Occurrence, distribution and risk assessment of organic micropollutants in the Saronikos Gulf, Greece, utilizing LC-TIMS-HRMS

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SUPPLEMENTARY INFORMATION

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1. Sampling stations

A sampling campaign was conducted by the Hellenic Centre for Marine research (HCMR) in March of 2023 with the research vessel (R/V) "Aegaeo" in the wider Saronikos Gulf and Elefsis Bay, collecting seawater samples (n=13) from various depths (surface, 50m and near bottom) and corresponding surface sediment samples (n=4), along with influent (n=2) and related effluent (n=2) wastewater samples from the Thriassio and Psyttalia wastewater treatment plants (WWTPs) operating in the study area. Detailed information regarding sampling stations, their oceanographic characteristics, and sampling depth for corresponding wastewater samples are presented in Tables S1 & S2.

Table S1: Location and characteristics of sampling stations

Sampling Station	Latitude	Longitude	Sampling Depth	Sediment
S1	38º 01.05' N	23º 33.27' E	2 m 18 m	√
S1-Biol (Thriassio WWTP)	38° 01.93' N	23° 34.30' E	10 m Influent + Effluent	-
S7	37º 55.42' N	23º 35.45' E	2 m 50 m 69 m	√
S7-Biol (Psyttalia WWTP)	37° 55.94'N	23° 35.50'E	63 m Influent + Effluent	-
S8	37º 53.00' N	23º 32.00' E	2 m 50 m 90 m	√
S11	37º 52.36' N	23º 38.30' E	2 m 50 m 73 m	√

38 **Table S2**: Physicochemical characteristics of the sampling stations in different sampling depths

Station	Depth (m)	T (°C)	Salinity	Dissolved Oxygen (mL L^{-1})	Particulate Organic Carbon (µmol L^{-1})	Chl-a (µg L^{-1})	Organic C in sediment (%)
S1	2	15.67	38.72	5.88	27.4	1.13	1.90
	18	14.52	38.77	5.25	16.1	1.11	
S7	2	15.10	38.22	5.48	10.5	1.05	2.08
	50	15.17	39.06	5.24	5.67	0.280	
	69	15.05	39.07	5.03	6.46	0.220	
S8	2	15.34	39.08	5.66	8.79	0.150	0.89
	50	15.25	39.08	5.57	5.16	0.290	
	90	15.06	39.07	5.24	3.61	0.510	
S11	2	15.34	38.72	5.73	8.79	0.670	0.30
	50	15.11	39.05	5.40	5.65	0.380	
	73	15.11	39.06	5.34	4.93	0.360	

2. Sample preparation

To identify the chemical imprint in tested seawaters, a previously reported generic sample preparation protocol with slight modifications was applied for seawater samples[1,2]. For the pre-treatment of considered sediment samples, a previously in-house developed method was followed[3,4], with minor modifications. Lastly, wastewater sample preparation was also based on a previously reported generic sample preparation protocol with slight modifications[5]. All three methodologies aimed to extract as many semi-polar to polar, thermally unstable, LC-amenable organic priority pollutants (PPs) and emerging contaminants (ECs), along with their respective metabolites and transformation products (TPs) as possible. Key points with detailed information regarding sample preparations are discussed subsequently.

2.1. Seawater samples preparation

Total volume of 1 L per seawater sample was stored in the dark at 4°C until sample preparation. Sample pH was adjusted to 6.5 (±0.2) with HCl 0.1 M and/or ammonium hydroxide 25% v/v. Consequently, an isotopically labelled (IS) mix was spiked in each sample for chromatographic quality control and quantification of detected analytes. A respective spiking procedure with reference standards mixture takes place, producing 6-level spiked samples, for quantification purposes. Samples were left to stand for 15 min and then, sample clean-up and pre-concentration was realized by SPE. Layered mixed-mode cartridges consisting of Oasis HLB (200 mg) and a mixture of Strata-X-AW (weak anion exchanger), Strata-X-CW (weak cation exchanger) and Isolute ENV+ (350 mg of total mixture) were used.

