim	<MDL	<MDL	<MDL	<MDL	<MDL	92.2	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Cetirizine	28.3	47.1	<MDL	<MDL	68.4	92.4	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	87.8
Chloramphenicol	48.2	35.8	<MDL	99.3	98.8	<MDL	<MDL	<MDL	93.1	54.5	<MDL	<MDL	89.4
Chloridazon	99.4	100.0	<MDL	99.4	<MDL	99.8	95.6	0.7	<MDL	<MDL	<MDL	96.3	<MDL
Citalopram	<MDL	96.3	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	90.0	<MDL
Clarithromycin	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	59.6
Climbazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Clomazone	56.6	55.0	<MDL	95.0	90.5	<MDL	<MDL	<MDL	92.4	63.4	85.8	<MDL	91.3
Clopidogrel	<MDL	<MDL	<MDL	<MDL	<MDL	98.8	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Codeine	57.2	69.4	<MDL	<MDL	86.8	<MDL	<MDL	<MDL	97.1	81.0	95.4	95.7	73.4
Cyanazine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Cybutryne	18.4	<0	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	86.2	<MDL
Cyprodinil	89.1	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
DEET	<MDL	98.4	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	87.6	<MDL	<MDL	92.1	<MDL
Diazepam	31.0	50.8	<0	99.2	94.4	<MDL	96.5	<MDL	91.0	54.6	<MDL	99.0	96.1
Dibutyl phosphate	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	98.0	<MDL
Diclofenac	<MDL	<MDL	<MDL	78.2	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Difenoconazole I	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	88.2	<MDL	<MDL	95.0	<MDL
Diuron	<0	34.9	<MDL	<MDL	<0	<MDL	74.6	5.8	75.1	<MDL	42.5	83.2	<MDL

(*continued on next page*)

Table A5 (*continued*)

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
Fexofenadine	99.2	100.0	3.9	99.9	94.7	97.0	96.8	<MDL	96.9	99.4	84.1	96.3	65.1
Fluconazole	32.1	26.4	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	55.0	<MDL	<MDL	95.0
Fludioxonil	<MDL	<MDL	<MDL	<MDL	<MDL	97.7	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Flufenacet	<MDL	94.4	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	97.0	<MDL
Flusilazole	<0	<0	<MDL	<0	<MDL	24.3	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Flutriafol	<MDL	7.9	<MDL	76.1	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Fuberidazole	<0	<0	4.8	22.3	0.5	17.6	<0	<0	<0	42.8	<0	13.5	27.5
Furosemide	<0	<0	<0	68.6	<MDL	69.5	<0	<MDL	60.1	<MDL	<0	56.5	33.4
Hexamethylcyclotrisiloxane	<0	<0	1.1	4.6	4.4	<0	<0	<MDL	<0	81.1	<0	<0	18.7
Hexazinone	3.5	5.2	<0	36.1	<MDL	78.3	<0	<MDL	8.9	15.7	<0	41.1	27.8
Imidacloprid	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Irbesartan	<0	1.9	<0	77.7	<MDL	91.9	9.3	7.4	77.1	<MDL	<0	93.4	45.6
Isoproturon	0.8	<0	9.5	46.2	<0	45.4	<0	<MDL	<0	61.4	<0	34.7	30.2
Ketoprofen	<MDL	<0	<MDL	<0	<MDL	<0	<MDL	<MDL	<MDL	<MDL	61.8	<0	<0
Lamotrigine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Levamisole	<MDL	<MDL	<MDL	99.5	<MDL	<MDL	<MDL	<MDL	95.7	<MDL	<MDL	<MDL	<MDL
Loratadine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	94.6	<MDL	<MDL	<MDL	<MDL
Losartan	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	89.7	<MDL	<MDL
Mandipropamid	<MDL	<MDL	<MDL	99.0	97.0	<MDL	89.2	<MDL	98.5	<MDL	88.0	<MDL	97.7
MCPA	<MDL	<MDL	<MDL	99.9	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	95.8	<MDL	<MDL
Mebendazole	<MDL	<MDL	<MDL	98.8	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	98.5
Mecoprop	<MDL	90.6	<0	99.2	99.1	<MDL	91.4	<MDL	95.6	<MDL	87.7	98.7	97.0
Metalaxyl	<MDL	<MDL	<MDL	99.8	98.6	<MDL	97.5	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Methabenzthiazuron	<MDL	<MDL	<MDL	99.8	99.8	<MDL	<MDL	<MDL	98.3	99.7	97.7	99.6	99.8
Methadone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	62.2	<MDL	<MDL	<MDL
Metolachlor	<MDL	<MDL	<MDL	99.9	98.7	<MDL	97.9	<MDL	72.3	<MDL	<MDL	<MDL	<MDL
Metoprolol	<MDL	<MDL	<MDL	99.9	100.0	<MDL	99.3	<MDL	99.7	<MDL	99.6	98.1	99.9
Metribuzin	92.5	97.1	<MDL	99.6	99.2	<MDL	96.4	<MDL	99.1	64.8	97.2	92.0	<MDL
Metronidazole	<MDL	<MDL	<MDL	95.8	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Metsulfuron methyl	<MDL	<MDL	<MDL	100.0	96.7	<MDL	<MDL	<MDL	96.3	<MDL	95.3	<MDL	<MDL
Mirtazapine	59.0	54.0	<MDL	99.3	<MDL	91.9	<MDL	<MDL	<MDL	<MDL	<MDL	86.2	<MDL
Monobutyl Phthalate	<MDL	<MDL	<MDL	85.1	80.6	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
N-Desmethylcitalopram	<MDL	<MDL	18.6	99.9	99.8	<MDL	99.7	<MDL	99.5	99.8	99.9	99.7	100.0
Nicotine	40.8	20.9	<MDL	95.0	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	62.0	64.8	<MDL
Niflumic acid	<MDL	<MDL	<MDL	87.7	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Ofloxacin	83.8	81.8	<MDL	100.0	99.9	<MDL	98.9	<MDL	99.9	<MDL	95.3	98.7	98.1
Oxazepam	<MDL	<MDL	<MDL	97.1	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Oxycodone	73.7	93.0	0.9	99.9	99.8	94.7	97.6	<MDL	99.3	<MDL	91.4	98.2	99.8
Perfluorobutane sulfonic acid (PFBS)	97.8	<MDL	<MDL	99.6	<MDL	<MDL	<MDL	<MDL	<MDL	97.7	<MDL	<MDL	<MDL
Perfluorodecanoic acid (PFDA)	<MDL	<MDL	<MDL	95.8	<MDL	<MDL	<MDL	<MDL	<MDL	60.0	<MDL	<MDL	<MDL

(*continued on next page*)

Table A5 (*continued*)

Compound	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
Perfluoroheptanoic acid (PFHpA)	<MDL	99.0	<MDL	100.0	99.4	<MDL	98.4	<MDL	98.9	98.7	95.0	98.6	99.5
Perfluorohexane sulfonic acid (PFHxS)	<MDL	<MDL	<MDL	93.9	<MDL	<MDL	<MDL	<MDL	<MDL	89.7	<MDL	<MDL	<MDL
Perfluorohexanoic acid (PFHxA)	<MDL	<MDL	<MDL	98.7	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Perfluorononanoic acid (PFNA)	94.1	<MDL	<MDL	98.0	99.7	<MDL	98.2	<MDL	99.2	<MDL	94.9	94.7	89.6
Perfluorooctane sulfonamide (FOSA)	57.6	<MDL	<MDL	96.8	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Perfluorooctane sulfonic acid (PFOS)	<MDL	<MDL	<MDL	99.5	97.0	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Perfluorooctanoic acid (PFOA)	<MDL	<MDL	<MDL	98.8	96.3	<MDL	90.7	<MDL	89.2	<MDL	<MDL	<MDL	<MDL
Perfluoropentanoic acid (PFPeA)	<MDL	<MDL	<MDL	<MDL	<MDL	95.0	<MDL	<MDL	95.6	84.3	94.2	97.0	<MDL
Perfluoroundecanoic acid (PFUnDA)	<MDL	<MDL	<MDL	99.6	<MDL	<MDL	<MDL	<MDL	89.4	<MDL	<0	<MDL	<MDL
Prochloraz	<MDL	<MDL	6.3	99.7	95.3	<MDL	92.6	<MDL	<MDL	<MDL	<MDL	98.1	<MDL
Progesterone	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	98.2	<MDL	<MDL
Propamocarb	<MDL	<MDL	<MDL	98.8	<MDL	<MDL	67.8	<MDL	72.8	<MDL	<MDL	<MDL	<MDL
Propiconazole	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	99.4
Propranolol	<MDL	<MDL	<MDL	<MDL	96.3	<MDL	<MDL	<MDL	85.3	<MDL	<MDL	<MDL	<MDL
Prothioconazole-desthio	<MDL	91.2	<MDL	99.4	97.5	<MDL	95.0	<MDL	89.1	94.0	85.5	95.0	97.9
Pyraclostrobin	99.3	98.2	<0	100.0	99.5	<0	99.6	<MDL	100.0	92.9	99.9	99.7	99.9
Pyroxsulam	<MDL	<MDL	<MDL	<MDL	98.7	<MDL	<MDL	<MDL	97.2	98.4	<MDL	95.9	98.9
Roxithromycin	<MDL	<MDL	<MDL	99.2	87.4	<MDL	<MDL	<MDL	78.4	<MDL	<MDL	98.3	99.2
Sotalol	<MDL	<MDL	<0	100.0	99.9	92.8	99.9	<MDL	98.1	99.0	98.2	99.7	97.9
Sucralose	96.4	98.6	<0	98.3	77.2	98.8	98.8	<MDL	98.6	99.4	97.4	87.9	99.8
Sulfamethoxazole	90.5	67.0	<MDL	98.4	89.4	82.4	93.9	<MDL	99.1	<MDL	90.2	98.4	72.4
TCEP	<MDL	<MDL	<0	100.0	99.7	<MDL	99.2	<MDL	98.4	96.4	97.3	99.6	97.1
Telmisartan	47.7	42.9	13.5	89.0	66.6	77.9	52.1	<MDL	47.0	86.5	39.4	63.4	73.5
Terbuthylazine	70.7	99.7	<0	91.1	89.7	11.2	95.0	<0	90.3	<0	95.7	78.8	94.7
Terbutryn	<MDL	<MDL	<MDL	97.5	<MDL	99.0	<MDL	<MDL	<MDL	<MDL	<MDL	91.7	<MDL
Theobromine	<MDL	<MDL	<MDL	96.0	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Thiabendazole	<0	0.4	<MDL	<MDL	<MDL	77.3	55.8	<MDL	<MDL	<MDL	74.8	<MDL	66.3
Thiamethoxam	<MDL	<MDL	<MDL	99.9	99.0	<MDL	<MDL	<MDL	<MDL	<MDL	97.5	<MDL	98.9
Tramadol	<MDL	96.9	<MDL	94.9	<MDL	99.2	<MDL	<MDL	<MDL	91.5	<MDL	<MDL	92.1
Triadimefon	92.5	82.8	<MDL	95.9	63.4	97.6	<MDL	<0	95.5	56.0	76.2	95.2	47.0
Triflusulfuron-methyl	77.1	55.3	<MDL	88.8	<MDL	72.2	<MDL	<MDL	<MDL	<MDL	<MDL	95.8	<MDL
Triisopropanolamine	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Valsartan	93.9	82.5	<MDL	<MDL	<MDL	92.6	<MDL	<MDL	<MDL	<MDL	54.4	89.8	71.3
Venlafaxine	99.4	99.6	<MDL	<MDL	<MDL	98.4	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL	97.5
Average - Total	**55.2**	**56.6**	**9.1**	**89.0**	**82.0**	**76.8**	**77.4**	**2.3**	**83.3**	**73.4**	**69.2**	**84.0**	**81.6**
Average - Pesticide	**55.6**	**61.5**	**24.1**	**93.4**	**74.1**	**96.4**	**90.3**	**3.3**	**87.5**	**67.4**	**66.2**	**88.4**	**87.3**
Average - PFAS	**0.6**	**1.7**	**2.6**	**36.8**	**1.7**	**40.9**	**1.5**	**3.7**	**24.3**	**50.3**	**8.8**	**34.2**	**26.2**
Average - Pharmaceutical	**80.5**	**81.0**	**3.2**	**98.2**	**96.3**	**79.4**	**95.1**	**<MDL**	**94.0**	**89.1**	**89.2**	**95.2**	**97.0**
Average - Misc	**72.3**	**73.9**	**0.0**	**94.9**	**84.0**	**80.9**	**75.4**	**0.0**	**92.9**	**86.5**	**39.4**	**63.4**	**73.5**
Sucralose	**47.7**	**42.9**	**13.5**	**89.0**	**66.6**	**77.9**	**52.1**	**<MDL**	**47.0**	**61.2**	**75.3**	**91.5**	**81.1**

Table A6
List of suspects (n = 500) screened for in the raw water and drinking water. The list was created using SusTool (Dürig et al., 2019).

Name	CAS#	Smiles	Monoisotopic Mass (Da)
(1-Methylethyl) dihydrogen 2-hydroxypropane-1,2,3-tricarboxylate	1321-57-9	CC(C)OC(=O)CC(O)(CC(O)=O)C(O)=O	234.073955
(2S-cis)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-3-hydroxy-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one	42399-40-6	CN(C)CCN1C(=O)C(O)C(Sc2ccccc12)c1ccc(cc1)OC	372.150763
(3-Chloro-2-hydroxypropyl)dimethyl[2-[(2-methyl-1-oxoallyl)oxy]ethyl]ammonium nitrate	67596-04-7	CC(=C)C(=O)OCC[N+](C)(C)CC(O)CCl	250.120996
(E)-3-Formyl-2,4,4-trichloro-2-butenoic acid	115340-67-5	OC(=O)C(Cl)=C(C=O)C(Cl)Cl	215.914776
(p-Ammoniophenyl)ethyl(2-hydroxyethyl)ammonium sulphate	4327-84-8	Nc1ccc(CCNCCO)cc1	180.126263
(Propylcarbonylthioethyl)trimethylammonium iodide	1866-16-6	CCCC(=O)SCC[N+](C)(C)C	190.126559
(R)-N-Methylsalsolinol	53622-84-7	CC1c2cc(O)c(O)cc2CCN1C	193.110279
(R)-S-(2-amino-2-carboxyethyl)-L-homocysteine	56-88-2	NC(CSCCC(N)C(O)=O)C(O)=O	222.067428
?-hydroxyhippuric acid	16555-77-4	OC(=O)C(O)NC(=O)c1ccccc1	195.053159
?-hydroxy-o-tolyl ?-D-glucopyranoside	138-52-3	OC1C(O)C(OC(CO)C1O)Oc1ccccc1CO	286.105255
[2-hydroxypropyl]dimethyl[2-[(2-methyl-1-oxoallyl)oxy]ethyl]ammonium nitrate	68928-62-1	CC(=C)C(=O)OCC[N+](C)(C)CC(C)O	216.159969
[R(R*,R*]-2-amino-1-[p-(methylsulphonyl)phenyl]propane-1,3-diol	51458-28-7	CS(=O)(=O)c1ccc(cc1)C(O)C(N)CO	245.072179
1-(2,4-Dinitrophenyl)pyridinium chloride	4185-69-7	[O-][N+](=O)c1cc(ccc1-[n+]1ccccc1)[N+]([O-])=O	246.051482
1-(2-Aminoethyl)piperazine	140-31-8	NCCN1CCNCC1	129.126597
1-(4-Fluorophenyl)piperazine dihydrochloride	64090-19-3	Fc1ccc(cc1)N1CCNCC1	180.106276
1,1-(But-2-en-1,4-diyl)bis[3,5,7-triaza-1-azoniatricyclo[3.3.1.13,7]decane] dichloride	51350-84-6	C1N2CN3C[N+]1(CN(C2)C3)CC=CC[N+]12CN3CN(C1)CN(C2)C3	334.259342
1,1-Diethoxy-2-methylbutane	3658-94-4	NC1=NC(=O)C2N=C(COP(O)(=O)OP(O)(O)=O)CNC2=N1	355.008289
1,1′-Oxybis-2-propanol	110-98-5	CC(O)COCC(C)O	134.094295
1,2,4-Benzenetrisulfonic acid, 5,6-dihydroxy-, trisodium salt	112935-85-0	Oc1c(cc(c(c1O)S(O)(=O)=O)S(O)(=O)=O)S(O)(=O)=O	349.907225
1,2-Bis[hydroxymethoxy]ethane	3586-55-8	OCOCCOCO	122.05791
1,2-Ethanediamine, N-(2-aminoethyl)-N-[(ethenylphenyl)methyl]-, polymer with diethenylbenzene	65945-33-7	C=Cc1ccccc1CN(CCN)CCN	219.173547
1,2-Propylene glycol	57-55-6	CC(O)CO	76.05243
1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol	4719-04-4	OCCN1CN(CN(C1)CCO)CCO	219.158292
1,3-Benzenedimethanamine	1477-55-0	NCc1cc(CN)ccc1	136.100048
1,3-Benzenedisulfonic acid, 4-hydroxy-	96-77-5	Oc1ccc(cc1S(O)(=O)=O)S(O)(=O)=O	253.955495
1,3-Dimethylol-5,5-dimethylhydantoin	6440-58-0	CC1(C)C(=O)N(CO)C(=O)N1CO	188.079708
1,4-BENZENDIOL, 2-(PHENYLMETHYL)-	1706-73-6	Oc1cc(Cc2ccccc2)c(O)cc1	200.08373
1,4-Diazabicyclo[2.2.2]octane	280-57-9	C1CN2CCN1CC2	112.100048
16ALPHA-HYDROXYESTRONE	566-76-7	CC12CCC3C(CCc4cc(O)ccc43)C1CC(O)C2=O	286.156895
16-Ketoestradiol	566-75-6	CC12CCC3C(CCc4cc(O)ccc43)C1CC(=O)C2O	286.156895
17-Alpha-estradiol	57-91-0	c1c(O)cc2CCC3C4CCC(O)C4(C)CCC3c2c1	272.17763
17-Beta-estradiol	50-28-2	CC12CCC3C(CCc4cc(O)ccc43)C1CCC2O	272.17763
1-Amino-2-propanol	78-96-6	CC(O)CN	75.068414
1-Methoxy-4-(1,2,2,2-tetrachloroethyl)benzene	51495-87-5	COc1ccc(cc1)C(Cl)C(Cl)(Cl)Cl	271.932923
1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., chlorides, sodium salts	61789-39-7	C[N+](C)(CCCN)CC(O)=O	161.129003
1-Propanesulfonic acid, 2-hydroxy-3-(2-propenyloxy)-, monosodium salt	52556-42-0	C=CCOCC(O)CS(O)(=O)=O	196.040545
1-Propanol, 3,3′,3′′-phosphinylidynetris-	51805-42-6	OCCCP(=O)(CCCO)CCCO	224.117747
2-(2,7-Dichloro-6-hydroxy-3-oxo-3H-xanthen-9-yl)benzoic acid	76-54-0	Oc1cc2Oc3cc(O)c(Cl)cc3C3(OC(=O)c4ccccc34)c2cc1Cl	399.990529
2-(4,5-Dibromo-3,6-dihydroxy-2,7-dinitroxanthen-9-yl)-benzoic acid, disodium salt	548-24-3	[O-][N+](=O)c1cc2C(c3ccccc3C(O)=O)=C3C=C(C(=O)C(Br)=C3Oc2c(Br)c1O)[N+]([O-])=O	577.859655
2-(4-Hydroxybenzyl)phenol	2467-03-0	Oc1ccc(Cc2ccccc2O)cc1	200.08373
2-(Hydroxymethyl)-2-nitro-1,3-propanediol	126-11-4	[O-][N+](=O)C(CO)(CO)CO	151.048074
2,2,2-[Methylidynetris(thio)]trisacetic acid	34914-39-1	OC(=O)CSC(SCC(O)=O)SCC(O)=O	285.96395
2,2′-[[3-Methyl-4-[[4-[[2-(sulphooxy)ethyl]sulphonyl]phenyl]azo]phenyl]imino] bisethyl bis(hydrogen sulphate), sodium salt	94157-82-1	Cc1cc(ccc1N=Nc1ccc(cc1)S(=O)(=O)CCOS(O)(=O)=O)N(CCOS(O)(=O)=O)CCOS(O)(=O)=O	647.021937
2,2-Bis(4-hydroxyphenyl)-1,1,1-trichloroethane	2971-36-0	Oc1ccc(cc1)C(c1ccc(O)cc1)C(Cl)(Cl)Cl	315.982461
2,3-DICHLOROPROPIONIC ACID	565-64-0	OC(=O)C(Cl)CCl	141.958834
2,3-Dihydroxyfumaric acid	133-38-0	OC(C(=O)C(O)=O)C(O)=O	148.00079
2,3-NAPHTHALENEDIOL, 6-ETHYL-	136944-43-9	CCc1cc2cc(O)c(O)cc2cc1	188.08373
2,4,4′-Trihydroxybenzophenone	1470-79-7	Oc1cc(O)ccc1C(=O)c1ccc(O)cc1	230.05791
2,4,6-Tris(dimethylaminomethyl)phenol	90-72-2	CN(C)Cc1cc(CN(C)C)c(O)c(CN(C)C)c1	265.215412

(continued on next page)

Table A6 (*continued*)