Conditioning of the cartridges was initially performed with 3 mL methanol followed by 3 mL of water. Elution of the analytes trapped within the sorbent materials was facilitated using a sequence of basic solution [6 mL of ethyl acetate/methanol (50/50 *v/v*), containing 2% v/v ammonium hydroxide], followed by an acidic solution [4 mL of ethyl acetate/methanol (50/50 v/v), containing 1.7% v/v formic acid]. Extracts were evaporated to dryness under a gentle

nitrogen stream (at 40°C) and reconstituted to a final volume of 200 μL (methanol/milli-Q, 50/50 v/v). Extracts were finally filtered directly into 2 mL glass vials equipped with inserts using syringes fitted with 0.22 μm RC membrane filters. attaining a 5,000-fold pre-concentration factor.

2.2. Sediment samples preparation

Sediment samples were initially freeze-dried at a temperature of -55^{o}C at 5×10^{-5} bar. A total mass of 1 g of each lyophilized sediment sample was stored in 15 mL centrifuge tube in the dark at room temperature until extraction. An IS mix was spiked in each sample as before, and a respective spiking procedure took place with the reference standards mixture, again producing 6-level spiked samples. The samples were left to stand for 15 min. For the extraction step 3 mL of extraction solvent mixture were added to each sample, followed by hand shaking for 1 min, until the entire sediment mass was wet and then shaken by vortex for another 1 min. Then, ultrasonic assisted extraction (UAE) at 50^{o}C for 15 min took place at an adjusted bath temperature of 50^{o}C. Samples were then centrifuged at 4,000 rpm for 10 min, and each supernatant liquid was collected in dedicated glass test tubes. The extraction step was repeated 2 more times, collecting a total of 9 mL supernatant liquid. Final extracts were evaporated to dryness under a gentle nitrogen stream (at 40°C) and reconstituted to a final volume of 200 μL (methanol/milli-Q, 50/50 v/v). As before, the extracts were filtered directly into a 2 mL glass vial equipped with insert. using syringes fitted with 0.22 μm RC membrane filters, attaining a 5-fold pre-concentration factor.

The extraction solvent used for UAE consisted of a MeOH/H_2O 50/50 v/v mix with 0.5% v/v formic acid and 0.1% w/v EDTA. It was prepared on the day of the extraction and stored in the dark until use.

2.3. Wastewater samples preparation

A total volume of 100 mL of each wastewater sample were stored in the freezer at -20°C pending sample preparation, same as in seawater samples. pH was adjusted to 6.5 ± 0.2 and then an IS mixture was spiked in each wastewater sample. Samples were left to stand for 15 min and then, as in seawater preparation, sample clean-up and pre-concentration was realized by SPE, utilizing the same layered mixed-mode cartridges and conditioning parameters as mentioned above. Analyte elution was realized using the same eluent mixtures as in seawater samples and after solvent evaporation via N_2 stream, extracts were again filtered directly into 2 mL glass vials equipped with inserts using syringes fitted with 0.22 μm RC membrane filters, attaining a 500-fold pre-concentration factor.

3. Instrumental analysis

Extracted analytes were separated using ultra-high potential liquid chromatography (UHPLC) (Elute LC series, Bruker Daltonics, Bremen, Germany), coupled to a hybrid trapped ion mobility-quadrupole time-of-flight (TIMS-QTOF) spectrometer (timsTOF Pro 2, Bruker Daltonics, Bremen, Germany). The gradient elution program is presented in **Table S3**.

Table S3: Gradient elution parameters for HRMS analysis

Time (min)	Flow (mL/min)	%A	%B
0.00	0.200	96.0	4.0
0.10	0.200	96.0	4.0
1.00	0.200	81.7	18.3
2.50	0.223	50.0	50.0
14.00	0.400	0.1	99.9
16.00	0.480	0.1	99.9
16.10	0.480	96.0	4.0
19.00	0.480	96.0	4.0
19.10	0.200	96.0	4.0
20.00	0.200	96.0	4.0

Solvents used for mobile phases in positive (+) ionization mode were:

A. MeOH/H_2O (99/1 v/v), 0.01% formic acid, 0.005 M ammonium formate

B. MeOH, 0.01% formic acid, 0.005 M ammonium formate

Solvents used for mobile phases in negative (–) ionization mode were:

A. MeOH/H_2O (99/1 v/v), 0.005 M ammonium acetate

B. MeOH, 0.005 M ammonium acetate

Prior to instrumental analysis, calibration of both mobility and mass accuracy took place. For mobility calibration, collision cross-section (CCS) values of certain compound ions included in an IMS calibration mix were evaluated and accepted only when %ΔCCS value did not exceed 1% (more than 99% accuracy). For mass accuracy, masses of cluster sodium formate ions produced within the ion source were considered. Mass accuracy was considered acceptable if Δm/z values did not exceed ± 0.1 mDa (more than 99% accuracy).