Name	CAS#	Smiles	Monoisotopic Mass (Da)
2,5-Dichloro-4′-biphenylol	53905-28-5	Oc1ccc(cc1)-c1cc(Cl)ccc1Cl	237.995219
2,5-Pyrrolidinedione, 1-[2-[[2-[[2-[(2-aminoethyl)amino]ethyl]amino]ethyl]amino]ethyl]-, monopolyisobutenyl derivs.	67762-72-5	CC(=C)CC1CC(=O)N(CCNCCNCCNCCN)C1=O	325.247775
2-Amino-2-methylpropan-1-ol	124-68-5	CC(C)(N)CO	89.084064
2-Chloro-4-phenylphenol	92-04-6	Oc1cc(Cl)c(cc1)-c1ccccc1	204.034192
2-Chloro-6-hydroxynaphthalene	40604-49-7	Oc1cc2ccc(Cl)cc2cc1	178.018542
2-chloro-9-[3-(dimethylamino)propyl]thioxanthen-9-ol	4295-65-2	CN(C)CCCC1(O)c2ccccc2Sc2ccc(Cl)cc12	333.095411
2-Deoxyguanosine-5-Triphosphate	2564-35-4	NC1Nc2c([n]c[n]2C2CC(O)C(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)O2)C(=O)N=1	506.995751
2-Deoxyinosine	890-38-0	OC1CC(OC1CO)[n]1c[n]c2c1NC=NC2=O	252.085856
2-Ethyl-2-(hydroxymethyl)-1,3-propanediol	77-99-6	CCC(CO)(CO)CO	134.094295
2-Furanmethanol, 2-formate	13493-97-5	CC1OCC(O)C(O1)C(O)C(O)C=O	206.07904
2-hydroxy-5-carboxymethylmuconate semialdehyde	2461-62-3	OC(=O)C(=O)C=CC(CC(O)=O)C=O	200.03209
2-Hydroxy-estradiol	362-05-0	CC12CCC3C(CCc4cc(O)c(O)cc43)C1CCC2O	288.172545
2-Hydroxyethanesulfonic acid maleate, disodium	51678-73-0	OC(=O)C=CC(=O)OCCS(O)(=O)=O	223.999075
2-Keto-3-deoxy-6-phosphogluconate	27244-54-8	OC(=O)C(=O)CC(O)C(O)COP(O)(O)=O	258.014072
2-Methoxyestradiol	362-07-2	CC12CCC3C(CCc4cc(O)c(cc43)OC)C1CCC2O	302.188195
2-Propenoic acid, polymer with 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonic acid	40623-75-4	CCC(C)(NC(=O)C=C)S(O)(=O)=O	207.056529
3-(2-Aminoethyl)indol-5-ol	50-67-9	NCCc1c[nH]c2ccc(O)cc21	176.094963
3-(2-Chloro-phenoxy)-propane-1,2-diol	5112-21-0	OCC(O)COc1ccccc1Cl	202.039672
3-(Dimethylamino)propylamine	109-55-7	CN(C)CCCN	102.115698
3-(Trimethoxysilyl)-N-[3-(trimethoxysilyl)propyl]propan-1-amine	82985-35-1	CO[Si](CCCNCCC[Si](OC)(OC)OC)(OC)OC	341.168993
3-(Trimethoxysilyl)propan-1-amine	13822-56-5	CO[Si](CCCN)(OC)OC	179.097771
3,3,3-Trichloro-2-hydroxy-propionic acid	599-01-9	OC(C(O)=O)C(Cl)(Cl)Cl	191.914776
3,3′-Dichloro-5,5′-dinitro-2,2′-biphenol	15595-24-1	[O-][N+](=O)c1cc(Cl)c(O)c(c1)-c1cc(cc(Cl)c1O)[N+]([O-])=O	343.960292
3,3′-Dimethylbisphenol A	79-97-0	CC(C)(c1cc(C)c(O)cc1)c1cc(C)c(O)cc1	256.14633
3,4-Dihydroxyphenyllactic acid	23028-17-3	OC(Cc1cc(O)c(O)cc1)C(O)=O	198.052825
3,6,9,12-Tetraoxahexadecan-1-ol	1559-34-8	CCCCOCCOCCOCCOCCO	250.178025
3-[(6-Deoxy-?-L-mannopyranosyl)oxy]-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-benzopyran-4-one	17912-87-7	CC1OC(OC2C(=O)c3c(cc(O)cc3O)OC=2c2cc(O)c(O)c(O)c2)C(O)C(O)C1O	464.09548
3-Benzylsydnone-4-acetamide	14504-15-5	NC(=O)Cc1c(O)o[n][n+]1Cc1ccccc1	234.087867
3-Deazaadenosine	6736-58-9	Nc1[n]ccc2c1[n]c[n]2C1OC(CO)C(O)C1O	266.101506
3-Deoxyestradiol	2529-64-8	CC12CCC3C(CCc4ccccc43)C1CCC2O	256.182715
3-HYDROXY-4-OXO-4H-PYRAN-2,6-DICARBOXYLIC ACID	497-59-6	OC(=O)C1=CC(=O)C(=O)C(O1)C(O)=O	199.995705
3-Hydroxykynurenine	484-78-6	Nc1c(cccc1O)C(=O)CC(N)C(O)=O	224.079708
3-Ketolactose	15990-62-2	OC(CO)C(OC1OC(CO)C(O)C(=O)C1O)C(O)C(O)C=O	340.100565
3-O-Ethylascorbic acid	86404-04-8	CCOC1C(OC(=O)C1=O)C(O)CO	204.06339
4-((Dimethylamino)methyl)phenol	103-87-7	CN(C)Cc1ccc(O)cc1	151.099714
4-(4-Acetylpiperazin-4-yl)phenol	67914-60-7	CC(=O)N1CCN(CC1)c1ccc(O)cc1	220.121178
4(G)-alpha-glucopyranosyl-rutin	130603-71-3	CC1OC(OCC2OC(OC3C(=O)c4c(cc(O)cc4O)OC=3c3cc(O)c(O)cc3)C(O)C(O)C2OC2OC(CO)C(O)C(O)C2O)C(O)C(O)C1O	772.206215
4,4′-(3H-2,1-benzoxathiol-3-ylidene)bis[2-chlorophenol] S,S-dioxide	4430-20-0	Oc1ccc(cc1Cl)C1(OS(=O)(=O)c2ccccc12)c1cc(Cl)c(O)cc1	421.978249
4,4′-(Oxydiethylene)bis(morpholine)	6425-39-4	C1COCCN1CCOCCN1CCOCC1	244.178693
4,4′-Biphenyldiol	92-88-6	Oc1ccc(cc1)-c1ccc(O)cc1	186.06808
4,4′-Dihydoxybenzophenone	611-99-4	Oc1ccc(cc1)C(=O)c1ccc(O)cc1	214.062995
4,4′-Dihydroxydiphenyl ether	1965-09-9	Oc1ccc(cc1)Oc1ccc(O)cc1	202.062995
4,4-Dithiobis[2-aminobutyric] acid	462-10-2	NC(CCSSCCC(N)C(O)=O)C(O)=O	268.055148
4,4-Iminodianiline	537-65-5	Nc1ccc(cc1)Nc1ccc(N)cc1	199.110947
4,4′-Oxydianiline	101-80-4	Nc1ccc(cc1)Oc1ccc(N)cc1	200.094963
4,4′-Propane-1,1-diyldiphenol	1576-13-2	CCC(c1ccc(O)cc1)c1ccc(O)cc1	228.11503
4,4′-Thiodibenzene-1,3-diol	97-29-0	Oc1cc(O)c(cc1)Sc1ccc(O)cc1O	250.02998
4-[(4-Amino-3-methylphenyl)amino]-phenol, reaction products with sodium sulfide (Na2(Sx))	1327-57-7	Cc1cc(ccc1N)Nc1ccc(O)cc1	214.110613
4-[(4-Iminocyclohexa-2,5-dien-1-ylidene)benzyl]aniline monohydrochloride	3442-83-9	Nc1ccc(cc1)C(c1ccccc1)=C1C=CC(=N)C=C1	272.131348
4-Amino-4′-hydroxybiphenyl	1204-79-1	Nc1ccc(cc1)-c1ccc(O)cc1	185.084064
4-Benzylphenol	101-53-1	Oc1ccc(Cc2ccccc2)cc1	184.088815
4-Chloro-2-[(Z)-(methoxycarbonyl)methoxyimino]-3-oxobutyric acid	84080-70-6	COC(=O)CON=C(C(=O)CCl)C(O)=O	237.004016
4-Chloro-4′-biphenylol	28034-99-3	Oc1ccc(cc1)-c1ccc(Cl)cc1	204.034192
4-Cyclohexylphenol	1131-60-8	Oc1ccc(cc1)C1CCCCC1	176.120115
4-Hydroxybenzophenone	1137-42-4	Oc1ccc(cc1)C(=O)c1ccccc1	198.06808
4-Hydroxy-estradiol	5976-61-4	CC12CCC3C(CCc4c3ccc(O)c4O)C1CCC2O	288.172545
4-Hydroxyphenylpyruvic acid	156-39-8	OC(=O)C(=O)Cc1ccc(O)cc1	180.04226
4-Phenylphenol	92-69-3	Oc1ccc(cc1)-c1ccccc1	170.073165

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Table A6 (*continued*)

Name	CAS#	Smiles	Monoisotopic Mass (Da)
4-phenylpiracetam	77472-70-9	NC(=O)CN1CC(CC1=O)c1ccccc1	218.105528
5-(3-Dimethylaminopropyl)-10,11-dihydrodibenzo[a,d]cyclohepten-5-ol	1159-03-1	CN(C)CCCC1(O)c2ccccc2CCc2ccccc12	295.193614
5-Amino-3-sulfosalicylic acid	6201-87-2	Nc1cc(c(O)c(c1)C(O)=O)S(O)(=O)=O	232.999409
5-Bromo-4-chloroindol-3-yl-?-D-galactopyranoside	7240-90-6	OCC1OC(Oc2c[nH]c3ccc(Br)c(Cl)c23)C(O)C(O)C1O	406.977127
5-Bromouridine	957-75-5	OCC1OC(C(O)C1O)N1C=C(Br)C(=O)NC1=O	321.980049
5-Fluorouridine	316-46-1	OCC1OC(C(O)C1O)N1C=C(F)C(=O)NC1=O	262.060116
5H-Thiachromine-8-ethanol, 2,7-dimethyl-	92-35-3	CC1=C(CCO)SC2=Nc3[n]c(C)[n]cc3CN12	262.088831
6,6-Dihydroxy-3,3-diarsene-1,2-diyldianilinium dichloride	139-93-5	Nc1cc(ccc1O)[As]=[As]c1cc(N)c(O)cc1	365.933066
6a,7-dihydro-3,4,6a,10-tetrahydroxybenz[b]indeno[1,2-d]pyran-9(6H)-one	475-25-2	Oc1ccc2c(OCC3(O)CC4=CC(=O)C(=O)CC4=C32)c1O	300.06339
6-Alpha-hydroxy-estradiol	1229-24-9	CC12CCC3C(CC(O)c4cc(O)ccc43)C1CCC2O	288.172545
6-Azacytidine	3131-60-0	NC1C=NN(C2OC(CO)C(O)C2O)C(=O)N=1	244.080771
6-AZAURIDINE	54-25-1	OCC1OC(C(O)C1O)N1N=CC(=O)NC1=O	245.064787
6-Phosphonoglucono-delta-lactone	2641-81-8	OC1C(COP(O)(O)=O)OC(=O)C(O)C1O	258.014072
7-Aminonaphthalene-1,3,6-trisulphonic acid	118-03-6	Nc1cc2c(cc(cc2cc1S(O)(=O)=O)S(O)(=O)=O)S(O)(=O)=O	382.943944
7-Thia-8-oxoguanosine	122970-40-5	NC1=NC(=O)C2SC(=O)N(C3OC(CO)C(O)C3O)C2=N1	316.047756
8-Azidoadenosine	4372-67-2	Nc1[n]c[n]c2c1[n]c(N=[N+]=N)[n]2C1OC(CO)C(O)C1O	309.105977
8-Bromo-cAMP	23583-48-4	Nc1[n]c[n]c2c1[n]c(Br)[n]2C1OC2COP(O)(=O)OC2C1O	406.963033
8-Hydroxyguanosine	3868-31-3	NC1=NC(=O)C2NC(=O)N(C3OC(CO)C(O)C3O)C2=N1	299.086585
9-Deazainosine	89458-19-5	OCC1OC(C(O)C1O)c1c[nH]c2C(=O)N=CNc21	267.085522
Acetarsol	97-44-9	CC(=O)Nc1cc(ccc1O)[As](O)(O)=O	274.977493
Acetophenazine	2751-68-0	CC(=O)c1cc2c(cc1)Sc1ccccc1N2CCCN1CCN(CCO)CC1	411.198047
ACETRYPTINE	3551-18-6	CC(=O)c1cc2c(CCN)c[nH]c2cc1	202.110613
Acetylpromazine	61-00-7	CN(C)CCCN1c2cc(ccc2Sc2ccccc12)C(C)=O	326.145283
ACONINE	509-20-6	CCN1CC2(COC)C3C(OC)C4C1C3(C1CC3(O)C(OC)C(O)C4(O)C1C3O)C(CC2O)OC	499.278134
Acrylic acid	79-10-7	C=CC(O)=O	72.02113
Adenosine 5-(trihydrogen diphosphate)	58-64-0	Nc1[n]c[n]c2c1NCN2C1OC(COP(O)(=O)OP(O)(O)=O)C(O)C1O	429.045069
Adenosine 5′-(trihydrogen diphosphate), monosodium salt	1172-42-5	Nc1[n]c[n]c2c1[n]c[n]2C1OC(COP(O)(=O)OP(O)(O)=O)C(O)C1O	427.029419
Adenosine Phosphosulfate	485-84-7	Nc1[n]c[n]c2c1[n]c[n]2C1OC(COP(O)(=O)OS(O)(=O)=O)C(O)C1O	427.019902
Adesulfone sodium	144-75-2	OS(=O)CNc1ccc(cc1)S(=O)(=O)c1ccc(cc1)NCS(O)=O	404.017048
Alcohols, C13-15, ethoxylated	64425-86-1	CC1C(CCc2cccc(O)c21)N(CCC)CCC	261.209264
ALENTEMOL	112891-97-1	CCCN(CCC)C1Cc2cc(O)cc3cccc(C1)c23	283.193614
Alginic acid	9005-32-7	COC1C(OC(OC2C(OC(OC)C(O)C2O)C(O)=O)C(O)C1O)C(O)=O	398.106045
Allantoin	97-59-6	NC(=O)NC1NC(=O)NC1=O	158.043991
Alloxantin	76-24-4	OC1(C(=O)NC(=O)NC1=O)C1(O)C(=O)NC(=O)NC1=O	286.018566
Alpha-amanitin	23109-05-9	CCC(C)C1NC(=O)CNC(=O)C2Cc3c4ccc(O)cc4[nH]c3S(=O)CC(NC(=O)CNC1=O)C(=O)NC(CC(N)=O)C(=O)N1CC(O)CC1C(=O)NC(C(C)C(O)CO)C(=O)N2	918.35417
Alpha-D-glucose 1,6-bisphosphate	10139-18-1	OC1C(OP(O)(O)=O)OC(COP(O)(O)=O)C(O)C1O	339.996054
Alpha-D-glucose-1-phosphate	59-56-3	OCC1OC(OP(O)(O)=O)C(O)C(O)C1O	260.029722
Amidephrine mesylate	1421-68-7	CNCC(O)c1cc(ccc1)NS(C)(=O)=O	244.088163
Aminoimidazole ribotide	25635-88-5	Nc1c[n]c[n]1C1OC(COP(O)(O)=O)C(O)C1O	295.056939
Amiterol	54063-25-1	CC(CC)NCC(O)c1ccc(N)cc1	208.157563
AMMONIUM ZIRCONIUM HYDROXY CITRATE	149564-62-5	OC(=O)CC(O)(CC(=O)OO)C(O)=O	208.02192
Amopyroquine	550-81-2	Oc1ccc(cc1CN1CCCC1)Nc1cc[n]c2cc(Cl)ccc21	353.129489
Amygdalin	29883-15-6	N#CC(OC1OC(COC2OC(CO)C(O)C(O)C2O)C(O)C(O)C1O)c1ccccc1	457.158414
Anthrarobin	577-33-3	Oc1ccc2c(cc3ccccc3c2O)c1O	226.062995
Aphidicolin	38966-21-1	CC12CCC(O)C(C)(CO)C1CCC1CC3CC21CCC3(O)CO	338.24571
Arbutin	497-76-7	Oc1ccc(cc1)OC1OC(CO)C(O)C(O)C1O	272.089605
Ascorbic acid 2-O-glucoside	129499-78-1	OC(CO)C1OC(=O)C(OC2OC(CO)C(O)C(O)C2O)C1=O	338.084915
ASPARTOCIN	4117-65-1	CC(C)CC(NC(=O)C1CCCN1C(=O)C1CSSCC(N)C(=O)NC(Cc2ccc(O)cc2)C(=O)NC(C(C)CC)C(=O)NC(CC(N)=O)C(=O)NC(CC(N)=O)C(=O)N1)C(=O)NCC(N)=O	992.420808
Asperuloside	14259-45-1	CC(=O)OCC1=CC2OC(=O)C3=COC(OC4OC(CO)C(O)C(O)C4O)C1C32	414.116215
Azidamfenicol	13838-08-9	N=[N+]=NCC(=O)NC(CO)C(O)c1ccc(cc1)[N+]([O-])=O	296.099495
Benaxibine	27661-27-4	OC(=O)c1ccc(cc1)NC1OCC(O)C(O)C1O	269.089939
Benzenemethanaminium, ar-ethenyl-N-(2-hydroxyethyl)-N,N-dimethyl-, chloride, polymer with diethenylbenzene	63181-94-2	C[N+](C)(CCO)Cc1ccccc1C=C	206.154489
Benzenesulfonamide,3-F-4-[3-HOPr-thio]-	108966-74-1	NS(=O)(=O)c1cc(F)c(cc1)SCCCO	265.024262
benzyl(3-chloro-2-hydroxypropyl)dimethylammonium Chloride	67304-25-0	C[N+](C)(CC(O)CCl)Cc1ccccc1	228.115516
Benzylmorphine	14297-87-1	CN1CCC23C4C=CC(O)C2Oc2c3c(CC14)ccc2OCc1ccccc1	375.183444
Bergenin	477-90-7	COc1c(O)cc2C(=O)OC3C(OC(CO)C(O)C3O)c2c1O	328.079435
Beta-mercaptolactate cysteine disulfide	18841-42-4	NC(CSSCC(O)C(O)=O)C(O)=O	241.007864
Biflorin	89701-85-9	CC1=CC(=O)c2c(cc(O)c(C3OC(CO)C(O)C(O)C3O)c2O)O1	354.095085

(*continued on next page*)

Table A6 (*continued*)

Name	CAS#	Smiles	Monoisotopic Mass (Da)
Bipenamol	79467-22-4	NCc1ccccc1Sc1ccccc1CO	245.087434
Bis(2-hydroxyethyl)methyloctylammonium toluene-p-sulphonate	58767-50-3	CCCCCCCC[N+](C)(CCO)CCO	232.227654
Bis(4-hydroxyphenyl)methane	620-92-8	Oc1ccc(Cc2ccc(O)cc2)cc1	200.08373
Bisphenol A	80-05-7	CC(C)(c1ccc(O)cc1)c1ccc(O)cc1	228.11503
Bisphenol B	77-40-7	CCC(C)(c1ccc(O)cc1)c1ccc(O)cc1	242.13068
Bisphenol E	2081-08-5	CC(c1ccc(O)cc1)c1ccc(O)cc1	214.09938
Bithionoloxide	844-26-8	Oc1c(cc(Cl)cc1Cl)S(=O)c1cc(Cl)cc(Cl)c1O	369.879173
BOTIACRINE	4774-53-2	OCC1OC(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1O	484.08531
Bufotenine	487-93-4	CN(C)CCc1c[nH]c2ccc(O)cc12	204.126263
Busulfan	55-98-1	CS(=O)(=O)OCCCCOS(C)(=O)=O	246.02318
Butanedioic acid, [(ethoxythioxomethyl)thio]-	22119-15-9	CCOC(=S)SC(CC(O)=O)C(O)=O	237.996965
Butanedioic acid, 2,3-dihydroxy- R-(R*,R*) -, m	608-89-9	CCOC(=O)C(O)C(O)C(O)=O	178.04774
C.I. Basic Red 9	479-73-2	Nc1ccc(cc1)C(c1ccc(N)cc1)=C1C=CC(=N)C=C1	287.142247
C6-galactose mustard	105618-02-8	OC1OC(CN(CCCl)CCCl)C(O)C(O)C1O	303.064028
Caftaric acid	67879-58-7	OC(C(OC(=O)C=Cc1cc(O)c(O)cc1)C(O)=O)C(O)=O	312.048135
Carboxymethyl cellulose	9000-11-7	OC1C(COCC(O)=O)OC(O)C(O)C1O	238.06887
Cartap	15263-53-3	CN(C)C(CSC(N)=O)CSC(N)=O	237.060567
Chloralose	15879-93-3	OCC(O)C1OC2OC(OC2C1O)C(Cl)(Cl)Cl	307.962121
Chloramphenicol sodium succinate	982-57-0	[O-][N+](=O)c1ccc(cc1)C(O)C(COC(=O)CCC(O)=O)NC(=O)C(Cl)Cl	422.028372
Chloroacetic acid	79-11-8	OC(=O)CCl	93.982157
Chlorogenic acid	327-97-9	OC(=O)C1(O)CC(O)C(O)C(C1)OC(=O)C=Cc1cc(O)c(O)cc1	354.095085
Cianidanol	154-23-4	OC1Cc2c(cc(O)cc2O)OC1c1cc(O)c(O)cc1	290.07904
CINAPROXEN	89163-44-0	CC(=O)NC(CSC(=O)C(C)c1cc2ccc(cc2cc1)OC)C(O)=O	375.114044
Citric acid, monoester with glycerol	36291-32-4	OCC(O)COC(=O)CC(O)(CC(O)=O)C(O)=O	266.063785
CLIROPAMINE	109525-44-2	Cc1ccc(cc1O)C(O)C(C)NCCCc1ccccc1	299.188529
CLOFEVERINE	54340-63-5	CCCCC(=O)c1cc(F)c(O)c(Br)c1	274.000469
Copper diethylamine oxyquinoline sulfonate	13007-93-7	Oc1c2[n]cccc2c(cc1S(O)(=O)=O)S(O)(=O)=O	304.966394
Cordycepin triphosphate	73-04-1	Nc1[n]c[n]c2c1[n]c[n]2C1OC(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)CC1O	491.000836
Corilagin	23094-69-1	Oc1c2-c3c(cc(O)c(O)c3O)C(=O)OCC3OC(OC(=O)c4cc(O)c(O)c(O)c4)C(O)C(OC(=O)c2cc(O)c1O)C3O	634.08062
Crisnatol	96389-68-3	CC(CO)(CO)NCc1cc2c3ccccc3ccc2c2ccccc21	345.172879
Cyclocytidine	31698-14-3	N=C1C=CN2C3OC(CO)C(O)C3OC2=N1	225.074957
Cyclouridine	3736-77-4	OC1C2OC3=NC(=O)C=CN3C2OC1CO	226.058973
Cytidine-5-Diphosphate	63-38-7	NC1C=CN(C2OC(COP(O)(=O)OP(O)(O)=O)C(O)C2O)C(=O)N=1	403.018186
D-(-)threo-2-amino-1-(p-nitrophenyl)propane-1,3-diol	716-61-0	NC(CO)C(O)c1ccc(cc1)[N+]([O-])=O	212.079708
DACINOSTAT	404951-53-7	ONC(=O)C=Cc1ccc(CN(CCO)CCc2c[nH]c3ccccc23)cc1	379.189592
DACOPAFANT	125372-33-0	NC(=O)c1cc[n]2C(SCc21)c1c[n]ccc1	245.062282
D-arabino-2-hexulosonic acid, methyl ester	21063-40-1	COC(=O)C(=O)C(O)C(O)C(O)CO	208.058305
DATELLIPTIUM CHLORIDE	105118-14-7	Cc1c2[nH]c3ccc(O)cc3c2c(C)c2c[n+](CCN(CC)CC)ccc12	362.223237
Deaminodicarba-Gly-oxytocin	33605-67-3	CC(C)CC(NC(=O)CNC(=O)C1CCCCCC(=O)NC(Cc2ccc(O)cc2)C(=O)NC(C(C)CC)C(=O)NC(CCC(N)=O)C(=O)NC(CC(N)=O)C(=O)N1)C(=O)NCC(N)=O	915.481419
Delsoline	509-18-2	CCN1CC2(CCC(O)C34C2C(OC)C(O)(C31)C1(O)CC(OC)C2CC4C1C2OC)COC	467.288304
Demoxytocin	113-78-0	CC(C)CC(NC(=O)C1CCCN1C(=O)C1CSSCCC(=O)NC(Cc2ccc(O)cc2)C(=O)NC(C(C)CC)C(=O)NC(CCC(N)=O)C(=O)NC(CC(N)=O)C(=O)N1)C(=O)NCC(N)=O	991.425559
Deoxyuridine triphosphate	1173-82-6	OP(O)(=O)OP(O)(=O)OP(O)(=O)OCC1OC(CC1O)N1C=CC(=O)NC1=O	467.973619
Desethylhydroxychloroquine	4298-15-1	CC(CCCNCCO)Nc1cc[n]c2cc(Cl)ccc21	307.145139
Desmopressin	16679-58-6	N1(CCC[C@@H]1C(=O)N[C@@H](C(NCC(N)=O)=O)CCCNC(N)=N)C([C@@H]1CSSCCC(N[C@@H](C(N[C@@H](C(=O)N[C@@H](CCC(=O)N)C(=O)N[C@@H](C(N1)=O)CC(N)=O)Cc1ccccc1)=O)Cc1ccc(cc1)O)=O)=O	1068.42696
Dexelvucitabine	134379-77-4	NC1=NC(=O)N(C=C1F)C1C=CC(CO)O1	227.07062
Dezocine	53648-55-8	CC12CCCCCC(Cc3ccc(O)cc13)C2N	245.177964
D-fructose 1-(dihydrogen phosphate)	15978-08-2	OCC(O)C(O)C(O)C(=O)COP(O)(O)=O	260.029722
D-fructose 6-(dihydrogen phosphate)	643-13-0	OC1COC(O)(COP(O)(O)=O)C(O)C1O	260.029722
D-Fructose, 3-O-.alpha.-D-glucopyranosyl-	547-25-1	OC1COC(O)(CO)C(OC2OC(CO)C(O)C(O)C2O)C1O	342.116215
-D-Galactopyranoside, 5-bromo-4-chloro-1H-indol-3-yl 6-deoxy-	17016-46-5	CC1OC(Oc2c[nH]c3ccc(Br)c(Cl)c23)C(O)C(O)C1O	390.982212
D-Galacturonic acid	685-73-4	OC(C=O)C(O)C(O)C(O)C(O)=O	194.042655
D-Glucitol	50-70-4	OC(CO)C(O)C(O)C(O)CO	182.07904
D-gluco-Heptonic acid, (2?)-, ester with boric acid (H3BO3), sodium salt	58450-10-5	OCC(O)C(O)C(O)C(O)C(OB(O)O)C(O)=O	270.07583
D-gluconic acid 6-(dihydrogen phosphate)	921-62-0	OC(COP(O)(O)=O)C(O)C(O)C(O)C(O)=O	276.024637
D-gluconic acid, cyclic 4,5-ester with boric acid, calcium salt (2:1)	5743-34-0	OCC1OB(O)OC1C(O)C(O)C(O)=O	222.0547