Two separate reversed-phase chromatographic runs for positive and negative vacuum insulated probe - heated electrospray ionization (VIP-HESI) modes were conducted. Auto sampler injection volume was set at 1 μL for positive ionization and at 3 μL for negative ionization mode. ensuring up to par peak intensity for detected analyte ions and their respective fragments. Data Independent Acquisition (DIA) scan mode was applied for data acquirement, called broadband Collision Induced Dissociation (bbCID). In DIA scan mode, low collision energy (4 eV) produces a full scan spectrum. followed by high collision energy (25 eV) producing MS/MS fragment ion spectra. Data produced in DIA scan mode were utilized for quantification purposes in the wide-scope target screening procedure.

Samples were analyzed in TIMS-ON mode, making use of the instrumentation's added value, which provides an additional dimension of separation, granting the ability of 4D-separation of isomeric compounds in without the need to apply specific chromatographic parameters[6]. This instrumentation also amplifies peak capacity and increases sensitivity. Data received from the TIMS-ON analysis were translated into CCS values[6,7]. Experimental CCS

values were then considered for %ΔCCS calculation, adding an additional identification parameter to the already strict ones selected for HRMS application[8].

4. QA/QC procedures

To ensure quality assurance of received data, QA/QC procedures were followed. Procedural and field blanks were analyzed along with each environmental matrix. A sample for each batch, which was expected to be the least chemically burdened, was used for spiking, producing 6-level spiked samples, as mentioned above. These 6-level spiked samples were used for quantification purposes, aiming to bypass different matrices' effects. Relative areas in each sample were compared with those of the 6-level spiking curve. The spike level with the closest relative area to the sample was used for quantification.

Analytes were confirmed for determination only if their relative area was equal or above 150% of each blank sample's relative area, provided that the analyte is also confirmed in the blanks. Every sample and blank analyzed was also spiked with an IS mixture, aiming to evaluate the instrumentation's sensitivity during analysis and facilitate quantifications. The list of chosen compounds for the IS mix utilized in this study is presented in **Table S4**.

Table S4: List of isotopically labelled internal standards used for quality assurance

Ionization mode	I.S.	Formula	m/z (Da)	RT (min)	CCS (Å²)
+	Amitriptyline D3	$C_{20}D_3H_{20}N$	281.2092	7.40	168.45
+	Atenolol D7	$C_{14}D_7H_{15}N_2O_3$	274.2143	3.49	159.39
+	Atrazine D5	$C_8D_5H_9ClN_5$	221.1324	7.59	150.30
+	Caffeine D9	$C_8D_9HN_4O_2$	204.1441	4.32	141.18
+	Cetirizine D8	$C_{21}D_8H_{17}ClN_2S$	397.2129	8.16	200.17
+	Citalopram D4	$C_{20}D_4H_{17}FN_2O$	329.1962	5.72	181.99
+	Diazepam D5	$C_{16}D_5H_8ClN_2O$	290.1103	8.94	166.70
+	Diuron D6	$C_9D_6H_4Cl_2N_2O$	239.0620	7.82	151.55

Ionization mode	I.S.	Formula	m/z (Da)	RT (min)	CCS (Å²)
+	Flunixin D3	$C_{14}D_3H_8F_3N_2O_2$	300.1034	8.90	164.24
+	Mefenamic acid D3	$C_{15}D_3H_{12}NO_2$	245.1364	11.22	155.82
+	Meloxicam D3	$C_{14}D_3H_{10}N_3O_4S_2$	355.0609	6.74	178.94
+	Metoprolol D7	$C_{15}D_7H_{18}NO_3$	275.2347	4.66	173.40
+	Sertraline D3	$C_{17}D_3H_{14}Cl_2N$	309.0999	8.05	169.32
+	Sulfadiazine D4	$C_{10}D_4H_6N_4O_2S$	255.0848	3.83	155.15
+	Sulfamerazine D4	$C_{11}D_4H_8N_4O_2S$	269.1005	4.12	160.06
+	Tramadol D6	$C_{16}D_6H_{19}NO_2$	270.2335	4.64	162.57
+	Venlafaxine D6	$C_{17}D_6H_{21}NO_2$	284.2491	5.54	172.27
–	Bisphenol A D16	$C_{15}D_{14}H_2O_2$	241.1956	7.57	161.84
–	Diuron D6	$C_9D_6H_4Cl_2N_2O$	237.0474	7.89	147.85
–	Flunixin D3	$C_{14}D_3H_8F_3N_2O_2$	298.0888	7.43	160.94
–	Meloxicam D3	$C_{14}D_3H_{10}N_3O_4S_2$	353.0463	5.77	177.48