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Table A6 (*continued*)

Name	CAS#	Smiles	Monoisotopic Mass (Da)
D-Glucose	50-99-7	OCC1OC(O)C(O)C(O)C1O	180.06339
Dhurrin	499-20-7	N#CC(OC1OC(OO)C(O)C(O)C1O)c1ccc(O)cc1	313.079769
Diazolidinyl urea	78491-02-8	OCNC(=O)N(CO)C1C(=O)N(CO)C(=O)N1CO	278.086251
Dichlorophen	97-23-4	Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O	268.005784
Dichlorprop	120-36-5	CC(Oc1ccc(Cl)cc1Cl)C(O)=O	233.985049
Diethanolamine	111-42-2	OCCNCCO	105.078979
Diethylene glycol	111-46-6	OCCOCCO	106.062995
Diethylenetriamine	111-40-0	NCCNCCN	103.110947
Digallic acid	536-08-3	OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1	322.032485
Dihydroequilin	3563-27-7	CC12CCC3c4ccc(O)cc4CC=C3C1CCC2O	270.16198
Dihydroxymethoxychlor olefin	14868-03-2	Oc1ccc(cc1)C(c1ccc(O)cc1)=C(Cl)Cl	280.005784
Dimaprit	65119-89-3	CN(C)CCCSC(N)=N	161.098667
Dimethylaminoethanol	108-01-0	CN(C)CCO	89.084064
Dimethylolurea	140-95-4	OCNC(=O)NCO	120.053493
Diphemethoxidine	13862-07-2	OCCN1CCCCC1C(c1ccccc1)c1ccccc1	295.193614
Disodium 3,4,5,6-tetraoxocyclohex-1-en-1,2-ylene dioxide	523-21-7	OC1C(=O)C(=O)C(=O)C(=O)C1=O	169.98514
Disodium 3-hydroxy-4-nitrosonaphthalene-2,7-disulphonate	525-05-3	Oc1c(N=O)c2ccc(cc2cc1S(O)(=O)=O)S(O)(=O)=O	332.961309
Disodium 3-hydroxynaphthalene-2,7-disulfonate	135-51-3	Oc1cc2ccc(cc2cc1S(O)(=O)=O)S(O)(=O)=O	303.971145
Disodium ethylenediaminediacetate	38011-25-5	OC(=O)CNCCNCC(O)=O	176.079708
DOPA sulfate	96253-55-3	NC(Cc1cc(OS(O)(=O)=O)c(O)cc1)C(O)=O	277.025624
Dopaquinone	4430-97-1	NC(CC1=CC(=O)C(=O)C=C1)C(O)=O	195.053159
Dothiepin	113-53-1	CN(C)CCC=C1c2ccccc2CSc2ccccc21	295.139469
Droxidopa	23651-95-8	NC(C(O)c1ccc(O)c(O)c1)C(O)=O	213.063724
Echinacoside	82854-37-3	CC1OC(OC2C(OC(=O)C=Cc3cc(O)c(O)cc3)C(COC3OC(CO)C(O)C(O)C3O)OC(OCCc3cc(O)c(O)cc3)C2O)C(O)C(O)C1O	786.25825
Ecopipam	112108-01-7	CN1CCc2cc(Cl)c(O)cc2C2C1CCc1ccccc12	313.123341
Ellagic acid	476-66-4	Oc1cc2c3-c4c(OC2=O)c(O)c(O)cc4C(=O)Oc3c1O	302.00627
Elliptinium	58337-34-1	Cc1c2[nH]c3ccc(O)cc3c2c(C)c2c[n+](C)ccc12	277.134088
Emiglitate	80879-63-6	CCOC(=O)c1ccc(cc1)OCCN1CC(O)C(O)C(O)C1CO	355.163104
Endrin aldehyde	7421-93-4	O=CC1CC2C3C1C1(Cl)C4(Cl)C2C4(Cl)C3(Cl)C1(Cl)Cl	377.870627
EO 9	114560-48-4	C[n]1c(C=CCO)c(CO)c2c1C(=O)C=C(C2=O)N1CC1	288.111008
Epilactose	50468-56-9	OC(CO)C(OC1OC(CO)C(O)C(O)C1O)C(O)C(O)C=O	342.116215
Eptifibatide	188627-80-7	NC(=O)C1CSSCCC(=O)NC(CCCCNC(N)=N)C(=O)NCC(=O)NC(CC(O)=O)C(=O)NC(Cc2c[nH]c3ccccc23)C(=O)N2CCCC2C(=O)N1	831.315614
Erythrose 4-phosphate	585-18-2	OC(C=O)C(O)COP(O)(O)=O	200.008592
Esculamine	2908-75-0	CC1=CC(=O)Oc2c1cc(O)c(O)c2CN(CCO)CCO	309.121239
Estriol	50-27-1	CC12CCC3C(CCc4cc(O)ccc43)C1CC(O)C2O	288.172545
Estrone	53-16-7	CC12CCC3C(CCc4cc(O)ccc43)C1CCC2=O	270.16198
ETANTEROL	93047-39-3	CC(Cc1ccc(O)cc1)NCC(O)c1cc(N)cc(CO)c1	316.178693
Ethanedithioamide, N,N'-bis(2-hydroxyethyl)-	120-86-5	OCCNC(=S)C(=S)NCCO	208.034018
Ethanolamine	141-43-5	NCCO	61.052764
Ethidium chloride (ET)	602-52-8	CC[n+]1c(c2cc(N)ccc2c2ccc(N)cc12)-c1ccccc1	314.165722
Ethylene glycol	107-21-1	OCCO	62.03678
Ethylenebis[tris(2-cyanoethyl)phosphonium] dibromide	10310-38-0	N#CCC[P+](CC[P+](CCC#N)(CCC#N)CCC#N)(CCC#N)CCC#N	414.185068
Ethylenediamine	107-15-3	NCCN	60.068748
Exifone	52479-85-3	Oc1ccc(C(=O)c2cc(O)c(O)c(O)c2)c(O)c1O	278.042655
Felypressin	56-59-7	N1([C@@H](C(N[C@@H](C(NCC(N)=O)=O)=O)CCCCN)=O)CCC1)C([C@@H]1NC([C@@H](NC([C@@H](NC([C@@H](Cc2ccccc2)NC([C@@H](NC([C@@H](CSSC1)N)=O)Cc1ccccc1)=O)=O)=O)CCC(N)=O)=O)CC(N)=O)=O)=O	1039.43679
Fenalcomine	34616-39-2	CC(Cc1ccccc1)NCCOc1ccc(cc1)C(O)CC	313.204179
Fenchlorphos	299-84-3	COP(=S)(Oc1cc(Cl)c(Cl)cc1Cl)OC	319.899733
Fenoldopam	67227-56-9	Oc1c(Cl)c2CCNCC(c2cc1O)c1ccc(O)cc1	305.081871
Fenticlor	97-24-5	Oc1ccc(Cl)cc1Sc1cc(Cl)ccc1O	285.962204
Fepradinol	63075-47-8	CC(C)(CO)NCC(O)c1ccccc1	209.141579
FERRIC (59 FE) CITRATE	54063-42-2	OC(=O)CC(O)(C(O)=O)C(O)=O	178.011355
Flurocitabine	37717-21-8	N=C1N=C2OC3C(OC(CO)C3O)N2C=C1F	243.065535
Formaldehyde, polymer with 1,3-benzenediol, [1,1′-biphenyl]-ar,ar'-diol and [1,1′-biphenyl]triol	65876-95-1	Oc1ccc(-c2ccccc2)c(O)c1O	202.062995
Formic acid	64-18-6	OC=O	46.00548
FOSCOLIC ACID	2398-95-0	CC(O)(C(O)=O)P(O)(=O)C(C)(O)C(O)=O	242.019157
FRAKEFAMIDE	188196-22-7	CC(NC(=O)C(N)Cc1ccc(O)cc1)C(=O)NC(Cc1ccc(F)cc1)C(=O)NC(Cc1ccccc1)C(N)=O	563.254398
Fuculose 1-phosphate	16562-58-6	CC1OC(OP(O)(O)=O)C(O)C(O)C1O	244.034807
Fulvic acid	479-66-3	CC1(O)CC2Oc3cc(O)c(O)c(c3C(=O)C=2CO1)C(O)=O	308.05322
Gallic acid	149-91-7	OC(=O)c1cc(O)c(O)c(O)c1	170.021525
Gamma-glutamylcysteine	636-58-8	NC(CCC(=O)NC(CS)C(O)=O)C(O)=O	250.062343
Gemcitabine	95058-81-4	NC1C=CN(C2OC(CO)C(O)C2(F)F)C(=O)N=1	263.071763
Ginkgolide-A	15291-75-5	CC(C)(C)C1CC2OC(=O)C34OC5OC(=O)C(O)C51C32CC1OC(=O)C(C)C41O	408.142035

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Table A6 (*continued*)

Name	CAS#	Smiles	Monoisotopic Mass (Da)
Ginkgolide-C	15291-76-6	CC(C)(C)C1C(O)C2OC(=O)C34OC5OC(=O)C(O)C51C32C(O)C1OC(=O)C(C)C41O	440.131865
Ginkgolide-J	107438-79-9	CC(C)(C)C1C(O)C2OC(=O)C34OC5OC(=O)C(O)C51C32CC1OC(=O)C(C)C41O	424.13695
Ginkgolide-M	15291-78-8	CC(C)(C)C1C(O)C2OC(=O)C34OC5OC(=O)C(O)C51C32C(O)C1OC(=O)C(C)C41	424.13695
Gluconolactone	90-80-2	OCC1OC(=O)C(O)C(O)C1O	178.04774
Glucose 6-(disodium phosphate)	3671-99-6	OC(COP(O)(O)=O)C(O)C(O)C(O)C=O	260.029722
Glucose-6-Phosphate	56-73-5	OC1OC(COP(O)(O)=O)C(O)C(O)C1O	260.029722
GLUFOSFAMIDE	132682-98-5	OCC1OC(OP(=O)(NCCCl)NCCCl)C(O)C(O)C1O	382.046344
Glycerol	56-81-5	OC(CO)CO	92.047345
Glycerol, propoxylated	25791-96-2	OC(COC(OCCC(O)CO)OCCC(O)CO)CO	314.157685
Glycine	56-40-6	NCC(O)=O	75.032029
Glycine, N,N'-(1,2-dithioxo-1,2-ethanediyl)bis-	95-99-8	OC(=O)CNC(=S)C(=S)NCC(O)=O	235.992548
Glycolic acid	79-14-1	OCC(O)=O	76.016045
Guanosine	118-00-3	NC1NC(=O)c2[n]c[n](C3OC(CO)C(O)C3O)c2N=1	283.09167
Guanosine-5-Diphosphate	146-91-8	NC1Nc2c([n]c[n]2C2OC(COP(O)(=O)OP(O)(O)=O)C(O)C2O)C(=O)N=1	443.024334
Helicin	618-65-5	OCC1OC(Oc2ccccc2C=O)C(O)C(O)C1O	284.089605
Hematoxylin	517-28-2	Oc1cc2C3c4ccc(O)c(O)c4OCC3(O)Cc2cc1O	302.07904
Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafl	1546-95-8	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F	345.986316
Hexahydro-1,3,5-tris(2-hydroxypropyl)-s-triazine	25254-50-6	CC(O)CN1CN(CN(C1)CC(C)O)CC(C)O	261.205242
Hexamethylolmelamine	531-18-0	OCN(CO)c1[n]c([n]c([n]1)N(CO)CO)N(CO)CO	306.128784
Hexanedioic acid	124-04-9	OC(=O)CCCCC(O)=O	146.05791
Homocitric acid	3562-74-1	OC(=O)C(O)(CC(O)=O)CCC(O)=O	206.042655
Hydromorphinol	2183-56-4	CN1CCC23C4Oc5c2c(CC1C3(O)CCC4O)ccc5O	303.147059
Hydroxyethylcellulose	9004-62-0	OCC1OC(O)C(OCCO)C(O)C1OC1OC(COCCO)C(O)C(COCCO)C1O	488.21051
HYDROXYPYRIDINE TARTRATE	7008-17-5	OC(=O)C(O)C(O)C(=O)Oc1cccc[n]1	227.042989
Hydroxystilbamidine Isethionate	533-22-2	NC(=N)C1C=CC(C=C1)=CC=C1C=CC(=CC1=O)C(N)=N	280.132411
Inosine 5-(trihydrogen diphosphate)	86-04-4	OP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1O)[n]1c[n]c2c1NC=NC2=O	428.013435
Isochorismic Acid	22642-82-6	C=C(OC1C=CC=C(C1O)C(O)=O)C(O)=O	226.04774
Isopropyl citrate	83966-24-9	CC(C)OC(=O)C(O)(CC(O)=O)CC(O)=O	234.073955
Isoquercitrin	21637-25-2	OCC(O)C1OC(OC2C(=O)c3c(cc(O)cc3O)OC=2c2cc(O)c(O)cc2)C(O)C1O	464.09548
Isoquinoline-6,7-diol, 1,2,3,4-tetrahydro-2-meth	63937-92-8	CN1Cc2cc(O)c(O)cc2CC1	179.094629
Isovalerylglucuronide	88070-93-3	CC(C)CC(=O)OC1OC(C(O)C(O)C1O)C(O)=O	278.10017
Keracyanin	18719-76-1	CC1OC(OCC2OC(Oc3cc4c(cc(O)cc4O)[o+]c3-c3cc(O)c(O)cc3)C(O)C(O)C2O)C(O)C(O)C1O	595.1663
KETORFANOL	79798-39-3	Oc1cccc2CC3C4CCC(=O)CC4(CCN3CC3CC3)c21	311.188529
Lactic acid	50-21-5	CC(O)C(O)=O	90.031695
Lactobionic acid	96-82-2	OC(CO)C(OC1OC(CO)C(O)C(O)C1O)C(O)C(O)C(O)=O	358.11113
Lactose	63-42-3	OC1OC(CO)C(OC2OC(CO)C(O)C(O)C2O)C(O)C1O	342.116215
L-Arginine	74-79-3	NC(=N)NCCCC(N)C(O)=O	174.111676
L-Ascorbic acid	50-81-7	OCC(O)C1OC(=O)C(=O)C1O	176.03209
L-Cystine	56-89-3	NC(CSSCC(N)C(O)=O)C(O)=O	240.023848
L-Dopa	59-92-7	NC(Cc1cc(O)c(O)cc1)C(O)=O	197.068809
Levallorphan	152-02-3	C=CCN1CCC23CCCCC2C1Cc1ccc(O)cc31	283.193614
L-Glutamic acid	56-86-0	NC(CCC(O)=O)C(O)=O	147.053159
Lithium carbonate	554-13-2	O=C(O[Li])O[Li]	74.01675074
Lodoxamide	53882-12-5	N#Cc1cc(NC(=O)C(O)=O)c(Cl)c(c1)NC(=O)C(O)=O	310.994514
Losigame	112856-44-7	COC1=CC(=O)OC1C(O)c1ccccc1Cl	254.034587
L-Tartaric acid	87-69-4	OC(=O)C(O)C(O)C(O)=O	150.01644
L-Threonine	72-19-5	CC(O)C(N)C(O)=O	119.058244
Maleic acid	110-16-7	OC(=O)C=CC(O)=O	116.01096
Maleylacetoacetic acid	5698-52-2	OC(=O)CC(=O)CC(=O)C=CC(O)=O	200.03209
Maltodextrin	9050-36-6	OCC(O)C(O)C(O)C(O)C=O	180.06339
MDL 11,939	107703-78-6	OC(C1CCN(CCc2ccccc2)CC1)c1ccccc1	295.193614
MDL 28574	121104-96-9	CCCC(=O)OC1CN2CCC(O)C2C(O)C1O	259.141974
Melamine	108-78-1	Nc1[n]c(N)[n]c(N)[n]1	126.065394
Melaminylthioarsenate	89141-50-4	Nc1[n]c(Nc2ccc(cc2)[As](SCCN)SCCN)[n]c(N)[n]1	428.054651
MEPROTIXOL	4295-63-0	COc1cc2c(cc1)Sc1ccccc1C2(O)CCCN(C)C	329.144949
Methanaminium, N-[4-[[4-(dimethylamino)phenyl][4-[(2-hydroxyethyl)amino]phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methyl-, acetate (salt)	82171-32-2	CN(C)c1ccc(cc1)C(c1ccc(cc1)NCCO)=C1C=CC(C=C1)=[N+](C)C	388.238887
Methanesulfonic acid	75-75-2	CS(O)(=O)=O	95.988115
Methoxyacetic acid	625-45-6	COCC(O)=O	90.031695
Methyl cellulose	9004-67-5	COCC1OC(O)C(O)C(O)C1O	194.07904
Methyl o-methoxyhippuric acid	27796-49-2	C[N+](C)(CCO)CCCC(=O)c1ccccc1	236.165054
Monomethyl phosphate	812-00-0	COP(O)(O)=O	111.992547
Monoxerutin	23869-24-1	CC1OC(OCC2OC(OC3=C(Oc4cc(cc(O)c4C3=O)OCCO)c3cc(O)c(O)cc3)C(O)C(O)C2O)C(O)C(O)C1O	654.179605
Morphine	57-27-2	CN1CCC23C4Oc5c2c(CC1C3C=CC4O)ccc5O	285.136494

(*continued on next page*)

Table A6 (*continued*)

Name	CAS#	Smiles	Monoisotopic Mass (Da)
Morphine methylbromide	125-23-5	C[N+]1(C)CCC23C4Oc5c2c(CC1C3C=CC4O)ccc5O	300.159969
Morphine-6-glucuronide	20290-10-2	CN1CCC23C4Oc5c2c(CC1C3C=CC4OC1OC(C(O)C(O)C1O)C(O)=O)ccc5O	461.168584
Morpholine	110-91-8	C1COCCN1	87.068414
Mucic acid	526-99-8	OC(=O)C(O)C(O)C(O)C(O)C(O)=O	210.03757
Myricetin	529-44-2	Oc1cc2OC(c3cc(O)c(O)c(O)c3)C(=O)C(=O)c2c(O)c1	318.03757
N-(3-acetyl-5-fluoro-2-hydroxyphenyl)-1H-tetrazole-5-carboxamide	70977-46-7	CC(=O)C1=CC(F)=CC(=NC(=O)C2NNNN=2)C1=O	265.061118
N-(3-Chloroallyl)hexaminium chloride	4080-31-3	ClC=CC[N+]12CN3CN(C1)CN(C2)C3	215.106348
N-(4-pyridinylmethyl)-4-pyridinemethanamine, 2-hydroxy-1,2,3-propanetricarboxylate	1539-39-5	C(NCc1cc[n]cc1)c1cc[n]cc1	199.110947
N-(4-sodiooxyphenyl)-p-benzoquinone monoimine	5418-32-6	Oc1ccc(cc1)N=C1C=CC(=O)C=C1	199.063329
N,N,N',N'-Tetrakis(2-Hydroxypropyl)ethylenediamine	102-60-3	CC(O)CN(CC(C)O)CCN(CC(C)O)CC(C)O	292.236208
N,N'-Bis[3-(trimethoxysilyl)propyl]ethane-1,2-diamine	68845-16-9	CO[Si](CCCNCCNCCC[Si](OC)(OC)OC)(OC)OC	384.211192
N,N-Diethylethanolamine	100-37-8	CCN(CCO)CC	117.115364
N-[3-(Trimethoxysilyl)propyl]ethane-1,2-diamine	1760-24-3	CO[Si](CCCNCCN)(OC)OC	222.13997
N-1-hydroxymethyl-2,3-dihydroxypropyl-2,2,5,5-tetramethylpyrrolidin-1-oxyl-3-carboxamide	97546-74-2	CC1(C)CC(C(=O)NC(CO)C(O)CO)C(C)(C)N1O	290.184173
N-Acetyl-P-Nitrophenylserinol	15376-53-1	CC(=O)NC(CO)C(O)c1ccc(cc1)[N+]([O-])=O	254.090273
Nadolol	42200-33-9	CC(C)(C)NCC(O)COc1cccc2CC(O)C(O)Cc21	309.194009
Nalmefene	55096-26-9	C=C1CCC2(O)C3Cc4ccc(O)c5OC1C2(CCN3CC1CC1)c45	339.183444
Neoarsphenamine	457-60-3	Nc1cc(ccc1O)[As]=[As]c1cc(NCS(O)=O)c(O)cc1	443.910616
Neopterin	2009-64-5	NC1Nc2[n]cc([n]c2C(=O)N=1)C(O)C(O)CO	253.081105
Nifuratrone	19561-70-7	[O-][N+](=O)c1ccc(C=[N+]([O-])CCO)o1	200.043323
Nitrocellulose	9004-70-0	[O-][N+](=O)OC1C(O[N+]([O-])=O)C(O)OC(CO[N+]([O-])=O)C1O	315.018627
NITROGEN	93037-13-9	NC1Nc2c([n]c(Br)[n]2C2OC(CO)C(OP(O)(O)=O)C2O)C(=O)N=1	440.968513
N-Methyldiethanolamine	105-59-9	CN(CCO)CCO	119.094629
N-methylserotonin	1134-01-6	CNCCc1c[nH]c2ccc(O)cc12	190.110613
N'-Nitrosonornicotine-1-N-oxide	78246-24-9	[O-][n+]1cc(ccc1)C1CCCN1N=O	193.085127
Norcodeine	467-15-2	COc1ccc2CC3NCCC45C(Oc1c42)C(O)C=CC53	285.136494
Normorphine	466-97-7	Oc1ccc2CC3NCCC45C(Oc1c42)C(O)C=CC53	271.120844
NSC 224131	51321-79-0	OC(=O)CC(NC(=O)CP(O)(O)=O)C(O)=O	255.014406
NULL	119179-66-7	Oc1cc2OC(=O)C=C(c2cc1Cl)C(F)(F)F	263.980106
ODAPIPAM	131796-63-9	CN1CC(c2cc(O)c(Cl)cc2CC1)c1cccc2CCOc21	329.118256
OMAPATRILAT	167305-00-2	OC(=O)C1CCCC2SCCC(NC(=O)C(S)Cc3ccccc3)C(=O)N12	408.117748
Oteracil	937-13-3	OC(=O)c1[n]c(O)[n]c(O)[n]1	157.012357
Oxalosuccinic acid	1948-82-9	OC(=O)C(=O)C(CC(O)=O)C(O)=O	190.011355
Oxalyl dichloride	79-37-8	O=C(Cl)C(=O)Cl	125.927534
OXONAZINE	5580-22-3	C=CC[N+](CC=C)(CC=C)c1[n]c(N)[n]c(N)[n]1	222.122909
Oxytocin	50-56-6	N3C(=O)C(NC(=O)C(CSSCC(C(=O)N2C(C(=O)NC(C(=O)NCC(=O)N)CC(C)C)CCC2)NC(=O)C(NC(=O)C(CCC(=O)N)NC(=O)C3C(CC)C)CC(=O)N)N)Cc1ccc(cc1)O	1006.43646
p-(1-phenylethyl)phenol	1988-89-2	CC(c1ccccc1)c1ccc(O)cc1	198.104465
PANCRATISTATIN	96203-70-2	Oc1c2OCOc2cc2C3C(NC(=O)c12)C(O)C(O)C(O)C3O	325.079769
Panobinostat	404950-80-7	Cc1[nH]c2ccccc2c1CCNCc1ccc(C=CC(=O)NO)cc1	349.179027
Peldesine	133432-71-0	NC1Nc2c(Cc3c[n]ccc3)c[nH]c2C(=O)N=1	241.09636
Pentaerythritol	115-77-5	OCC(CO)(CO)CO	136.07356
Persilic acid	4444-23-9	OS(=O)(=O)c1cc(O)c(cc1O)S(O)(=O)=O	269.95041
Phalloidin	17466-45-4	CC(O)C1NC(=O)C(C)NC(=O)C(CC(C)(O)CO)NC(=O)C2Cc3c4ccccc4[nH]c3SCC(NC1=O)C(=O)N1CC(O)CC1C(=O)NC(C)C(=O)N2	788.316327
Phenanthridinium, 3,8-diamino-5-methyl-6-phenyl-	518-67-2	C[n+]1c(c2cc(N)ccc2c2ccc(N)cc12)-c1ccccc1	300.150072
PHENOL, 2-CHLORO-4-CYCLOHEXYL-	3964-61-2	Oc1ccc(cc1Cl)C1CCCCC1	210.081142
Phenol, 4-((phenylmethyl)amino)-	103-14-0	Oc1ccc(cc1)NCc1ccccc1	199.099714
Phenol, 4,4′-(3H-2,1-benzoxathiol-3-ylidene)bis[2,6-dinitro-, S,S-dioxide	57564-54-2	[O-][N+](=O)c1cc(cc(c1O)[N+]([O-])=O)C1(OS(=O)(=O)c2ccccc12)c1cc(c(O)c(c1)[N+]([O-])=O)[N+]([O-])=O	533.996511
Phenol, 4,4′-iminobis-	1752-24-5	Oc1ccc(cc1)Nc1ccc(O)cc1	201.078979
PHENOLPHTHALOL	81-92-5	OCc1ccccc1C(c1ccc(O)cc1)c1ccc(O)cc1	306.125595
Pholcodine	509-67-1	CN1CCC23C4C=CC(O)C2Oc2c3c(CC14)ccc2OCCN1CCOCC1	398.220558
Phosmethylan	83733-82-8	CCCC(=O)N(CSP(=S)(OC)OC)c1ccccc1Cl	367.023248
Phosphonic acid, [[(2-hydroxyethyl)imino]bis(methylene)]bis-	5995-42-6	OCCN(CP(O)(O)=O)CP(O)(O)=O	249.016728
Phosphonic acid, [[bis(2-hydroxyethyl)amino]methyl]-, diethyl ester	2781-11-5	CCOP(=O)(CN(CCO)CCO)OCC	255.123561
Phosphorothioic acid, O-(dichloro(methylthio)phe	60238-56-4	CSc1ccc(OP(=S)(OC)OC)c(Cl)c1Cl	331.926426
Picrotoxin	124-87-8	CC(C)(O)C1C2C(=O)OC1C1OC(=O)C34OC3CC2(O)C41C	310.105255
Piridoxylate	24340-35-0	Cc1[n]cc(CO)c(CO)c1OC(O)C(O)=O	243.074289
Plasma protein fraction	55963-80-9	C=COCC(COP(O)(O)=O)OC=O	226.024242
Pluronic F-127	9003-11-6	CC(COCCO)OCCO	164.10486
Poly[oxy(methyl-1,2-ethanediyl)], ?-hydro-?-hydroxy-, ether with 2,2-bis(hydroxymethyl)-1,3-propanediol (4:1), 2-hydroxy-3-mercaptopropyl ether	72244-98-5	OCCCOCC(COCCCO)(COCCCO)COCCCO	368.24102

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Table A6 (*continued*)

Name	CAS#	Smiles	Monoisotopic Mass (Da)
Polyoxin	11113-80-7	NC(C=O)C1OC(C(O)C1O)N1C=C(C(=O)NC1=O)C(O)=O	315.070267
Polyoxyethylene sorbitol tetraoleate	63089-86-1	OCCOC(COCCO)C(OCCO)C(OCCO)C(COCCO)OCCO	446.23633
Polyoxypropylenediamine	9046-10-0	CC(COCCCN)COCCN	190.168128
Potassium dichloroisocyanurate	2244-21-5	OC1=NC(=O)N(Cl)C(=O)N1Cl	196.939496
potassium N-ethyl-N-[(nonafluorobutyl)sulphonyl]glycinate	67584-51-4	CCN(CC(O)=O)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	385.003031
Potassium sorbate / Sorbistat-K	24634-61-5	O[K]C(=O)C=CC=CC	151.016136
Potassium citrate	6100-05-6	O=C(CC(C(O)=O)(CC(O)=O)O)O	192.027005
Primapterin	2582-88-9	CC(O)C(O)c1c[n]c2C(=O)N=C(N)Nc2[n]1	237.08619
Propionic acid	79-09-4	CCC(O)=O	74.03678
Propyl gallate	121-79-9	CCCOC(=O)c1cc(O)c(O)c(O)c1	212.068475
Psilocin	520-53-6	CN(C)CCc1c[nH]c2cccc(O)c12	204.126263
Puberulic Acid	99-23-0	OC(=O)C1=CC(=O)C(=O)C(O)C(O)=C1	198.01644
Purpurogallin	569-77-7	Oc1c(O)cc2C=CCC(=O)C(=O)c2c1O	220.037175
Pyrazofurin	30868-30-5	NC(=O)c1[n][nH]c(C2OC(CO)C(O)C2O)c1O	259.080437
Pyridine-2-thiol 1-oxide, sodium salt	3811-73-2	n1(=O)c(S[Na])cccc1	148.9911292
Pyridoxine-5-Phosphate	447-05-2	Cc1[n]cc(COP(O)(O)=O)c(CO)c1O	249.040226
Pyrisuccideanol	33605-94-6	Cc1[n]cc(COC(=O)CCC(=O)OCCN(C)C)c(CO)c1O	340.163438
Pyrithioxine	1098-97-1	Cc1[n]cc(CSSCc2c[n]c(C)c(O)c2CO)c(CO)c1O	368.086448
Quercetin-3-glucoside	482-35-9	OCC1OC(OC2C(=O)c3c(cc(O)cc3O)OC=2c2cc(O)c(O)cc2)C(O)C(O)C1O	464.09548
Ractopamine hydrochloride	90274-24-1	CC(CCc1ccc(O)cc1)NCC(O)c1ccc(O)cc1	301.167794
Ribavirin	36791-04-5	NC(=O)c1[n][n](c[n]1)C1OC(CO)C(O)C1O	244.080771
Ribavirin Monophosphate	40925-28-8	NC(=O)c1[n][n](c[n]1)C1OC(COP(O)(O)=O)C(O)C1O	324.047103
Rribose 1-phosphate	14075-00-4	OCC1OC(OP(O)(O)=O)C(O)C1O	230.019157
Ribose-5-phosphate	3615-55-2	OC(C(O)COP(O)(O)=O)C(O)C=O	230.019157
Ribose-5-Phosphate	4151-19-3	OCC(=O)C(O)C(O)COP(O)(O)=O	230.019157
Risedronic acid	105462-24-6	OC(Cc1c[n]ccc1)(P(O)(O)=O)P(O)(O)=O	283.001078
Robinin	301-19-9	CC1OC(Oc2cc(O)c3C(=O)C(OC4OC(COC5OC(C)C(O)C(O)C5O)C(O)C(O)C4O)=C(Oc3c2)c2ccc(O)cc2)C(O)C(O)C1O	740.216385
Rutin trihydrate	153-18-4	CC1OC(OCC2OC(OC3C(=O)c4c(cc(O)cc4O)OC=3c3cc(O)c(O)cc3)C(O)C(O)C2O)C(O)C(O)C1O	610.15339
Salidroside	10338-51-9	Oc1ccc(CCOC2OC(CO)C(O)C(O)C2O)cc1	300.120905
Sedoheptulose 7-phosphate	2646-35-7	OCC(=O)C(O)C(O)C(O)C(O)COP(O)(O)=O	290.040287
Sepiapterin	17094-01-8	CC(O)C(=O)C1CNC2=NC(N)=NC(=O)C2N=1	237.08619
SEVITROPIUM MESILATE	88199-75-1	C[N+]1(C)C2CC(CC1C1OC21)OC1c2ccccc2CSc2ccccc21	380.168424
SILTENZEPINE	98374-54-0	OCCN(CC(=O)N1c2ccc(Cl)cc2NC(=O)c2ccccc12)CCO	389.114234
Sinalbin	20196-67-2	Oc1ccc(CC(=NOS(O)(=O)=O)SC2OC(CO)C(O)C(O)C2O)cc1	425.045039
SKF 77434	104422-04-0	C=CCN1CC(c2cc(O)c(O)cc2CC1)c1ccccc1	295.157229
SKF 81297	71636-61-8	Oc1c(Cl)c2CCNCC(c2cc1O)c1ccccc1	289.086956
SKF 83566	99295-33-7	CN1CC(c2cc(O)c(Br)cc2CC1)c1ccccc1	331.057175
SKF 83959 hydrobromide	67287-95-0	Cc1cc(ccc1)C1CN(C)CCc2c(Cl)c(O)c(O)cc21	317.118256
Sodium 2-(2,4,5-trichlorophenoxy)ethyl sulfate	3570-61-4	OS(=O)(=O)OCCOc1cc(Cl)c(Cl)cc1Cl	319.907976
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	54970-72-8	Oc1c(Cl)cc(Cl)cc1S(O)(=O)=O	241.920734
Sodium 4-(3,5-dichloro-4-oxocyclohexa-2,5-dienylideneamino)phenoxide	620-45-1	Oc1ccc(cc1)N=C1C=C(Cl)C(=O)C(Cl)=C1	266.985383
Sodium 6,7-dihydroxynaphthalene-2-sulphonate	135-53-5	OS(=O)(=O)c1cc2cc(O)c(O)cc2cc1	240.009245
Sodium alginate	9005-38-3	OC1OC(C(O)C(O)C1O)C(O)=O	194.042655
SOLPECAINOL	68567-30-6	CC(COc1ccccc1)NC(CO)C(O)c1ccccc1	301.167794
Sucralose	56038-13-2	OCC1OC(OC2(CCl)OC(CCl)C(O)C2O)C(O)C(O)C1Cl	396.014551
Sucrose	57-50-1	OC1C(OC(CO)C(O)C1O)OC1(CO)OC(CO)C(O)C1O	342.116215
Sulmarin	29334-07-4	CC1=CC(=O)Oc2cc(OS(O)(=O)=O)c(cc21)OS(O)(=O)=O	351.95589
Sydnophen	22293-47-6	CC(Cc1ccccc1)[N+]1=CC(=N)ON1	204.113687
Tagetitoxin	87913-21-1	CC(=O)OC1C2OC(CSC2(O)C(N)=O)(C(OP(O)(O)=O)C1N)C(O)=O	416.02907
Taxifolin	480-18-2	OC1C(Oc2cc(O)cc(O)c2C1=O)c1cc(O)c(O)cc1	304.058305
TCPSA	65600-62-6	OS(=O)(=O)CC(Cl)=C(Cl)Cl	223.886846
Terbutaline	23031-25-6	CC(C)(C)NCC(O)c1cc(O)cc(O)c1	225.136494
Tetraacetylethylenediamine	10543-57-4	CC(=O)N(CCN(C(C)=O)C(C)=O)C(C)=O	228.111008
Tetraethylenepentamine	112-57-2	NCCNCCNCCNCCN	189.195345
tetrahydro-1,3,4,6-tetrakis(hydroxymethyl)imidazo[4,5-d]imidazole-2,5(1H,3H)-dione	5395-50-6	OCN1C2C(N(CO)C(=O)N2CO)N(CO)C1=O	262.091336
Tetrahydro-1,3,6-thiadiazepine-2,7-dithione	5782-83-2	S=C1NCCNC(=S)S1	177.969308
Tetrasodium iminidisuccinate	144538-83-0	OC(=O)CC(NC(CC(O)=O)C(O)=O)C(O)=O	249.048469
Tetronic 701	11111-34-5	CC(CN(CC(C)OCCO)CCN(CC(C)OCCO)CC(C)OCCO)OCCO	468.341068
Tetroquinone	319-89-1	OC1C(=O)C(=O)C(O)C(=O)C1=O	172.00079
Theaflavin	4670-05-7	OC1C=C(C2Oc3cc(O)cc(O)c3CC2O)C2=CC(=CC(=O)C(=O)C2C=1O)C1Oc2cc(O)cc(O)c2CC1O	564.12678
Theaflavin-3-gallate	28543-07-9	OC1Cc2c(cc(O)cc2O)OC1C1C=C2C(C(=O)C(=O)C=1)C(O)=C(O)C=C2C1Oc2cc(O)cc(O)c2CC1OC(=O)c1cc(O)c(O)c(O)c1	716.13774
THIACETARSAMIDE SODIUM	14433-82-0	NC(=O)c1ccc(cc1)[As](SCC(O)=O)SCC(O)=O	376.937283
Tiaramide	32527-55-2	OCCN1CCN(CC1)C(=O)CN1c2cc(Cl)ccc2SC1=O	355.075739

(*continued on next page*)

Table A6 (*continued*)

Name	CAS#	Smiles	Monoisotopic Mass (Da)
TIFLOREX	53993-67-2	CCNC(C)Cc1cc(ccc1)SC(F)(F)F	263.095553
Tiron	149-45-1	Oc1cc(cc(c1O)S(O)(=O)=O)S(O)(=O)=O	269.95041
Toyocamycin	606-58-6	Nc1[n]c[n]c2c1c(c[n]2C1OC(CO)C(O)C1O)C#N	291.096755
trans-4-hydroxystilbene	6554-98-9	Oc1ccc(cc1)C=Cc1ccccc1	196.088815
Trehalose-6-phosphate	4484-88-2	OCC1OC(OC2OC(COP(O)(O)=O)C(O)C(O)C2O)C(O)C(O)C1O	422.082547
Triethanolamine	102-71-6	OCCN(CCO)CCO	149.105194
Triethylene glycol	112-27-6	OCCOCCOCCO	150.08921
Triethylenetetramine	112-24-3	NCCNCCNCCN	146.153146
Trihydroxybiphenyl	29222-39-7	Oc1ccc(cc1)-c1cc(O)cc(O)c1	202.062995
Triisopropanolamine	122-20-3	CC(O)CN(CC(C)O)CC(C)O	191.152144
Trimethoquinol	18559-59-6	COc1c(cc(CC2NCCc3cc(O)c(O)cc32)cc1OC)OC	345.157624
Trimethyl(2-propionylthioethyl)ammonium chloride	1866-73-5	CCC(=O)SCC[N+](C)(C)C	176.110909
Tris[(dimethylamino)methyl]phenol	26444-72-4	CN(C)Cc1c(CN(C)C)c(O)ccc1CN(C)C	265.215412
Trisodium 5-[(3-carboxylato-5-methyl-4-oxo-2,5-cyclohexadien-1-ylidene)(2,6-dichloro-3-sulphonatophenyl)methyl]-2-hydroxy-3-methylbenzoate	1667-99-8	Cc1cc(cc(c1O)C(O)=O)C(c1c(Cl)c(ccc1Cl)S(O)(=O)=O)=C1C=C(C(=O)C(C)=C1)C(O)=O	537.989209
Trisodium 7-[[2-[(aminocarbonyl)amino]-4-[[4-fluoro-6-[(2-methylphenyl)amino]-1,3,5-triazin-2-yl]amino]phenyl]azo]naphthalene-1,3,6-trisulphonate	63817-39-0	Cc1ccccc1Nc1[n]c(F)[n]c(Nc2cc(NC(N)=O)c(cc2)N=Nc2cc3c(cc(cc3cc2S(O)(=O)=O)S(O)(=O)=O)S(O)(=O)=O)[n]1	747.063579
Trisodium citrate	68-04-2	OC(=O)C(O)(CC(O)=O)CC(O)=O	192.027005
Trisodium ethylenediaminetriacetate	19019-43-3	OC(=O)CNCCN(CC(O)=O)CC(O)=O	234.085188
Tritac	1861-44-5	CC(O)COCc1c(Cl)c(Cl)ccc1Cl	267.982461
Tromethamine	77-86-1	NC(CO)(CO)CO	121.073894
Troxerutin	7085-55-4	CC1OC(OCC2OC(OC3C(=O)c4c(cc(cc4O)OCCO)OC=3c3cc(OCCO)c(cc3)OCCO)C(O)C(O)C2O)C(O)C(O)C1O	742.232035
Tubercidin	69-33-0	Nc1[n]c[n]c2c1cc[n]2C1OC(CO)C(O)C1O	266.101506
UK-373911	291305-06-1	CNC1CCC(c2ccc(cc21)S(N)(=O)=O)c1cc(Cl)c(Cl)cc1	384.046602
Urea	57-13-6	NC(N)=O	60.032363
Uridine-5-diphosphate	58-98-0	OP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1O)N1C=CC(=O)NC1=O	404.002202
Urochloralic Acid	97-25-6	OC1C(O)C(OC(OCC(Cl)(Cl)Cl)C1O)C(O)=O	323.957036
Vacciniin	90-75-5	OC1OC(COC(=O)c2ccccc2)C(O)C(O)C1O	284.089605
Vanillactic acid	2475-56-1	COc1cc(CC(O)C(O)=O)ccc1O	212.068475
Xanthosine	146-80-5	OCC1OC(C(O)C1O)[n]1c[n]c2c1NC(=O)NC2=O	284.075686
Xanthosine monophosphate	523-98-8	OC1C(COP(O)(O)=O)OC(C1O)[n]1c[n]c2c1NC(=O)NC2=O	364.042018
Xylitol	87-99-0	OC(C(O)CO)C(O)CO	152.068475
Zelandopam	139233-53-7	Oc1c2CNCC(c2ccc1O)c1cc(O)c(O)cc1	273.100109
Zincpyrithione	13463-41-7	c2(n(cccc2)=O)S[Zn]Sc1n(cccc1)=O	315.931863
Zoledronate	118072-93-8	OC(C[n]1c[n]cc1)(P(O)(O)=O)P(O)(O)=O	271.996327

Table A7
All 208 detected features (175 unique suspects) in the raw (section a) and drinking water (section b) samples from all DWTPs (n = 13). 0=No detection in the triplicate, 1=one detection, 2=two detections, "number"= average response (area) of the three detections.

a)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Raw Water	China - 2 - Raw Water	Sweden - Raw Water	Spain - Raw Water	Czech Republic - Raw Water	Netherlands - Raw Water	Switzerland - Raw Water	Germany - Raw Water	Italy - 2 - Raw Water	Vietnam - Raw Water	Italy - 1 - Raw Water	Belgium - Raw Water	Japan - Raw Water
(1-Methylethyl) dihydrogen 2-hydroxypropane-1,2,3-tricarboxylate	+	5,98	234,0740	22278	0	0	0	0	0	0	0	0	0	0	0	0
(p-ammoniophenyl)ethyl(2-hydroxyethyl)ammonium sulphate	+	3,07	180,1263	0	0	0	3125	0	0	0	0	0	0	0	0	0
(R)-N-Methylsalsolinol	-	3,30	193,1103	0	3062	0	0	0	0	0	0	0	0	0	0	0
(R)-S-(2-amino-2-carboxyethyl)-L-homocysteine	+	4,77	222,0674	9344	24548	0	5947	0	0	0	0	10635	27311	0	0	4170
?-Hydroxy-o-tolyl ?-D-glucopyranoside	-	0,60	286,1053	2315	2541	4223	0	2908	2	1	5782	1	10018	3087	5066	5453
[R(R*,R*]-2-amino-1-[p-(methylsulphonyl)phenyl]propane-1,3-diol	+	2,82	245,0722	0	0	0	10117	0	0	0	0	0	0	0	0	0
1-(2,4-Dinitrophenyl)pyridinium chloride	-	0,51	246,0515	1	0	0	2070	3035	0	0	0	1	1	0	0	0
1,3-Benzenedimethanamine	+	2,73	136,1000	4071	0	0	0	0	0	0	0	0	0	0	0	0
1,3-Benzenedisulfonic acid, 4-hydroxy-	-	5,02	253,9555	1187	0	0	0	0	0	0	0	0	0	0	0	0
1,4-BENZENDIOL, 2-(PHENYLMETHYL)-	+	8,61	200,0837	0	0	0	3392	0	0	0	0	0	0	0	0	0
17-Alpha-estradiol	-	3,26	272,1776	0	0	0	0	0	0	0	0	2473	0	0	0	0
17-Alpha-estradiol	+	12,53	272,1776	0	0	0	281112	0	0	0	0	0	0	0	0	41704
1-methoxy-4-(1,2,2,2-tetrachloroethyl)benzene	-	4,52	271,9329	0	0	0	3052	0	0	0	0	0	1844	0	0	2872
1-Propanol, 3,3′,3′′-phosphinylidynetris-	+	0,65	224,1177	0	0	0	0	0	0	161169	0	0	1	0	0	0
1-Propanol, 3,3′,3′′-phosphinylidynetris-	+	12,38	224,1177	0	0	0	6143	0	0	0	0	0	1	0	0	0
2-(4-Hydroxybenzyl)phenol	+	8,61	200,0837	0	0	0	3392	0	0	0	0	0	0	0	0	0
2,4,4′-Trihydroxybenzophenone	-	2,35	230,0579	0	0	2234	0	0	0	0	1	0	0	0	0	0
2,4,4′-Trihydroxybenzophenone	+	5,29	230,0579	4412	4834	1	0	0	0	0	0	0	0	0	0	0
2,5-Pyrrolidinedione, 1-[2-[[2-[[2-[(2-aminoethyl)amino]ethyl]amino]ethyl]amino]ethyl]-, monopolyisobutenyl derivs.	+	5,90	325,2478	40539	27310	0	0	0	0	0	0	0	0	0	0	0
2-Chloro-9-[3-(dimethylamino)propyl]thioxanthen-9-ol	+	9,06	333,0954	0	0	2753	0	0	0	0	0	0	0	0	2556	0