5. Data treatment

5.1. Screening parameters

Acquired raw data were treated using the TASQ software (Bruker Daltonics). The occurrence of more than 2,500 analytes from different chemical classes was investigated through wide-scope target screening, by applying the following strict identification criteria:

1. **Mass accuracy:** Calculated m/z should not differ from expected m/z more than ±2 mDa.
2. **RT shift:** Determined RT should not differ from expected RT by more than ±0.2 min.
3. **Isotope profile matching:** The fit of experimental spectrum versus the theoretical one is expressed by the software as mSigma value. The lower the mSigma is, the better mSigma value < 100 is considered acceptable.
4. **Qualifier ions detection:** All mandatory ions included in the database should be detected with similar peak shape to the one projected by the principal ion. Mandatory ions are

produced by MS and MS/MS scan modes, exceeding precursor ion peak intensity by 50%. The principal mandatory ion ratio should be the same in real samples as in the STD mix.

5. **CCS value matching:** Experimental CCS values should not differ from expected CCS values by more than 2%.

Assessed peaks not abiding by all criteria were not reported in this study, as they were considered false positive. Possession of reference standards for each determined analyte provides the ability to conduct a wide-scope target screening of compounds, by attaining a level 1 identification level, as proposed in the literature[9].

For compounds included in the suspect screening database, retention time shift criteria were loosened to ± 0.6 min, to be able to detect possible peak candidates for further evaluation. Absence of respective reference standards lowers confidence in respect to identification level, but the availability of fragmentation data (inclusion of more than one mandatory ion) in online mass libraries sets the confidence for reported suspect compounds to a level 2a identification level[9,10].

5.2. Target and suspect screening databases

More than 2,500 analytes are included in the HRMS target screening database of the Laboratory of Analytical Chemistry, Department of Chemistry. National and Kapodistrian University of Athens, Greece, such as coffee and tobacco related compounds, pharmaceuticals, along with their human consumption metabolites and TPs, industrial chemicals, per- and polyfluorinated alkyl substances (PFAS), plant protection products and their TPs, artificial sweeteners and surfactants[11]. Among them are PPs controlled by European legislation for the preservation of the marine environment, while most analytes are classified as ECs, not yet prioritized or regulated by national and supranational legislation, neither included in respective watch lists for marine ecosystems.

Besides target screening of ECs and PPs, a suspect screening listing more than 600 surfactants, antiseptics and cleansers was utilized, further enhancing the investigated chemical domain of this study. For the development of the suspect list, mass bank data and in-silico prediction models for retention time generation were utilized. Detailed information on the employed suspect list has been previously reported in the literature[10,12].

5.3. Quantification procedure

For the quantification of ECs detected in tested samples through the target screening database application, 6-level spiked sample curves were utilized. In detail, the relative areas calculated in the samples were compared with those calculated for each spike level. The closest spike relative area to the one calculated in the tested sample was used for quantification of each analyte.

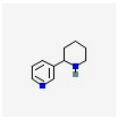
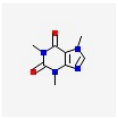
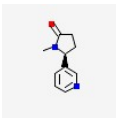
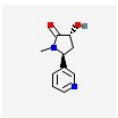
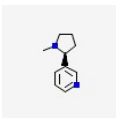
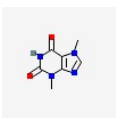
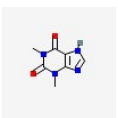
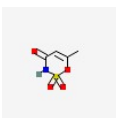
Regarding suspect-list surfactants, semi quantification procedure was followed. In detail, reported alcohol ethoxy sulfates (AES) were semi-quantified based on the signal of AES-C14, n=1, linear alkylbenzene sulfonates (LAS) and OP2EC were semi-quantified based on the signal of C10-LAS, and finally, alkyl phosphate esters and spirocyclic phosphoric acids (SPAs) were quantified based on the signal of C12 alkyl phosphate ester, for which reference standards were available.