(*continued on next page*)

Table A7 (*continued*)

a)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Raw Water	China - 2 - Raw Water	Sweden - Raw Water	Spain - Raw Water	Czech Republic - Raw Water	Netherlands - Raw Water	Switzerland - Raw Water	Germany - Raw Water	Italy - 2 - Raw Water	Vietnam - Raw Water	Italy - 1 - Raw Water	Belgium - Raw Water	Japan - Raw Water
2-Deoxyinosine	+	5,08	252,0859	0	0	0	21647	8693	9211	1	0	2	0	2	8264	2
2-Furanmethanol, 2-formate	+	2,82	206,0790	0	0	0	14860	8166	0	8419	0	1	0	2	10344	12495
3-(2-Aminoethyl)indol-5-ol	+	2,15	176,0950	110827	195846	50619	170670	70393	18583	37364	1	68690	168520	55028	112031	132329
3-Benzylsydnone-4-acetamide	+	8,29	234,0879	0	1	0	11398	0	0	0	0	0	0	0	0	0
3-HYDROXY-4-OXO-4H-PYRAN-2,6-DICARBOXYLIC ACID	-	0,47	199,9957	0	0	1	0	1533	0	0	5822	1	2446	0	1	0
3-O-Ethylascorbic acid	-	0,51	204,0634	1	0	1	0	1	0	0	3030	0	2	0	1	2
4-((Dimethylamino)methyl)phenol	+	1,55	151,0997	0	5377	0	1	0	0	0	0	0	1	0	0	0
4-((Dimethylamino)methyl)phenol	+	1,24	151,0997	0	3678	0	0	0	0	0	0	0	0	0	0	0
4,4′-Dihydroxydiphenyl ether	-	3,71	202,0630	0	0	0	1325	0	0	0	0	0	17300	0	0	0
4,4-Dithiobis[2-aminobutyric] acid	-	0,50	268,0551	0	0	1467	0	2	0	0	2	0	2	0	1	0
4,4-Iminodianiline	+	8,50	199,1109	2584	13165	0	7147	0	0	0	0	26479	3254	0	135201	0
4,4′-Propane-1,1-diyldiphenol	-	4,43	228,1150	0	0	0	4693	0	0	0	0	0	0	0	0	4890
4,4′-Thiodibenzene-1,3-diol	-	4,79	250,0300	1574	5437	0	6426	0	0	0	0	3219	4664	0	2010	1707
4-Amino-4′-hydroxybiphenyl	-	4,43	185,0841	0	0	0	0	0	0	0	0	0	1330	0	0	0
4-Amino-4′-hydroxybiphenyl	+	2,84	185,0841	0	0	0	19784	0	0	1	0	0	0	0	0	0
4-Benzylphenol	-	3,34	184,0888	0	0	0	1465	0	0	0	0	0	0	0	0	1889
4-Cyclohexylphenol	-	2,62	176,1201	0	0	0	0	0	0	0	0	0	0	0	0	0
4-Hydroxybenzophenone	-	3,69	198,0681	0	3898	0	0	0	0	0	0	0	1	0	0	0
4-hydroxyphenylpyruvic acid	-	1,88	180,0423	2	0	0	5290	1	0	0	1	11299	2	1	8439	0
4-Hydroxyphenylpyruvic acid	-	1,98	180,0423	9548	2	3397	5290	3486	5329	1	1	11299	7051	2	8439	4380
4-Phenylphenol	-	3,86	170,0732	0	1	1499	11263	1185	1	1	3405	2846	2235	1230	2	1307
5-Amino-3-sulfosalicylic acid	-	8,68	232,9994	3097	1943	0	0	0	0	0	0	0	0	0	0	0
5-Amino-3-sulfosalicylic acid	-	3,35	232,9994	9679	49092	2	0	2919	0	2342	3082	5497	36130	1492	10550	52786
5-Fluorouridine	-	2,92	262,0601	0	0	0	0	0	0	0	0	0	0	1476	2	0
5H-Thiachromine-8-ethanol, 2,7-dimethyl-	+	1,89	262,0888	3844	0	0	10680	2	0	0	0	1	0	0	0	2
6a,7-dihydro-3,4,6a,10-tetrahydroxybenz[b]indeno[1,2-d]pyran-9(6H)-one	+	3,59	300,0634	0	6224	0	0	0	0	0	0	0	1	0	0	0
7-Aminonaphthalene-1,3,6-trisulphonic acid	-	6,59	382,9439	0	0	0	0	0	0	0	0	0	0	0	0	0
8-Hydroxyguanosine	-	3,70	299,0866	0	0	0	0	0	0	0	0	0	2389	0	0	0
9-Deazainosine	+	4,74	267,0855	4790	0	0	0	0	0	0	0	0	0	0	0	0
Acetophenazine	+	3,96	411,1980	127037	103383	184825	205768	253364	0	29361	228174	2	2	66761	31841	32018
Acetophenazine	+	3,70	411,1980	1	103785	177210	109165	233448	0	0	2	2	2	66104	1	0
ACETRYPTINE	+	4,95	202,1106	77468	41154	0	0	0	130227	0	0	0	1	0	0	0
Alcohols, C13-15, ethoxylated	+	4,70	261,2093	0	0	0	0	0	0	0	0	0	0	0	0	19222
Alginic acid	-	6,26	398,1060	1455	0	0	0	0	0	0	0	0	0	0	0	0
Alloxantin	-	3,84	286,0186	0	0	0	0	0	0	0	0	0	0	0	0	0
Aminoimidazole ribotide	+	0,54	295,0569	4033	0	0	0	0	0	0	0	0	0	0	0	0
Amiterol	+	2,22	208,1576	8475	11556	0	9385	0	5418	0	0	0	1	2	3899	9704
Amiterol	+	3,28	208,1576	0	2	0	1	0	0	0	0	0	1	2	1	3898
AMMONIUM ZIRCONIUM HYDROXY CITRATE	+	6,17	208,0219	0	0	0	5458	0	0	0	0	0	0	0	0	0

(*continued on next page*)

Table A7 (*continued*)

a)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Raw Water	China - 2 - Raw Water	Sweden - Raw Water	Spain - Raw Water	Czech Republic - Raw Water	Netherlands - Raw Water	Switzerland - Raw Water	Germany - Raw Water	Italy - 2 - Raw Water	Vietnam - Raw Water	Italy - 1 - Raw Water	Belgium - Raw Water	Japan - Raw Water
Anthrarobin	-	3,80	226,0630	2	2	0	2	2261	0	0	0	1612	8398	0	2	2
Anthrarobin	+	7,17	226,0630	0	0	0	0	0	0	0	0	0	5843	0	0	0
Aphidicolin	-	5,17	338,2457	0	0	0	0	0	0	0	0	0	5990	0	3447	0
Aphidicolin	-	5,37	338,2457	21572	20383	0	2	3244	0	0	0	0	0	0	0	0
Aphidicolin	-	6,05	338,2457	44456	28605	1537	11817	7872	0	0	1874	3557	2988	4848	9209	4666
Aphidicolin	+	10,27	338,2457	232039	123966	0	2	2	0	0	0	0	0	25479	0	0
Arbutin	+	0,65	272,0896	0	0	0	0	0	0	0	0	0	0	0	0	0
Asperuloside	-	0,60	414,1162	1	0	1	0	0	0	0	4260	0	2	0	1	0
Asperuloside	+	4,88	414,1162	13167	10537	38558	0	0	0	0	0	0	14779	9225	0	0
Azidamfenicol	-	5,70	296,0995	0	0	0	10120	0	0	0	0	0	0	0	0	0
Benaxibine	-	3,26	269,0899	0	0	0	1659	0	0	0	0	0	0	0	0	0
Benaxibine	+	4,93	269,0899	0	0	0	22817	5854	0	2732	0	0	0	0	0	2
benzyl(3-chloro-2-hydroxypropyl)dimethylammonium chloride	-	4,43	228,1155	0	0	0	4693	0	0	0	0	0	0	0	0	4890
Benzylmorphine	+	9,18	375,1834	0	0	0	22393	1	0	0	0	0	0	0	0	16567
Bergenin	-	0,62	328,0794	0	0	0	0	0	0	0	0	0	0	0	0	0
Biflorin	-	0,62	354,0951	2	2	2	0	3479	1810	1	4935	1	4551	1	2258	1
Bipenamol	-	3,67	245,0874	0	1532	0	0	0	0	0	2332	0	0	0	2	0
Butanedioic acid, [(ethoxythioxomethyl)thio]-	-	0,64	237,9970	2594	0	0	1	0	0	0	1	3951	0	0	0	0
Butanedioic acid, 2,3-dihydroxy- R-(R*,R*) -, m	-	0,51	178,0477	0	0	0	0	0	0	0	1929	0	0	0	0	1
C6-galactose mustard	+	7,79	303,0640	0	0	0	2643	0	0	0	0	0	0	0	0	0
Caftaric acid	+	10,06	312,0481	8918	28847	0	0	0	0	0	0	0	11395	0	0	0
Carboxymethyl cellulose	-	5,84	238,0689	0	0	0	2	0	2165	0	0	2	0	1	2	0
Chloralose	+	5,34	307,9621	6304	0	0	0	0	0	0	0	0	0	0	0	0
Chlorogenic acid	-	0,60	354,0951	2	2	3394	0	3479	1810	1	4935	1	4551	1	2258	1
Cianidanol	-	0,60	290,0790	0	1434	0	0	0	2	2	2	1	1	2	2	1119
Cianidanol	+	5,13	290,0790	0	0	0	0	0	4646	0	0	0	0	0	0	0
Citric acid, monoester with glycerol	+	4,25	266,0638	0	0	0	21413	0	0	0	0	0	0	0	0	0
Cyclouridine	-	4,28	226,0590	3550	13127	0	1	0	0	0	1184	1787	2	1430	0	2601
Desethylhydroxychloroquine	+	9,83	307,1451	18667	64467	0	5303	4273	0	0	0	9997	13461	0	12961	34141
Dexelvucitabine	+	7,12	227,0706	9558	86174	0	0	0	0	0	0	0	0	0	0	0
Dezocine	+	9,43	245,1780	0	0	0	5583	0	0	0	0	0	0	0	0	0
Dezocine	+	6,91	245,1780	0	2275	0	0	0	0	0	0	0	0	0	0	0
D-gluco-Heptonic acid, (2?)-, ester with boric acid (H3BO3), sodium salt	-	0,51	270,0758	0	0	1887	0	2445	0	0	3769	0	2335	0	0	1
D-gluconic acid 6-(dihydrogen phosphate)	+	7,77	276,0246	1	0	0	1	0	1	0	0	5414	0	2	0	1
D-gluconic acid, cyclic 4,5-ester with boric acid, calcium salt (2:1)	+	5,01	222,0547	35908	31196	0	0	0	13626	0	0	0	0	0	0	6559
D-Glucose	+	2,22	180,0634	0	0	0	2	12237	0	0	0	10178	9468	1	1	13814
Dhurrin	-	3,71	313,0798	2	6580	1	0	0	0	0	1	0	0	0	0	0
Dhurrin	+	4,60	313,0798	6530	0	0	0	0	0	0	0	0	0	0	0	0
Dichlorprop	-	4,30	233,9850	0	0	0	0	0	0	0	0	0	0	0	0	0

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Table A7 (*continued*)

a)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Raw Water	China - 2 - Raw Water	Sweden - Raw Water	Spain - Raw Water	Czech Republic - Raw Water	Netherlands - Raw Water	Switzerland - Raw Water	Germany - Raw Water	Italy - 2 - Raw Water	Vietnam - Raw Water	Italy - 1 - Raw Water	Belgium - Raw Water	Japan - Raw Water
Digallic acid	-	0,47	322,0325	0	0	0	0	0	0	0	2	0	3072	0	0	0
Dihydroequilin	+	11,65	270,1620	0	0	0	0	0	0	0	0	0	0	0	0	3471
Dimaprit	+	0,64	161,0987	0	0	0	0	0	4795	0	0	0	0	0	0	0
Disodium 3-hydroxy-4-nitrosonaphthalene-2,7-disulphonate	-	5,60	332,9613	0	0	0	0	0	27987	0	0	0	0	0	0	0
Disodium ethylenediaminediacetate	+	6,90	176,0797	119369	542418	38968	6903020	33305	0	48646	11119	26580	29597	27921	87130	255492
DOPA sulfate	-	3,47	277,0256	1843	8414	0	0	0	0	0	0	0	2	0	0	3544
Dopaquinone	-	3,76	195,0532	0	3181	0	0	0	0	0	0	0	0	0	0	2
EO 9	-	3,89	288,1110	0	0	0	0	0	0	0	0	0	0	0	9822	0
Epilactose	-	7,37	342,1162	0	0	0	3111	0	0	4777	0	0	0	0	9785	0
Eptifibatide	+	7,86	831,3156	1	0	0	0	0	0	0	0	0	0	3538	0	0
Estriol	+	6,36	288,1725	30247	107539	41687	0	165177	2	11524	62434	12811	122367	0	152441	1
Estriol	+	5,76	288,1725	1	2	0	25257	26598	0	0	75710	27068	165110	0	0	25531
ETANTEROL	+	6,15	316,1787	0	0	0	0	0	0	0	0	0	0	0	0	0
Ethidium chloride (ET)	+	7,24	314,1657	0	0	0	0	0	0	0	0	0	0	0	0	22402
Exifone	-	3,29	278,0427	0	0	3330	0	0	0	0	2	0	8673	0	0	0
Felypressin	-	15,80	1039,4368	0	0	0	0	0	0	0	0	0	0	2	0	0
Fenoldopam	+	4,06	305,0819	0	0	0	8755	0	0	0	0	0	0	0	0	0
Fepradinol	+	6,83	209,1416	0	0	0	0	0	0	0	0	0	0	0	0	0
Formaldehyde, polymer with 1,3-benzenediol, [1,1′-biphenyl]-ar,ar'-diol and [1,1′-biphenyl]triol	+	5,39	202,0630	0	0	18315	0	0	0	0	12052	0	2	0	0	0
Fulvic acid	-	0,51	308,0532	0	0	1	0	1	0	0	2	0	3465	0	0	0
Gamma-glutamylcysteine	-	4,50	250,0623	0	16544	0	0	0	0	0	0	0	0	0	0	0
Gamma-glutamylcysteine	-	4,67	250,0623	0	16544	0	0	0	0	0	0	0	0	0	0	0
Gamma-glutamylcysteine	+	5,93	250,0623	0	1	0	4056	0	0	0	0	0	0	0	0	0
Gemcitabine	+	4,79	263,0718	3195	0	0	0	0	0	0	0	0	0	0	0	0
Ginkgolide-A	-	0,60	408,1420	2	3928	2	0	2	4368	2	7014	2155	6513	3139	4093	2610
Ginkgolide-A	+	2,13	408,1420	0	4379	0	6647	28820	0	0	0	0	8788	0	0	1
Ginkgolide-C	-	0,61	440,1319	1126	1	1	0	1	2	1	4338	1	2	2	1	1324
Ginkgolide-J	-	0,61	424,1369	2	2630	4201	0	4078	2	2	6325	2	5065	1961	3720	2138
Ginkgolide-M	-	0,60	424,1369	2	2630	4201	0	4078	2	2	6325	2	5065	1961	3720	2138
Gluconolactone	-	0,49	178,0477	0	0	0	0	0	0	0	1929	0	0	0	0	1
GLUFOSFAMIDE	-	6,19	382,0463	0	0	0	0	0	2171	0	0	0	0	0	0	0
Glycine, N,N'-(1,2-dithioxo-1,2-ethanediyl)bis-	-	2,44	235,9925	0	59361	0	0	0	0	0	0	0	0	0	0	0
Guanosine	+	5,41	283,0917	0	0	0	6270	0	0	0	0	0	0	0	0	0
Helicin	-	0,60	284,0896	2	1749	2	0	2145	1489	2	5063	1	6535	1386	3039	2416
Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafl	-	5,39	345,9863	1187	4649	0	0	0	0	0	0	0	0	2	1	0

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Table A7 (*continued*)

a)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Raw Water	China - 2 - Raw Water	Sweden - Raw Water	Spain - Raw Water	Czech Republic - Raw Water	Netherlands - Raw Water	Switzerland - Raw Water	Germany - Raw Water	Italy - 2 - Raw Water	Vietnam - Raw Water	Italy - 1 - Raw Water	Belgium - Raw Water	Japan - Raw Water
Hexamethylolmelamine	+	0,66	306,1288	0	0	1	0	0	0	0	0	0	0	0	0	0
Hexanedioic acid	-	0,49	146,0579	0	0	0	0	0	0	0	2255	0	2487	1226	2	2
Hydroxystilbamidine Isethionate	+	8,06	280,1324	0	0	32202	0	0	0	0	0	0	0	0	0	0
Isochorismic Acid	-	0,49	226,0477	0	0	0	0	1	0	0	1887	0	2249	0	0	0
Isochorismic Acid	+	3,32	226,0477	0	0	0	2869	0	0	0	0	0	0	0	0	0
Isopropyl citrate	+	5,98	234,0740	22278	0	0	0	0	0	0	0	0	0	0	0	0
Isoquinoline-6,7-diol, 1,2,3,4-tetrahydro-2-meth	+	5,23	179,0946	0	37012	0	0	0	0	0	0	0	0	0	0	0
Lactobionic acid	+	5,35	358,1111	16918	0	0	0	0	0	0	0	0	0	0	0	0
Lactose	-	7,37	342,1162	0	0	0	3111	0	0	4777	0	0	0	0	9785	0
L-Dopa	-	2,69	197,0688	1	10415	0	0	0	0	0	0	0	2662	0	0	2480
Levallorphan	+	7,16	283,1936	0	0	0	11410	0	0	0	0	0	0	0	0	0
L-Glutamic acid	+	6,90	147,0532	0	0	0	8553	0	0	0	0	0	0	0	0	0
Lodoxamide	-	5,46	310,9945	0	0	0	2466	0	0	0	0	0	0	0	0	0
Maleylacetoacetic acid	-	3,13	200,0321	1792	1	0	0	0	0	0	0	0	0	0	0	0
Maltodextrin	+	2,49	180,0634	0	0	2	0	0	0	0	0	0	0	0	6710	0
MDL 28574	+	7,48	259,1420	16500	0	0	0	0	0	0	0	0	0	0	0	0
Methanaminium, N-[4-[[4-(dimethylamino)phenyl][4-[(2-hydroxyethyl)amino]phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methy	+	8,59	388,2389	0	0	0	1	0	0	0	0	0	0	0	0	129267
Morphine	+	6,93	285,1365	0	0	0	0	0	0	0	0	0	0	0	0	0
Morphine methylbromide	+	4,92	300,1600	0	2	0	1353631	0	0	0	0	0	0	0	0	1
N-(3-Chloroallyl)hexaminium chloride	+	7,51	215,1063	0	0	0	16204	0	0	0	0	0	0	0	0	0
N,N,N',N'-Tetrakis(2-Hydroxypropyl)ethylenediamine	-	4,18	292,2362	0	0	0	3258	0	0	0	0	0	0	0	0	0
Nadolol	-	4,51	309,1940	0	0	0	0	0	0	0	0	0	0	0	0	0
Nitrocellulose	-	3,45	315,0186	4006	7386	0	0	0	0	0	0	0	10159	0	0	0
Nitrocellulose	+	4,94	315,0186	2797	4391	0	0	0	0	0	0	0	3774	0	0	0
N'-Nitrosonornicotine-1-N-oxide	+	4,86	193,0851	1	2	2	0	3382	0	0	0	0	0	2	0	0
Norcodeine	+	9,24	285,1365	0	0	0	29209	2	0	0	0	0	12238	0	0	4390
Normorphine	-	2,89	271,1208	0	0	0	0	0	0	0	0	0	1814	0	0	0
OXONAZINE	-	3,87	222,1229	2	0	0	2	1	0	0	0	1	2	0	2	0
p-(1-phenylethyl)phenol	-	5,97	198,1045	0	1	0	2040	0	0	0	0	0	11078	0	0	5477
PANCRATISTATIN	-	3,75	325,0798	0	1513	0	0	0	0	0	0	0	0	0	0	0
Phenanthridinium, 3,8-diamino-5-methyl-6-phenyl-	+	6,90	300,1501	2	2	0	0	0	0	1	0	13208	0	2	0	2
Phenol, 4,4′-iminobis-	+	6,05	201,0790	0	2	0	0	0	0	0	0	2	0	1	0	37252
PHENOLPHTHALOL	+	9,56	306,1256	3331	2	2	5818	2813	0	0	0	0	2	0	6498	2
Phosphonic acid, [[(2-hydroxyethyl)imino]bis(methylene)]bis-	+	4,41	249,0167	0	6086	0	0	0	0	0	0	0	0	0	0	0
Picrotoxin	-	3,83	310,1053	28351	5204	0	4591	1	0	0	1	2	0	1	0	0

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Table A7 (*continued*)

a)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Raw Water	China - 2 - Raw Water	Sweden - Raw Water	Spain - Raw Water	Czech Republic - Raw Water	Netherlands - Raw Water	Switzerland - Raw Water	Germany - Raw Water	Italy - 2 - Raw Water	Vietnam - Raw Water	Italy - 1 - Raw Water	Belgium - Raw Water	Japan - Raw Water
Picrotoxin	+	0,67	310,1053	0	0	1	0	0	0	0	0	0	0	0	0	0
Plasma protein fraction	-	2,89	226,0242	8774	20853	0	0	0	0	1	2517	6055	0	2	2	3707
Potassium citrate	-	0,51	192,0270	0	0	0	0	1	0	3966	2	0	0	1	0	0
Propyl gallate	-	4,37	212,0685	0	0	0	0	0	0	0	0	2535	0	0	0	0
Puberulic acid	-	0,49	198,0164	2	0	2449	0	3042	2	0	6519	1	6872	1	2137	2
Purpurogallin	-	1,54	220,0372	0	0	0	0	0	0	0	0	2148	2	0	0	0
Purpurogallin	-	2,52	220,0372	0	0	1	0	1	0	0	0	0	7867	0	0	0
Pyrazofurin	+	4,58	259,0804	0	0	0	0	1	1	0	1	1	0	1	0	0
Ractopamine hydrochloride	-	6,09	301,1678	1	1893	7164	0	0	0	0	0	0	0	0	0	0
Ribavirin monophosphate	-	0,50	324,0471	0	0	0	0	2	0	0	2445	0	3443	0	0	0
Ribavirin monophosphate	+	6,71	324,0471	1	2	0	1	0	0	0	1	2	2	1	1	1
Risedronic acid	-	10,06	283,0011	0	0	0	0	0	0	0	0	0	1033	0	0	0
Robinin	-	8,10	740,2164	0	0	0	2407	0	0	0	0	0	0	0	0	1129
Salidroside	-	0,60	300,1209	2369	2886	2	0	3202	2224	2	6963	2	9196	3103	5141	4717
Salidroside	+	0,65	300,1209	0	0	0	0	0	0	0	0	0	0	0	0	0
Sedoheptulose 7-phosphate	+	3,13	290,0403	0	0	0	8372	0	0	0	0	0	0	0	0	0
SEVITROPIUM MESILATE	+	9,95	380,1684	0	0	0	24280	2	0	0	0	0	0	0	0	0
SKF 77434	+	10,43	295,1572	0	0	0	0	0	14310	0	0	14713	2	0	0	0
SKF 81297	+	4,28	289,0870	0	0	0	15081	2	1	0	0	0	0	0	0	0
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	-	4,06	241,9207	1	2052	0	0	0	0	0	0	0	0	0	0	0
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	-	2,47	241,9207	7662	0	0	0	0	0	0	0	0	1	0	0	0
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	-	4,26	241,9207	5733	3222	0	2	0	0	0	0	0	6609	0	0	0
Sucralose	-	2,98	396,0146	40578	29437	7619	138714	13755	12977	4776	0	5620	4762	3450	21107	64922
Sydnophen	-	2,94	204,1137	0	0	0	0	0	0	0	0	0	2	0	0	0
TCPSA	-	2,53	223,8868	1	0	0	0	0	0	0	0	0	0	0	0	0
tetrahydro-1,3,4,6-tetrakis(hydroxymethyl)imidazo[4,5-d]imidazole-2,5(1H,3H)-dione	+	1,90	262,0913	3844	0	0	10680	2	0	0	0	1	0	0	0	2
Tetrasodium iminidisuccinate	+	2,72	249,0485	2	0	0	0	0	13073	0	0	0	0	0	0	0
Tetronic 701	-	10,21	468,3411	0	0	0	0	0	0	0	2557	1100	818	0	0	0
Tetronic 701	-	10,09	468,3411	2	1	2	2	0	2	2102	0	1100	818	1989	2495	2
Theaflavin-3-gallate	-	2,99	716,1377	1473	0	0	1	0	0	0	0	0	0	0	1	1
Tiaramide	+	8,11	355,0757	0	0	0	0	0	0	0	0	0	0	0	0	0
TIFLOREX	+	7,81	263,0956	6759	2679	0	0	0	0	0	0	0	0	0	0	0
Triethylene glycol	+	11,49	150,0892	0	0	0	13646	0	0	0	0	0	0	0	0	0
Triisopropanolamine	+	0,65	191,1521	14436	20308	1	169731	27905	34561	33146	0	33680	59141	20977	23783	254516
Trisodium citrate	-	0,51	192,0270	0	0	0	0	1	0	3966	2	0	0	1	0	0
Vanillactic acid	-	0,62	212,0685	2	0	0	0	2	0	0	3520	2	3715	2	2241	2761
Vanillactic acid	+	7,13	212,0685	0	2	0	2	0	1	2	0	10017	0	0	2	0
Xanthosine	+	5,46	284,0757	6038	2	0	0	0	6551	0	0	0	0	0	0	0
Xanthosine	+	7,61	284,0757	2770	3907	0	0	0	0	0	0	0	0	0	0	0
Zelandopam	-	3,28	273,1001	0	0	0	1805	0	0	0	0	0	0	0	0	0

Table A7
(Continued).

b)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Drinking Water	China - 2 - Drinking Water	Sweden - Drinking Water	Spain - Drinking Water	Czech Republic - Drinking Water	Netherlands - Drinking Water	Switzerland - Drinking Water	Germany - Drinking Water	Italy - 2 - Drinking Water	Vietnam - Drinking Water	Italy - 1 - Drinking Water	Belgium - Drinking Water	Japan - Drinking Water
(1-MMethylethyl) dihydrogen 2-hydroxypropane-1,2,3-tricarboxylate	+	5,98	234,0740	0	0	0	0	0	0	0	0	0	0	0	0	0
(p-Ammoniophenyl)ethyl(2-hydroxyethyl)ammonium sulphate	+	3,07	180,1263	0	0	0	0	0	0	0	0	0	0	0	0	0
(R)-N-methylsalsolinol	-	3,30	193,1103	0	0	0	0	0	0	0	0	0	0	0	0	0
(R)-S-(2-amino-2-carboxyethyl)-L-homocysteine	+	4,77	222,0674	4155	20055	0	0	0	0	0	0	0	13844	0	0	0
?-hydroxy-o-tolyl ?-D-glucopyranoside	-	0,60	286,1053	7622	8087	3918	1937	3884	2311	5238	5948	3491	6648	5504	6286	3842
[R(R*,R*]-2-amino-1-[p-(methylsulphonyl)phenyl]propane-1,3-diol	+	2,82	245,0722	0	0	0	0	0	0	0	0	0	0	0	0	0
1-(2,4-Dinitrophenyl)pyridinium chloride	-	0,51	246,0515	0	0	0	0	0	0	0	1	0	0	0	0	0
1,3-Benzenedimethanamine	+	2,73	136,1000	0	0	0	0	0	0	0	0	0	0	0	0	0
1,3-Benzenedisulfonic acid, 4-hydroxy-	-	5,02	253,9555	0	0	0	0	0	0	0	0	0	0	0	0	0
1,4-BENZENDIOL, 2-(PHENYLMETHYL)-	+	8,61	200,0837	0	0	0	0	0	0	0	0	0	0	0	0	0
17-Alpha-estradiol	-	3,26	272,1776	0	0	0	0	0	0	0	0	0	0	0	0	0
17-Alpha-Estradiol	+	12,53	272,1776	0	0	0	0	0	0	0	0	0	0	0	0	0
1-Methoxy-4-(1,2,2,2-tetrachloroethyl)benzene	-	4,52	271,9329	0	0	0	0	0	0	0	0	0	2	0	0	0
1-Propanol, 3,3′,3′′-phosphinylidynetris-	+	0,65	224,1177	0	0	2	0	3821	0	0	1	3788	0	0	2	0
1-Propanol, 3,3′,3′′-phosphinylidynetris-	+	12,38	224,1177	0	0	0	0	0	0	0	0	0	1	0	0	0
2-(4-Hydroxybenzyl)phenol	+	8,61	200,0837	0	0	0	0	0	0	0	0	0	0	0	0	0
2,4,4′-Trihydroxybenzophenone	-	2,35	230,0579	0	0	2920	0	0	0	0	0	0	0	0	0	0
2,4,4′-Trihydroxybenzophenone	+	5,29	230,0579	0	0	1	0	0	0	0	0	0	0	0	0	0
2,5-Pyrrolidinedione, 1-[2-[[2-[[2-[(2-aminoethyl)amino]ethyl]amino]ethyl]amino]ethyl]-, monopolyisobutenyl derivs.	+	5,90	325,2478	52178	34844	0	0	0	0	0	0	0	0	0	0	0
2-Chloro-9-[3-(dimethylamino)propyl]thioxanthen-9-ol	+	9,06	333,0954	0	0	2558	0	0	0	0	0	0	0	0	0	0
2-Deoxyinosine	+	5,08	252,0859	0	0	0	0	0	0	0	0	0	0	0	0	0
2-Furanmethanol, 2-formate	+	2,82	206,0790	0	0	0	0	0	0	0	0	0	0	0	0	0
3-(2-Aminoethyl)indol-5-ol	+	2,15	176,0950	110820	148073	52428	58866	28174	1	10654	2	19209	104601	19064	47630	34321
3-Benzylsydnone-4-acetamide	+	8,29	234,0879	0	0	0	0	0	0	0	0	0	0	0	0	0
3-HYDROXY-4-OXO-4H-PYRAN-2,6-DICARBOXYLIC ACID	-	0,47	199,9957	0	0	0	0	0	0	0	3954	0	2	0	0	0

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Table A7 (*continued*)

b)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Drinking Water	China - 2 - Drinking Water	Sweden - Drinking Water	Spain - Drinking Water	Czech Republic - Drinking Water	Netherlands - Drinking Water	Switzerland - Drinking Water	Germany - Drinking Water	Italy - 2 - Drinking Water	Vietnam - Drinking Water	Italy - 1 - Drinking Water	Belgium - Drinking Water	Japan - Drinking Water
3-O-Ethylascorbic acid	-	0,51	204,0634	1	0	0	0	0	0	0	2421	0	2	0	1	0
4-((Dimethylamino)methyl)phenol	+	1,55	151,0997	1	3186	0	0	0	0	0	0	0	0	0	0	0
4-((Dimethylamino)methyl)phenol	+	1,24	151,0997	0	1	0	0	0	0	0	0	0	0	0	0	0
4,4′-Dihydroxydiphenyl ether	-	3,71	202,0630	0	0	0	0	0	0	0	0	0	0	0	0	0
4,4-Dithiobis[2-aminobutyric] acid	-	0,50	268,0551	0	0	1477	0	0	0	0	2610	0	2	0	0	0
4,4-Iminodianiline	+	8,50	199,1109	0	0	0	0	0	0	0	0	0	0	0	0	0
4,4′-Propane-1,1-diyldiphenol	-	4,43	228,1150	0	0	0	0	0	0	0	0	0	0	0	0	0
4,4′-Thiodibenzene-1,3-diol	-	4,79	250,0300	0	1	0	0	0	0	0	0	0	0	0	0	0
4-Amino-4′-hydroxybiphenyl	-	4,43	185,0841	0	0	0	0	0	0	0	0	0	0	0	0	0
4-Amino-4′-hydroxybiphenyl	+	2,84	185,0841	0	0	0	0	0	0	0	0	0	0	0	0	0
4-Benzylphenol	-	3,34	184,0888	0	0	0	0	0	0	0	0	0	0	0	0	0
4-Cyclohexylphenol	-	2,62	176,1201	1	1	2556	0	0	0	0	0	0	0	0	1	0
4-Hydroxybenzophenone	-	3,69	198,0681	0	0	0	0	0	0	0	0	0	0	0	0	0
4-Hydroxyphenylpyruvic acid	-	1,88	180,0423	0	0	1	0	0	0	0	2	12921	1	0	2	1
4-Hydroxyphenylpyruvic acid	-	1,98	180,0423	5422	3597	5507	5572	4160	3224	4155	0	12912	27288	3729	5311	2932
4-Phenylphenol	-	3,86	170,0732	1	0	1672	0	0	0	2	4108	2489	2293	1405	0	0
5-Amino-3-sulfosalicylic acid	-	8,68	232,9994	1552	0	0	0	0	0	0	0	0	0	0	0	0
5-Amino-3-sulfosalicylic acid	-	3,35	232,9994	7347	29545	2830	0	0	0	0	3291	0	19182	0	0	6072
5-Fluorouridine	-	2,92	262,0601	0	0	0	0	0	0	0	0	0	2091	0	0	0
5H-Thiachromine-8-ethanol, 2,7-dimethyl-	+	1,89	262,0888	0	0	0	0	0	0	0	0	0	0	0	0	0
6a,7-dihydro-3,4,6a,10-tetrahydroxybenz[b]indeno[1,2-d]pyran-9(6H)-one	+	3,59	300,0634	0	0	0	0	0	0	0	0	0	0	0	0	0
7-Aminonaphthalene-1,3,6-trisulphonic acid	-	6,59	382,9439	0	0	0	1991	0	0	0	0	0	0	0	0	0
8-Hydroxyguanosine	-	3,70	299,0866	0	0	0	0	0	0	0	0	0	0	0	0	0
9-Deazainosine	+	4,74	267,0855	0	0	0	0	0	0	0	0	0	0	0	0	0
Acetophenazine	+	3,96	411,1980	0	2	0	0	0	0	0	0	1	1	0	1	0
Acetophenazine	+	3,70	411,1980	0	0	0	0	1	0	0	0	0	0	0	0	0
ACETRYPTINE	+	4,95	202,1106	0	0	0	76341	1	0	0	0	0	0	0	0	0
Alcohols, C13-15, ethoxylated	+	4,70	261,2093	0	0	0	0	0	0	0	0	0	0	0	0	0
Alginic acid	-	6,26	398,1060	0	0	0	0	0	0	0	0	0	0	0	0	0
Alloxantin	-	3,84	286,0186	0	0	0	0	0	0	0	0	0	5002	0	0	0
Aminoimidazole ribotide	+	0,54	295,0569	0	0	0	0	0	0	0	0	0	0	0	0	0
Amiterol	+	2,22	208,1576	8093	13206	0	0	0	2	0	0	0	4100	7839	0	5330
Amiterol	+	3,28	208,1576	0	1	0	0	0	0	0	0	0	1	2	0	1
AMMONIUM ZIRCONIUM HYDROXY CITRATE	+	6,17	208,0219	0	0	0	0	0	0	0	0	0	0	0	0	0
Anthrarobin	-	3,80	226,0630	0	0	0	0	0	0	0	0	0	0	0	0	0
Anthrarobin	+	7,17	226,0630	0	0	0	0	0	0	0	0	0	0	0	0	0
Aphidicolin	-	5,17	338,2457	0	0	0	0	0	0	0	0	0	0	0	0	0
Aphidicolin	-	5,37	338,2457	0	0	0	0	0	0	0	0	0	0	0	0	0
Aphidicolin	-	6,05	338,2457	0	0	1	0	0	0	0	2	0	0	0	0	0
Aphidicolin	+	10,27	338,2457	0	0	0	0	0	0	0	0	0	0	0	0	0
Arbutin	+	0,65	272,0896	0	2686	0	0	0	0	0	0	0	0	0	0	0
Asperuloside	-	0,60	414,1162	2	1	0	1	1	1	1	2	2	2	0	2	0

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Table A7 (*continued*)

b)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Drinking Water	China - 2 - Drinking Water	Sweden - Drinking Water	Spain - Drinking Water	Czech Republic - Drinking Water	Netherlands - Drinking Water	Switzerland - Drinking Water	Germany - Drinking Water	Italy - 2 - Drinking Water	Vietnam - Drinking Water	Italy - 1 - Drinking Water	Belgium - Drinking Water	Japan - Drinking Water
Asperuloside	+	4,88	414,1162	6971	9155	2	0	0	0	0	0	0	0	0	0	0
Azidamfenicol	-	5,70	296,0995	0	0	0	7115	1	0	0	0	3044	0	2	0	3371
Benaxibine	-	3,26	269,0899	0	0	0	0	0	0	0	0	0	0	0	0	0
Benaxibine	+	4,93	269,0899	0	0	0	0	0	0	0	0	0	0	0	0	0
benzyl(3-chloro-2-hydroxypropyl)dimethylammonium chloride	-	4,43	228,1155	0	0	0	0	0	0	0	0	0	0	0	0	0
Benzylmorphine	+	9,18	375,1834	0	0	0	0	0	0	0	0	0	0	0	0	0
Bergenin	-	0,62	328,0794	0	0	0	0	2962	0	0	0	0	0	0	1	0
Biflorin	-	0,62	354,0951	2236	2537	3395	0	5858	1	2013	2	1164	2373	2	1	1
Bipenamol	-	3,67	245,0874	0	0	0	0	0	0	0	0	0	0	0	0	0
Butanedioic acid, [(ethoxythioxomethyl)thio]-	-	0,64	237,9970	0	0	1	1	0	0	0	2	1	0	0	0	0
Butanedioic acid, 2,3-dihydroxy- R-(R*,R*) -, m	-	0,51	178,0477	0	0	0	0	0	0	0	1313	0	0	0	0	0
C6-galactose mustard	+	7,79	303,0640	0	0	0	0	0	0	0	0	0	0	0	0	0
Caftaric acid	+	10,06	312,0481	0	0	0	0	0	0	0	0	0	0	0	0	0
Carboxymethyl cellulose	-	5,84	238,0689	0	0	0	0	0	0	0	0	0	0	0	0	0
Chloralose	+	5,34	307,9621	2270	0	0	0	0	0	0	0	0	0	0	0	0
Chlorogenic acid	-	0,60	354,0951	2236	2537	3395	0	5858	1	2013	2	1164	2373	2	1	1
Cianidanol	-	0,60	290,0790	0	0	0	0	0	0	0	1	0	0	0	0	0
Cianidanol	+	5,13	290,0790	0	0	0	0	0	0	0	0	0	0	0	0	0
Citric acid, monoester with glycerol	+	4,25	266,0638	0	0	0	0	0	0	0	0	0	0	0	0	0
Cyclouridine	-	4,28	226,0590	0	0	0	0	0	0	0	1545	0	0	0	0	0
Desethylhydroxychloroquine	+	9,83	307,1451	4812	17360	0	0	0	0	0	0	0	4692	0	0	0
Dexelvucitabine	+	7,12	227,0706	0	0	0	0	0	0	0	0	0	0	0	0	0
Dezocine	+	9,43	245,1780	0	0	0	0	0	0	0	0	0	0	0	0	0
Dezocine	+	6,91	245,1780	0	0	0	0	0	0	0	0	0	0	0	0	0
D-gluco-Heptonic acid, (2?)-, ester with boric acid (H3BO3), sodium salt	-	0,51	270,0758	2	2416	2209	0	1984	0	0	2	0	2	0	1	0
D-gluconic acid 6-(dihydrogen phosphate)	+	7,77	276,0246	1	1	1	0	1	1	1	2	1	0	0	0	0
D-gluconic acid, cyclic 4,5-ester with boric acid, calcium salt (2:1)	+	5,01	222,0547	0	0	0	0	2	0	0	0	0	0	0	0	0
D-Glucose	+	2,22	180,0634	1	0	0	0	0	0	0	0	0	0	0	0	0
Dhurrin	-	3,71	313,0798	2125	4884	1	0	0	0	0	3379	0	0	0	0	0
Dhurrin	+	4,60	313,0798	0	0	0	0	0	0	0	0	0	0	0	0	0
Dichlorprop	-	4,30	233,9850	0	0	0	0	0	0	0	0	0	3744	0	0	0
Digallic acid	-	0,47	322,0325	0	0	0	0	0	0	0	0	0	0	0	0	0
Dihydroequilin	+	11,65	270,1620	0	0	0	0	0	0	0	0	3656	0	0	0	6498
Dimaprit	+	0,64	161,0987	0	0	0	0	0	2	0	0	0	0	0	0	0
Disodium 3-hydroxy-4-nitrosonaphthalene-2,7-disulphonate	-	5,60	332,9613	0	0	0	0	0	0	0	0	0	0	0	0	0

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Table A7 (*continued*)

b)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Drinking Water	China - 2 - Drinking Water	Sweden - Drinking Water	Spain - Drinking Water	Czech Republic - Drinking Water	Netherlands - Drinking Water	Switzerland - Drinking Water	Germany - Drinking Water	Italy - 2 - Drinking Water	Vietnam - Drinking Water	Italy - 1 - Drinking Water	Belgium - Drinking Water	Japan - Drinking Water
Disodium ethylenediaminediacetate	+	6,90	176,0797	38597	269091	43694	655750	16781	0	7979	12698	7508	12985	12445	16842	42599
DOPA sulfate	-	3,47	277,0256	2	6010	0	0	0	0	0	0	0	1	0	0	0
Dopaquinone	-	3,76	195,0532	1	2819	0	0	0	0	0	0	0	0	0	0	0
EO 9	-	3,89	288,1110	0	1	0	0	0	0	0	0	0	9521	0	2	25441
Epilactose	-	7,37	342,1162	0	0	0	0	0	0	0	0	0	0	0	0	0
Eptifibatide	+	7,86	831,3156	0	0	0	0	0	0	0	0	0	1	2270	0	0
Estriol	+	6,36	288,1725	145844	34241	1	0	2	0	0	134768	0	231287	0	1	0
Estriol	+	5,76	288,1725	145881	116957	0	0	0	0	0	133701	0	229650	4405	0	0
ETANTEROL	+	6,15	316,1787	0	0	0	0	0	0	0	0	6275	0	0	0	0
Ethidium chloride (ET)	+	7,24	314,1657	0	0	0	2	0	0	0	0	0	0	0	0	2
Exifone	-	3,29	278,0427	0	0	1	0	0	0	0	0	0	0	0	0	0
Felypressin	-	15,80	1039,4368	0	0	0	0	0	0	0	0	0	1	1213	1	1
Fenoldopam	+	4,06	305,0819	0	0	0	0	0	0	0	0	0	0	0	0	0
Fepradinol	+	6,83	209,1416	0	0	0	2505	0	0	0	0	0	0	0	0	0
Formaldehyde, polymer with 1,3-benzenediol, [1,1′-biphenyl]-ar,ar'-diol and [1,1′-biphenyl]triol	+	5,39	202,0630	0	0	40288	0	0	0	0	2	0	0	0	0	0
Fulvic acid	-	0,51	308,0532	0	0	0	0	0	0	0	1	0	1	0	0	0
Gamma-glutamylcysteine	-	4,50	250,0623	0	0	0	0	0	0	0	0	0	0	0	0	0
Gamma-glutamylcysteine	-	4,67	250,0623	0	0	0	0	0	0	0	0	0	0	0	0	0
Gamma-glutamylcysteine	+	5,93	250,0623	0	4615	0	4333	0	0	0	0	0	0	0	0	0
Gemcitabine	+	4,79	263,0718	0	0	0	0	0	0	0	0	0	0	0	0	0
Ginkgolide-A	-	0,60	408,1420	3176	4470	2	1437	8098	3122	2512	2	2231	2680	2217	4578	2
Ginkgolide-A	+	2,13	408,1420	0	0	0	0	0	0	0	0	0	0	0	0	0
Ginkgolide-C	-	0,61	440,1319	2	2	2	2	3817	1131	1627	2	1471	2	996	2204	1
Ginkgolide-J	-	0,61	424,1369	3111	3347	4508	2	6574	2217	2640	7060	2161	2589	1898	3719	2
Ginkgolide-M	-	0,60	424,1369	3111	3347	4508	2	6574	2217	2640	7060	2161	2589	1898	3719	2
Gluconolactone	-	0,49	178,0477	0	0	0	0	0	0	0	1313	0	0	0	0	0
GLUFOSFAMIDE	-	6,19	382,0463	0	0	0	0	0	0	0	0	0	0	0	0	0
Glycine, N,N'-(1,2-dithioxo-1,2-ethanediyl)bis-	-	2,44	235,9925	0	44400	0	0	0	0	0	0	0	0	0	0	0
Guanosine	+	5,41	283,0917	0	0	0	0	0	0	0	0	0	0	0	0	0
Helicin	-	0,60	284,0896	3984	5131	4104	2	3985	1464	2	5640	2	3966	1812	4403	2
Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafl	-	5,39	345,9863	2581	5223	0	2298	2	0	0	5644	5500	0	1	2	0
Hexamethylolmelamine	+	0,66	306,1288	1	2978	0	1	0	0	0	0	0	0	0	1	0
Hexanedioic acid	-	0,49	146,0579	2	0	0	0	0	0	0	2	0	2	1413	0	2
Hydroxystilbamidine Isethionate	+	8,06	280,1324	0	0	34283	0	0	0	0	0	0	0	0	0	0
Isochorismic acid	-	0,49	226,0477	0	0	0	0	0	0	0	1898	0	2	0	0	0
Isochorismic acid	+	3,32	226,0477	0	0	0	0	0	0	0	0	0	0	0	0	0
Isopropyl citrate	+	5,98	234,0740	0	0	0	0	0	0	0	0	0	0	0	0	0
Isoquinoline-6,7-diol, 1,2,3,4-tetrahydro-2-meth	+	5,23	179,0946	0	22065	0	0	0	0	0	0	0	0	0	0	0
Lactobionic acid	+	5,35	358,1111	0	0	0	0	0	0	0	0	0	0	0	0	0

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Table A7 (*continued*)

b)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Drinking Water	China - 2 - Drinking Water	Sweden - Drinking Water	Spain - Drinking Water	Czech Republic - Drinking Water	Netherlands - Drinking Water	Switzerland - Drinking Water	Germany - Drinking Water	Italy - 2 - Drinking Water	Vietnam - Drinking Water	Italy - 1 - Drinking Water	Belgium - Drinking Water	Japan - Drinking Water
Lactose	-	7,37	342,1162	0	0	0	0	0	0	0	0	0	0	0	0	0
L-Dopa	-	2,69	197,0688	0	0	0	0	0	0	0	0	0	0	0	0	0
Levallorphan	+	7,16	283,1936	0	0	0	0	0	0	0	0	0	0	0	0	0
L-Glutamic acid	+	6,90	147,0532	0	0	0	0	0	0	0	0	0	0	0	0	0
Lodoxamide	-	5,46	310,9945	0	0	0	0	0	0	0	0	0	0	0	0	0
Maleylacetoacetic acid	-	3,13	200,0321	0	0	0	0	0	0	0	0	0	0	0	0	0
Maltodextrin	+	2,49	180,0634	0	0	13056	0	0	0	0	0	0	0	0	0	0
MDL 28574	+	7,48	259,1420	0	0	0	0	0	0	0	0	0	0	0	0	0
Methanaminium, N-[4-[[4-(dimethylamino)phenyl][4-[(2-hydroxyethyl)amino]phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methy	+	8,59	388,2389	0	0	0	0	0	0	0	0	0	0	0	0	0
Morphine	+	6,93	285,1365	0	1	0	0	0	0	0	0	0	0	0	0	2407
Morphine methylbromide	+	4,92	300,1600	0	1	0	2	0	0	0	0	0	0	0	0	0
N-(3-Chloroallyl)hexaminium chloride	+	7,51	215,1063	0	0	0	0	0	0	0	0	0	0	0	0	0
N,N,N',N'-Tetrakis(2-Hydroxypropyl)ethylenediamine	-	4,18	292,2362	0	0	0	0	0	0	0	0	0	0	0	0	0
Nadolol	-	4,51	309,1940	0	0	0	0	0	0	0	0	0	2	0	0	1294
Nitrocellulose	-	3,45	315,0186	3037	5698	0	0	0	0	0	0	0	4943	0	0	0
Nitrocellulose	+	4,94	315,0186	2559	3474	0	0	0	0	0	0	0	1	0	0	0
N'-Nitrosonornicotine-1-N-oxide	+	4,86	193,0851	0	2	0	0	0	0	0	0	0	0	0	0	0
Norcodeine	+	9,24	285,1365	0	0	0	0	0	0	0	0	0	0	0	0	0
Normorphine	-	2,89	271,1208	0	0	0	0	0	0	0	0	0	0	0	0	0
OXONAZINE	-	3,87	222,1229	1	7584	1	1915	0	0	0	1	0	2	0	0	0
p-(1-phenylethyl)phenol	-	5,97	198,1045	0	0	0	0	0	0	0	0	0	0	0	0	0
PANCRATISTATIN	-	3,75	325,0798	0	1164	0	0	0	0	0	0	0	0	0	0	0
Phenanthridinium, 3,8-diamino-5-methyl-6-phenyl-	+	6,90	300,1501	17406	1	0	1	2	0	2904	0	2614	0	2	1	1
Phenol, 4,4′-iminobis-	+	6,05	201,0790	0	1	0	0	0	0	0	0	0	0	0	0	0
PHENOLPHTHALOL	+	9,56	306,1256	0	0	2	0	0	0	0	0	0	0	0	0	0
Phosphonic acid, [[(2-hydroxyethyl)imino]bis(methylene)]bis-	+	4,41	249,0167	4322	2	0	0	0	0	0	0	0	0	0	0	0
Picrotoxin	-	3,83	310,1053	1	1	0	0	0	0	0	0	0	0	0	0	0

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Table A7 (*continued*)

b)

Suspect name	Ion Mode	Observed RT (min)	Expected neutral mass (Da)	China - 1- Drinking Water	China - 2 - Drinking Water	Sweden - Drinking Water	Spain - Drinking Water	Czech Republic - Drinking Water	Netherlands - Drinking Water	Switzerland - Drinking Water	Germany - Drinking Water	Italy - 2 - Drinking Water	Vietnam - Drinking Water	Italy - 1 - Drinking Water	Belgium - Drinking Water	Japan - Drinking Water
Picrotoxin	+	0,67	310,1053	2	3335	1	0	0	0	0	0	0	0	0	0	0
Plasma protein fraction	-	2,89	226,0242	0	0	0	0	0	0	0	1	0	0	0	0	0
Potassium citrate	-	0,51	192,0270	0	0	0	0	0	0	0	0	0	0	0	0	0
Propyl gallate	-	4,37	212,0685	0	0	0	0	0	0	0	0	0	0	0	0	0
Puberulic acid	-	0,49	198,0164	0	0	1308	0	0	0	0	3971	0	2	0	0	0
Purpurogallin	-	1,54	220,0372	0	0	0	0	0	0	0	0	0	5399	0	0	0
Purpurogallin	-	2,52	220,0372	0	0	0	0	0	0	0	0	0	0	0	0	0
Pyrazofurin	+	4,58	259,0804	0	6258	0	0	1	0	0	0	0	1	1	1	0
Ractopamine hydrochloride	-	6,09	301,1678	0	1	7483	0	0	0	0	0	0	0	0	0	0
Ribavirin Monophosphate	-	0,50	324,0471	0	0	0	0	0	0	0	0	0	0	0	0	0
Ribavirin Monophosphate	+	6,71	324,0471	2	1	1	2	1	1	0	65854	0	1	1	1	1
Risedronic acid	-	10,06	283,0011	0	0	0	0	0	0	0	0	0	0	0	0	0
Robinin	-	8,10	740,2164	0	0	0	0	0	0	0	0	0	0	0	0	0
Salidroside	-	0,60	300,1209	7541	8785	2	1	4403	2883	5177	7319	3535	6100	4807	6221	3652
Salidroside	+	0,65	300,1209	0	2727	0	0	0	0	0	0	0	0	0	0	0
sedoheptulose 7-phosphate	+	3,13	290,0403	0	0	0	0	0	0	0	0	0	0	0	0	0
SEVITROPIUM MESILATE	+	9,95	380,1684	0	0	0	0	0	0	0	0	0	0	0	0	0
SKF 77434	+	10,43	295,1572	0	0	0	0	0	0	0	0	0	0	0	0	0
SKF 81297	+	4,28	289,0870	0	0	0	0	0	0	0	0	0	0	0	0	0
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	-	4,06	241,9207	0	0	0	0	0	0	0	0	0	0	0	0	0
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	-	2,47	241,9207	0	0	0	0	0	0	0	0	0	0	0	0	0
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	-	4,26	241,9207	2	1383	0	0	0	0	0	0	0	0	0	0	0
Sucralose	-	2,98	396,0146	40081	27049	9049	18897	6526	3511	3049	0	3809	2042	2483	12067	30967
Sydnophen	-	2,94	204,1137	1	2311	0	0	0	0	0	1	0	0	0	1	0
TCPSA	-	2,53	223,8868	2	0	0	0	0	0	0	0	0	7873	0	0	0
tetrahydro-1,3,4,6-tetrakis(hydroxymethyl)imidazo[4,5-d]imidazole-2,5(1H,3H)-dione	+	1,90	262,0913	0	0	0	0	0	0	0	0	0	0	0	0	0
Tetrasodium iminidisuccinate	+	2,72	249,0485	0	0	0	0	0	0	0	0	0	0	0	0	0
Tetronic 701	-	10,21	468,3411	0	0	0	0	0	0	0	2	0	0	0	0	0
Tetronic 701	-	10,09	468,3411	1	0	1565	2	1594	2	1	0	0	0	2	2579	1
Theaflavin-3-gallate	-	2,99	716,1377	1	1	0	0	0	0	0	0	0	0	0	0	0
Tiaramide	+	8,11	355,0757	0	0	0	0	0	0	0	0	0	0	0	2589	0
TIFLOREX	+	7,81	263,0956	0	0	0	0	0	0	0	0	0	0	0	0	0
Triethylene glycol	+	11,49	150,0892	0	0	0	0	0	0	0	0	0	0	0	0	0
Triisopropanolamine	+	0,65	191,1521	0	0	2650	2	5676	0	0	0	0	0	0	2	1
Trisodium citrate	-	0,51	192,0270	0	0	0	0	0	0	0	0	0	0	0	0	0
Vanillactic acid	-	0,62	212,0685	1875	1674	0	0	0	0	0	1	1392	3367	1887	2	1
Vanillactic acid	+	7,13	212,0685	0	0	0	0	0	0	0	0	0	0	0	0	0
Xanthosine	+	5,46	284,0757	0	0	0	0	0	0	0	0	0	0	0	0	0
Xanthosine	+	7,61	284,0757	0	0	0	0	0	0	0	0	0	0	0	0	0
Zelandopam	-	3,28	273,1001	0	0	0	0	0	0	0	0	0	0	0	0	0

Table A8
Estimated removal rate (%) for all suspect features at all DWTPs (n = 13).

Suspect	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
(1-Methylethyl) dihydrogen 2-hydroxypropane-1.2,3-tricarboxylate	99.6	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
(p-ammoniophenyl)ethyl(2-hydroxyethyl)ammonium sulphate	N/D	N/D	N/D	96.8	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
(R)-N-Methylsalsolinol	N/D	96.7	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
(R)-S-(2-amino-2-carboxyethyl)-L-homocysteine	55.5	18.3	N/D	98.3	N/D	N/D	N/D	N/D	99.1	49.3	N/D	N/D	97.6
?-hydroxy-o-tolyl ?-D-glucopyranoside	0.0	0.0	7.2	N/D	0.0	N/D	N/D	0.0	N/D	33.6	0.0	0.0	29.5
[R(R*.R*]-2-amino-1-[p-(methylsulphonyl)phenyl]propane-1,3-diol	N/D	N/D	N/D	99.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
1-(2,4-dinitrophenyl)pyridinium chloride	N/D	N/D	N/D	95.2	96.7	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
1,3-Benzenedimethanamine	97.5	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
1,3-Benzenedisulfonic acid, 4-hydroxy-	91.6	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
1,4-BENZENDIOL, 2-(PHENYLMETHYL)-	N/D	N/D	N/D	97.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
17-alpha-Estradiol	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	96.0	N/D	N/D	N/D	N/D
17-alpha-Estradiol	N/D	N/D	N/D	100.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.8
1-methoxy-4-(1,2,2,2-tetrachloroethyl)benzene	N/D	N/D	N/D	96.7	N/D	N/D	N/D	N/D	N/D	94.6	N/D	N/D	96.5
1-Propanol, 3,3′,3′′-phosphinylidynetris-	N/D	N/D	N/D	N/D	N/D	N/D	99.9	N/D	N/D	N/D	N/D	N/D	N/D
1-Propanol, 3,3′,3′′-phosphinylidynetris-	N/D	N/D	N/D	98.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
2-(4-Hydroxybenzyl)phenol	N/D	N/D	N/D	97.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
2,4,4′-Trihydroxybenzophenone	N/D	N/D	0.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
2,4,4′-Trihydroxybenzophenone	97.7	97.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
2,5-Pyrrolidinedione, 1-[2-[[2-[[2-[(2-aminoethyl)amino]ethyl]amino]ethyl]amino]ethyl]-, monopolyisobutenyl derivs,	0.0	0.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
2-chloro-9-[3-(dimethylamino)propyl]thioxanthen-9-ol	N/D	N/D	7.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	96.1	N/D
2-Deoxyinosine	N/D	N/D	N/D	99.5	98.8	98.9	N/D	N/D	N/D	N/D	N/D	98.8	N/D
2-Furanmethanol, 2-formate	N/D	N/D	N/D	99.3	98.8	N/D	98.8	N/D	N/D	N/D	N/D	99.0	99.2
3-(2-aminoethyl)indol-5-ol	0.0	24.4	0.0	65.5	60.0	99.5	71.5	N/D	72.0	37.9	65.4	57.5	74.1
3-Benzylsydnone-4-acetamide	N/D	N/D	N/D	99.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
3-HYDROXY-4-OXO-4H-PYRAN-2,6-DICARBOXYLIC ACID	N/D	N/D	N/D	N/D	93.5	N/D	N/D	32.1	N/D	95.9	N/D	N/D	N/D
3-O-Ethylascorbic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	20.1	N/D	N/D	N/D	N/D	N/D
4-((Dimethylamino)methyl)phenol	N/D	40.7	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
4-((Dimethylamino)methyl)phenol	N/D	97.3	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
4,4′-Dihydroxydiphenyl ether	N/D	N/D	N/D	92.5	N/D	N/D	N/D	N/D	N/D	99.4	N/D	N/D	N/D
4,4-dithiobis[2-aminobutyric] acid	N/D	N/D	0.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
4,4-iminodianiline	96.1	99.2	N/D	98.6	N/D	N/D	N/D	N/D	99.6	96.9	N/D	99.9	N/D
4,4′-Propane-1,1-diyldiphenol	N/D	N/D	N/D	97.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	98.0
4,4′-Thiodibenzene-1,3-diol	93.6	98.2	N/D	98.4	N/D	N/D	N/D	N/D	96.9	97.9	N/D	95.0	94.1
4-Amino-4′-hydroxybiphenyl	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	92.5	N/D	N/D	N/D
4-Amino-4′-hydroxybiphenyl	N/D	N/D	N/D	99.5	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
4-Benzylphenol	N/D	N/D	N/D	93.2	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	94.7

(*continued on next page*)

Table A8 (*continued*)

Suspect	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
4-cyclohexylphenol	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
4-Hydroxybenzophenone	N/D	97.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
4-hydroxyphenylpyruvic acid	N/D	N/D	N/D	98.1	N/D	N/D	N/D	N/D	0.0	N/D	N/D	98.8	N/D
4-hydroxyphenylpyruvic acid	43.2	N/D	0.0	0.0	0.0	39.5	N/D	N/D	0.0	0.0	N/D	37.1	33.1
4-Phenylphenol	N/D	N/D	0.0	99.1	91.6	N/D	N/D	0.0	12.5	0.0	0.0	N/D	92.3
5-Amino-3-sulfosalicylic acid	49.9	94.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
5-Amino-3-sulfosalicylic acid	24.1	39.8	N/D	N/D	96.6	N/D	95.7	0.0	98.2	46.9	93.3	99.1	88.5
5-Fluorouridine	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	93.2	N/D	N/D
5H-Thiachromine-8-ethanol, 2,7-dimethyl-	97.4	N/D	N/D	99.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
6a,7-dihydro-3,4,6a,10-tetrahydroxybenz[b]indeno[1,2-d]pyran-9(6H)-one	N/D	98.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
7-aminonaphthalene-1,3,6-trisulphonic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
8-hydroxyguanosine	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	95.8	N/D	N/D	N/D
9-Deazainosine	97.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Acetophenazine	99.9	99.9	99.9	100.0	100.0	N/D	99.7	100.0	N/D	N/D	99.9	99.7	99.7
Acetophenazine	N/D	99.9	99.9	99.9	100.0	N/D	N/D	N/D	N/D	N/D	99.8	N/D	N/D
ACETRYPTINE	99.9	99.8	N/D	N/D	N/D	99.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Alcohols, C13-15, ethoxylated	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.5
Alginic acid	93.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Alloxantin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Aminoimidazole ribotide	97.5	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Amiterol	4.5	0.0	N/D	98.9	N/D	98.2	N/D	N/D	N/D	N/D	N/D	97.4	45.1
Amiterol	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	97.4
AMMONIUM ZIRCONIUM HYDROXY CITRATE	N/D	N/D	N/D	98.2	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Anthrarobin	N/D	N/D	N/D	N/D	95.6	N/D	N/D	N/D	93.8	98.8	N/D	N/D	N/D
Anthrarobin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	98.3	N/D	N/D	N/D
Aphidicolin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	98.3	N/D	97.1	N/D
Aphidicolin	99.5	99.5	N/D	N/D	96.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Aphidicolin	99.8	99.7	93.5	99.2	98.7	N/D	N/D	94.7	97.2	96.7	97.9	98.9	97.9
Aphidicolin	100.0	99.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.6	N/D	N/D
Arbutin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Asperuloside	N/D	N/D	N/D	N/D	N/D	N/D	N/D	97.7	N/D	N/D	N/D	N/D	N/D
Asperuloside	47.1	13.1	99.7	N/D	N/D	N/D	N/D	N/D	N/D	99.3	98.9	N/D	N/D
Azidamfenicol	N/D	N/D	N/D	29.7	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Benaxibine	N/D	N/D	N/D	94.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Benaxibine	N/D	N/D	N/D	99.6	98.3	N/D	96.3	N/D	N/D	N/D	N/D	N/D	N/D
benzyl(3-chloro-2-hydroxypropyl)dimethylammonium chloride	N/D	N/D	N/D	97.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	98.0
Benzylmorphine	N/D	N/D	N/D	99.6	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.4
Bergenin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Biflorin	N/D	N/D	N/D	N/D	0.0	94.5	N/D	98.0	N/D	47.9	N/D	95.6	N/D
Bipenamol	N/D	93.5	N/D	N/D	N/D	N/D	N/D	95.7	N/D	N/D	N/D	N/D	N/D
Butanedioic acid, [(ethoxythioxomethyl)thio]-	96.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	97.5	N/D	N/D	N/D	N/D
Butanedioic acid, 2,3-dihydroxy-R-(R*,R*) -, m	N/D	N/D	N/D	N/D	N/D	N/D	N/D	31.9	N/D	N/D	N/D	N/D	N/D
C6-galactose mustard	N/D	N/D	N/D	96.2	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Caftaric acid	98.9	99.7	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.1	N/D	N/D	N/D
Carboxymethyl cellulose	N/D	N/D	N/D	N/D	N/D	95.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Chloralose	64.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Chlorogenic acid	N/D	N/D	0.0	N/D	0.0	94.5	N/D	98.0	N/D	47.9	N/D	95.6	N/D
Cianidanol	N/D	93.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	91.1

(*continued on next page*)

Table A8 (*continued*)

Suspect	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
Cianidanol	N/D	N/D	N/D	N/D	N/D	97.8	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Citric acid, monoester with glycerol	N/D	N/D	N/D	99.5	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Cyclouridine	97.2	99.2	N/D	N/D	N/D	N/D	N/D	0.0	94.4	N/D	93.0	N/D	96.2
Desethylhydroxychloroquine	74.2	73.1	N/D	98.1	97.7	N/D	N/D	N/D	99.0	65.1	N/D	99.2	99.7
Dexelvucitabine	99.0	99.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Dezocine	N/D	N/D	N/D	98.2	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Dezocine	N/D	95.6	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
D-gluco-Heptonic acid, (2?)-, ester with boric acid (H3BO3), sodium salt	N/D	N/D	0.0	N/D	18.9	N/D	N/D	97.3	N/D	95.7	N/D	N/D	N/D
D-gluconic acid 6-(dihydrogen phosphate)	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	98.2	N/D	N/D	N/D	N/D
D-gluconic acid, cyclic 4,5-ester with boric acid, calcium salt (2:1)	99.7	99.7	N/D	N/D	N/D	99.3	N/D	N/D	N/D	N/D	N/D	N/D	98.5
D-Glucose	N/D	N/D	N/D	N/D	99.2	N/D	N/D	N/D	99.0	98.9	N/D	N/D	99.3
Dhurrin	N/D	25.8	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Dhurrin	98.5	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Dichlorprop	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Digallic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	96.7	N/D	N/D	N/D
Dihydroequilin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	0.0
Dimaprit	N/D	N/D	N/D	N/D	N/D	97.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Disodium 3-hydroxy-4-nitrosonaphthalene-2,7-disulphonate	N/D	N/D	N/D	N/D	N/D	99.6	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Disodium ethylenediaminediacetate	67.7	50.4	0.0	90.5	49.6	N/D	83.6	0.0	71.8	56.1	55.4	80.7	83.3
DOPA sulfate	94.6	28.6	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	97.2
Dopaquinone	N/D	11.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
EO 9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.0	N/D
Epilactose	N/D	N/D	N/D	96.8	N/D	N/D	97.9	N/D	N/D	N/D	N/D	99.0	N/D
Eptifibatide	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	35.8	N/D	N/D
Estriol	0.0	68.2	99.8	N/D	99.9	N/D	99.1	0.0	99.2	0.0	N/D	99.9	N/D
Estriol	N/D	N/D	N/D	99.6	99.6	N/D	N/D	0.0	99.6	0.0	N/D	N/D	99.6
ETANTEROL	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Ethidium chloride (ET)	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.6
Exifone	N/D	N/D	97.0	N/D	N/D	N/D	N/D	N/D	N/D	98.8	N/D	N/D	N/D
Felypressin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Fenoldopam	N/D	N/D	N/D	98.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Fepradinol	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Formaldehyde, polymer with 1,3-benzenediol, [1,1′-biphenyl]-ar,ar'-diol and [1,1′-biphenyl]triol	N/D	N/D	0.0	N/D	N/D	N/D	N/D	99.2	N/D	N/D	N/D	N/D	N/D
Fulvic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	97.1	N/D	N/D	N/D
Gamma-glutamylcysteine	N/D	99.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Gamma-glutamylcysteine	N/D	99.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Gamma-glutamylcysteine	N/D	N/D	N/D	0.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Gemcitabine	96.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Ginkgolide-A	N/D	0.0	N/D	N/D	N/D	28.5	N/D	98.6	0.0	58.9	29.4	0.0	96.2
Ginkgolide-A	N/D	97.7	N/D	98.5	99.7	N/D	N/D	N/D	N/D	98.9	N/D	N/D	N/D
Ginkgolide-C	91.1	N/D	N/D	N/D	N/D	N/D	N/D	97.7	N/D	N/D	N/D	N/D	92.4
Ginkgolide-J	N/D	0.0	0.0	N/D	0.0	N/D	N/D	0.0	N/D	48.9	3.2	0.0	95.3
Ginkgolide-M	N/D	0.0	0.0	N/D	0.0	N/D	N/D	0.0	N/D	48.9	3.2	0.0	95.3
Gluconolactone	N/D	N/D	N/D	N/D	N/D	N/D	N/D	31.9	N/D	N/D	N/D	N/D	N/D

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Table A8 (*continued*)

Suspect	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
GLUFOSFAMIDE	N/D	N/D	N/D	N/D	N/D	95.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Glycine, N,N'-(1,2-dithioxo-1,2-ethanediyl)bis-	N/D	25.2	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Guanosine	N/D	N/D	N/D	98.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Helicin	N/D	0.0	N/D	N/D	0.0	1.7	N/D	0.0	N/D	39.3	0.0	0.0	95.9
Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafl	0.0	0.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Hexamethylolmelamine	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Hexanedioic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	95.6	N/D	96.0	0.0	N/D	N/D
Hydroxystilbamidine Isethionate	N/D	N/D	0.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Isochorismic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	0.0	N/D	95.6	N/D	N/D	N/D
Isochorismic acid	N/D	N/D	N/D	96.5	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Isopropyl citrate	99.6	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Isoquinoline-6,7-diol, 1,2,3,4-tetrahydro-2-meth	N/D	40.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Lactobionic acid	99.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Lactose	N/D	N/D	N/D	96.8	N/D	N/D	97.9	N/D	N/D	N/D	N/D	99.0	N/D
L-Dopa	N/D	99.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	96.2	N/D	N/D	96.0
Levallorphan	N/D	N/D	N/D	99.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
L-Glutamic acid	N/D	N/D	N/D	98.8	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Lodoxamide	N/D	N/D	N/D	95.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Maleylacetoacetic acid	94.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Maltodextrin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	98.5	N/D
MDL 28574	99.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Methanaminium, N-[4-[[4-(dimethylamino)phenyl][4-[(2-hydroxyethyl)amino]phenyl]methylene]-2,5-cyclohexadien-1-ylidene]-N-methy	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.9
Morphine	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Morphine methylbromide	N/D	N/D	N/D	100.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
N-(3-Chloroallyl)hexaminium chloride	N/D	N/D	N/D	99.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
N,N,N',N'-Tetrakis(2-Hydroxypropyl)ethylenediamine	N/D	N/D	N/D	96.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Nadolol	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Nitrocellulose	24.2	22.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	51.3	N/D	N/D	N/D
Nitrocellulose	8.5	20.9	N/D	N/D	N/D	N/D	N/D	N/D	N/D	97.4	N/D	N/D	N/D
N'-Nitrosonornicotine-1-N-oxide	N/D	N/D	N/D	N/D	97.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Norcodeine	N/D	N/D	N/D	99.7	N/D	N/D	N/D	N/D	N/D	99.2	N/D	N/D	97.7
Normorphine	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	94.5	N/D	N/D	N/D
OXONAZINE	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
p-(1-phenylethyl)phenol	N/D	N/D	N/D	95.1	N/D	N/D	N/D	N/D	N/D	99.1	N/D	N/D	98.2
PANCRATISTATIN	N/D	23.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Phenanthridinium, 3,8-diamino-5-methyl-6-phenyl-	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	80.2	N/D	N/D	N/D	N/D
Phenol, 4,4′-iminobis-	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.7
PHENOLPHTHALOL	97.0	N/D	N/D	98.3	96.4	N/D	N/D	N/D	N/D	N/D	N/D	98.5	N/D
Phosphonic acid, [[(2-hydroxyethyl)imino]bis(methylene)]bis-	N/D	98.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Picrotoxin	99.6	98.1	N/D	97.8	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Picrotoxin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Plasma protein fraction	98.9	99.5	N/D	N/D	N/D	N/D	N/D	96.0	98.3	N/D	N/D	N/D	97.3
Potassium citrate	N/D	N/D	N/D	N/D	N/D	N/D	97.5	N/D	N/D	N/D	N/D	N/D	N/D
Propyl gallate	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	96.1	N/D	N/D	N/D	N/D

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Table A8 (*continued*)

Suspect	China #1	China #2	Sweden	Spain	Czech Republic	Netherlands	Switzerland	Germany	Italy #2	Vietnam	Italy #1	Belgium	Japan
Puberulic acid	N/D	N/D	46.6	N/D	96.7	N/D	N/D	39.1	N/D	98.5	N/D	95.3	N/D
Purpurogallin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	95.3	N/D	N/D	N/D	N/D
Purpurogallin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	98.7	N/D	N/D	N/D
Pyrazofurin	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Ractopamine hydrochloride	N/D	94.7	0.0	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Ribavirin monophosphate	N/D	N/D	N/D	N/D	N/D	N/D	N/D	95.9	N/D	97.1	N/D	N/D	N/D
Ribavirin monophosphate	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Risedronic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	90.3	N/D	N/D	N/D
Robinin	N/D	N/D	N/D	95.8	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	91.1
Salidroside	0.0	0.0	N/D	N/D	0.0	0.0	N/D	0.0	N/D	33.7	0.0	0.0	22.6
Salidroside	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Sedoheptulose 7-phosphate	N/D	N/D	N/D	98.8	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
SEVITROPIUM MESILATE	N/D	N/D	N/D	99.6	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
SKF 77434	N/D	N/D	N/D	N/D	N/D	99.3	N/D	N/D	99.3	N/D	N/D	N/D	N/D
SKF 81297	N/D	N/D	N/D	99.3	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	N/D	95.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	98.7	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Sodium 3,5-dichloro-2-hydroxybenzenesulphonate	98.3	57.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	98.5	N/D	N/D	N/D
Sucralose	1.2	8.1	0.0	86.4	52.6	72.9	36.2	N/D	32.2	57.1	28.0	42.8	52.3
Sydnophen	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
TCPSA	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Tetrahydro-1,3,4,6-tetrakis(hydroxymethyl)imidazo[4,5-d]imidazole-2,5(1H,3H)-dione	97.4	N/D	N/D	99.1	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Tetrasodium iminidisuccinate	N/D	N/D	N/D	N/D	N/D	99.2	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Tetronic 701	N/D	N/D	N/D	N/D	N/D	N/D	N/D	96.1	90.9	87.8	N/D	N/D	N/D
Tetronic 701	N/D	N/D	N/D	N/D	N/D	N/D	95.2	N/D	90.9	87.8	95.0	0.0	N/D
Theaflavin-3-gallate	93.2	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Tiaramide	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
TIFLOREX	98.5	96.3	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Triethylene glycol	N/D	N/D	N/D	99.3	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Triisopropanolamine	99.3	99.5	N/D	99.9	79.7	99.7	99.7	N/D	99.7	99.8	99.5	99.6	100.0
Trisodium citrate	N/D	N/D	N/D	N/D	N/D	N/D	97.5	N/D	N/D	N/D	N/D	N/D	N/D
Vanillactic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	97.2	N/D	9.4	N/D	95.5	96.4
Vanillactic acid	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	99.0	N/D	N/D	N/D	N/D
Xanthosine	98.3	N/D	N/D	N/D	N/D	98.5	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Xanthosine	96.4	97.4	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Zelandopam	N/D	N/D	N/D	94.5	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D	N/D
Number of detected features	57	60	23	65	33	21	15	32	30	54	22	34	45
Average removal	74.8	63.8	28.3	93.2	67.0	81.4	91.1	50.4	80.2	74.4	54.1	72.7	87.2

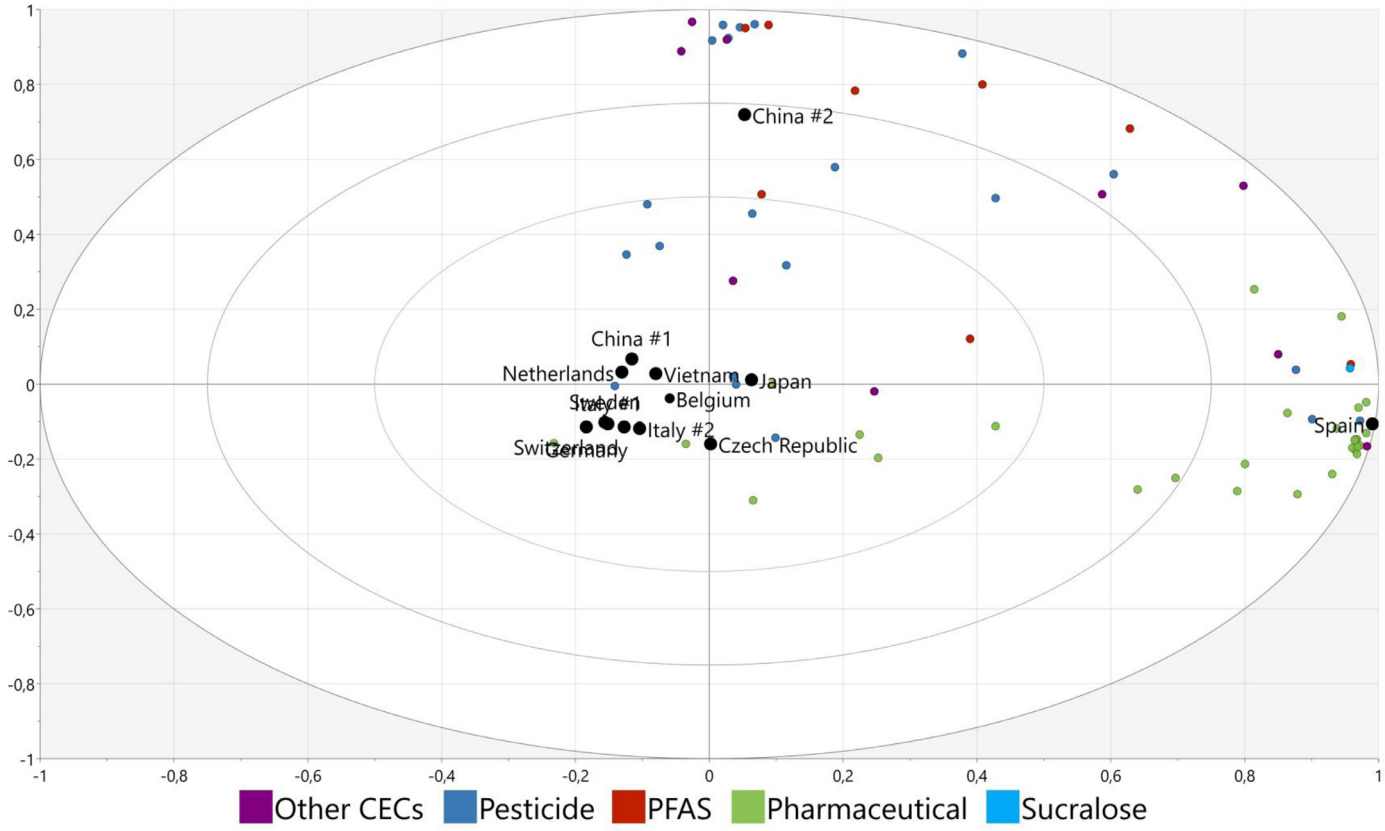

Fig. A1. PCA biplot of raw water concentrations of individual CECs at all DWTPs (n = 13). The first two principal components (PCs) jointly explained 61% of the data variance (PC1: 39%, PC2: 22%).

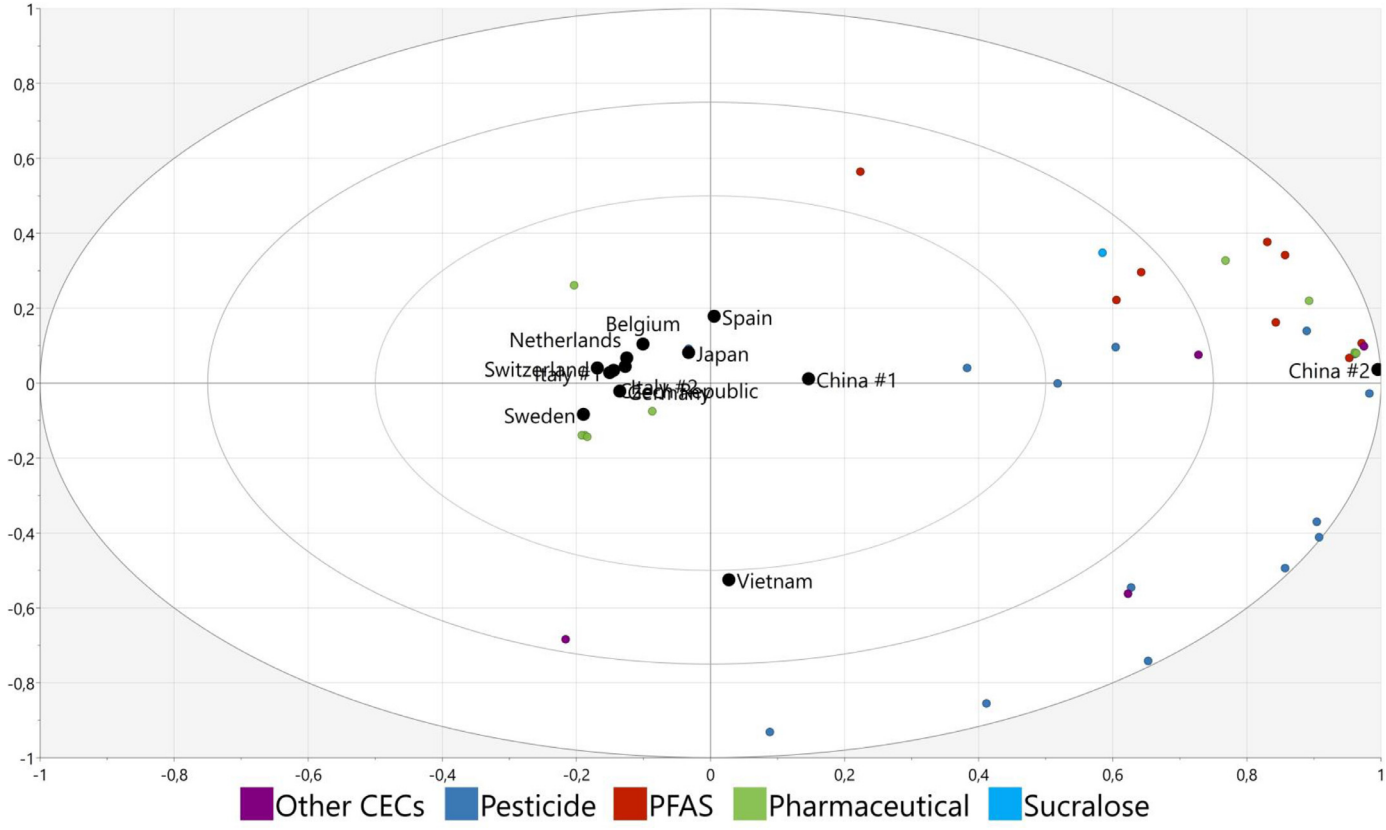

Fig. A2. PCA biplot of drinking water concentrations of individual CECs at all DWTPs (n = 13). The first two principal components (PCs) jointly explained 62% of the data variance (PC1: 48%, PC2: 14%).

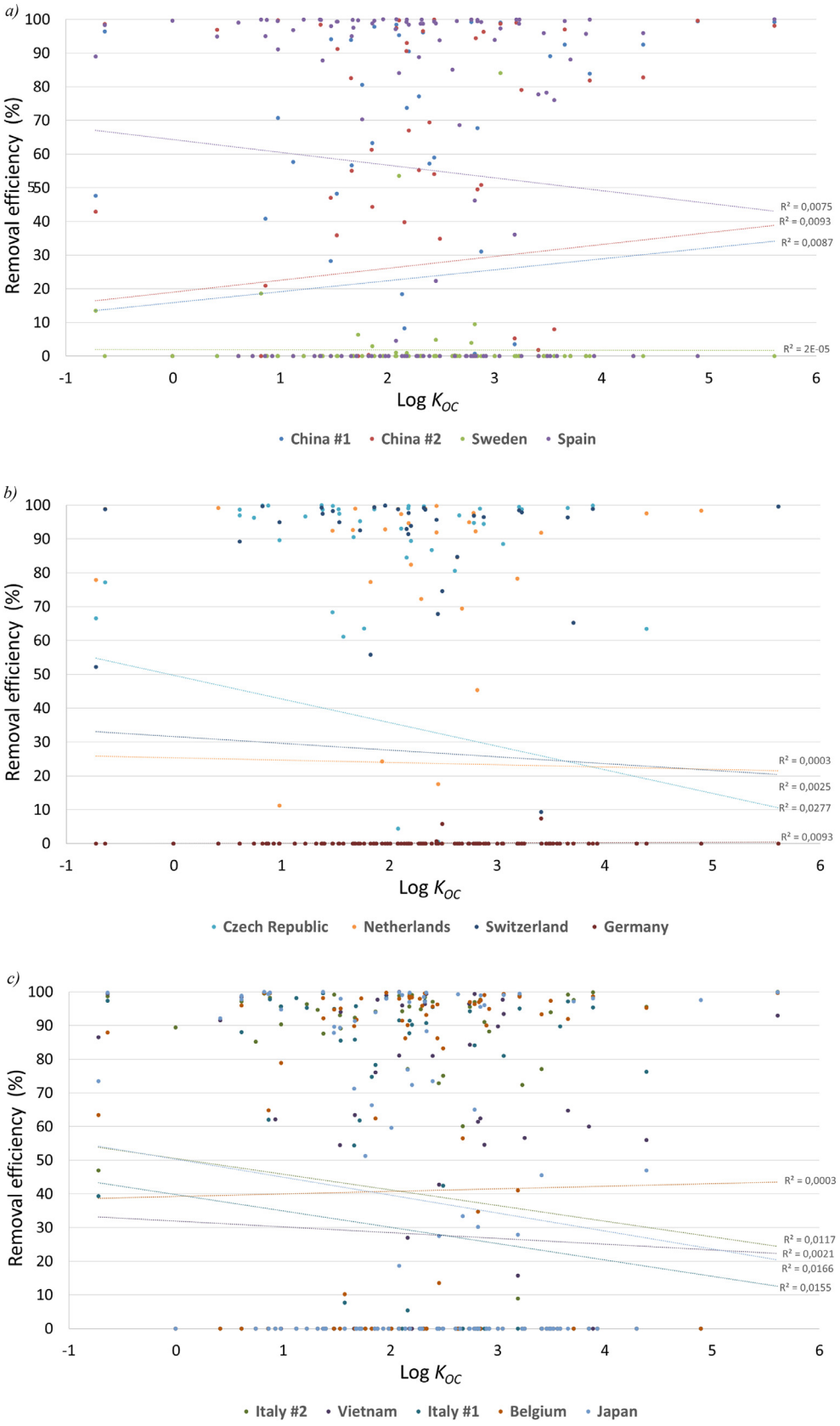

Fig. A3. Removal efficiency (%) plotted vs log K_{oc} for all individual CECs at all individual DWTPs (n = 13). Dotted lines represent regression lines for each individual DWTP. For visibility, the DWTPs was divided in sub-figure a-c.

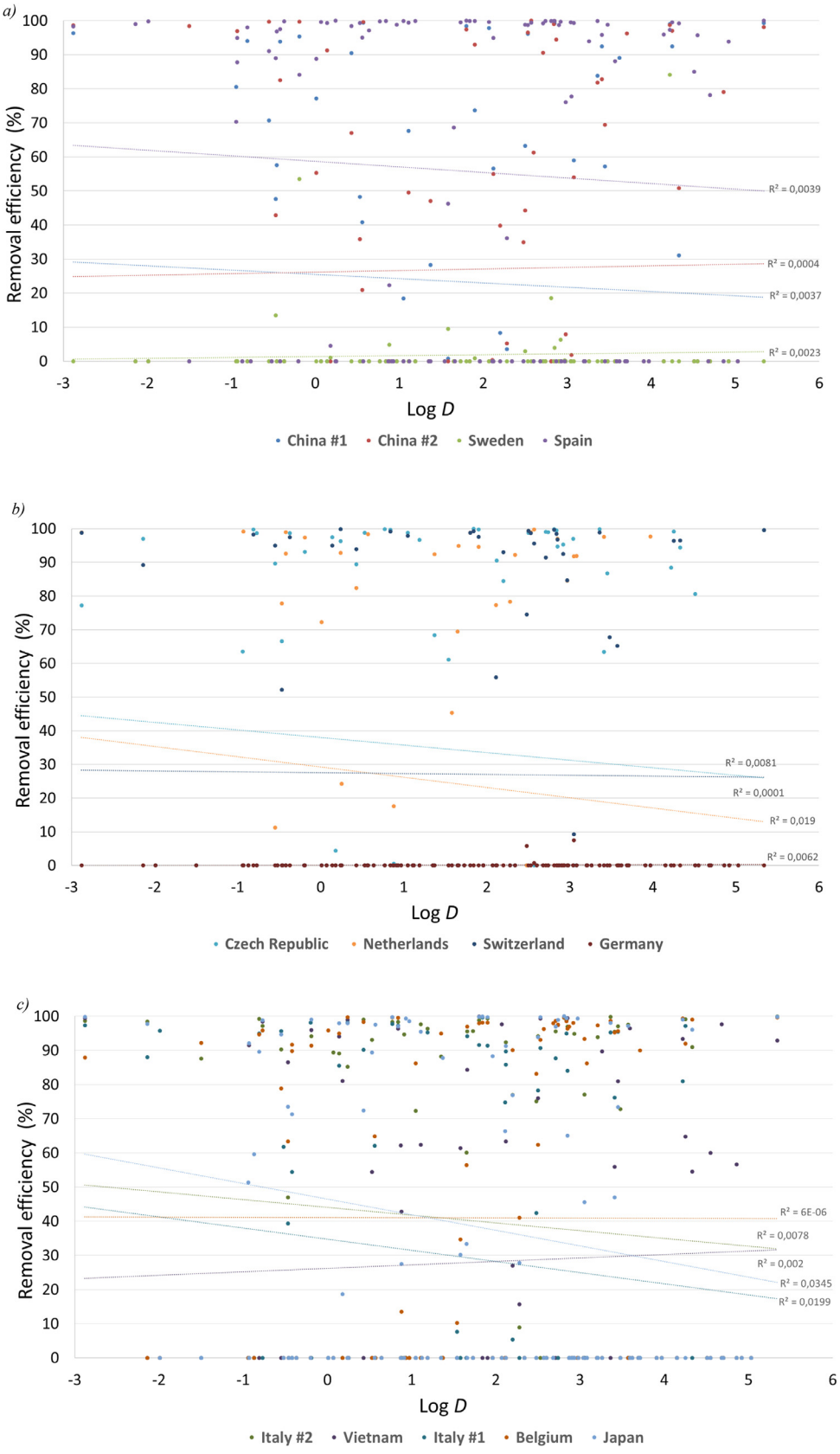

Fig. A4. Removal efficiency (%) plotted vs log *D* for all individual CECs at all individual DWTPs (n = 13). Dotted lines represent regression lines for each individual DWTP. For visibility, the DWTPs was divided in sub-figure a-c.

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