Finally, the limits of detection (LODs) and quantification (LOQs) were calculated based on the analyte signal-to-noise (S/N) ratio of the sample with the lowest analyte concentration. An S/N equal to 3 represents the LOD value, while an S/N equal to 10 represents the LOQ value. Compound concentrations not exceeding LOD concentrations were marked as "<LOD". while concentrations ranging between LOD and LOQ values were marked as "BQL" (below quantification limit) in the presented results of Tables S6 and S7. Aiming to generate a visualization of generated results in the main body of the manuscript, a statistical compromise was considered, where BQL values were replaced with concentrations equaling LOQ/2.

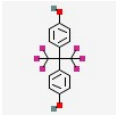
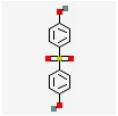
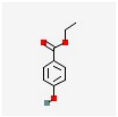
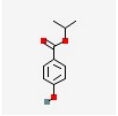
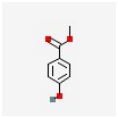
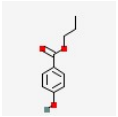
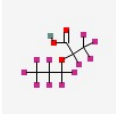
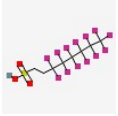
5.4. Ecotoxicological data

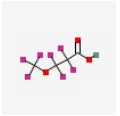
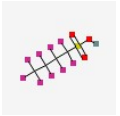
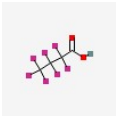
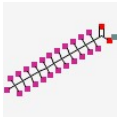
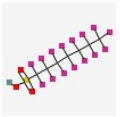
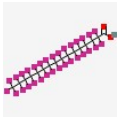
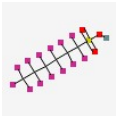
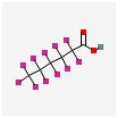
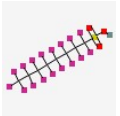
To prioritize determined chemical compounds based on their potential adverse effect towards the marine environment, information regarding lipophilicity, as well as predicted no effect concentration (PNEC) levels were utilized. To that end, a data mining tool was employed to produce lists of octanol/water partition coefficient (log P) values, recorded on PubChem. and PNEC values registered in the NORMAN network database[13–15]. Recorded PNEC values, which reflect on the toxicity of determined substances, derive from published experimental data, available in the literature, or from in silico information generated by the Quantitative Structure – Activity Relationship (QSAR) prediction model or were calculated utilizing recorded freshwater PNEC values. Ecotoxicological information of determined analytes, along with their chemical identifiers for both datasets, is presented in **Table S5**.

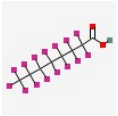
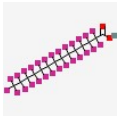
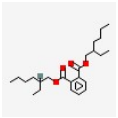
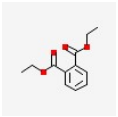
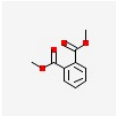
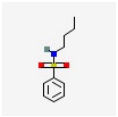
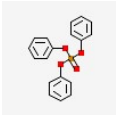
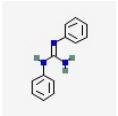
Table S5: Chemical identifiers of determined analytes, along with their logP values (lipophilicity) and registered PNEC values on the NORMAN network. PNEC values are derived from experimental data or generated by prediction model QSAR or calculated based on available freshwater PNEC values.

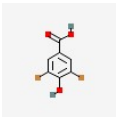
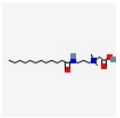
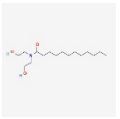
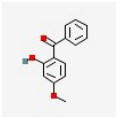
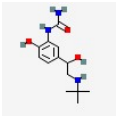
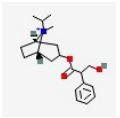
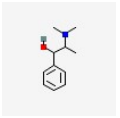
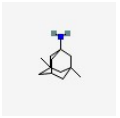
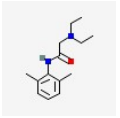
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Anabasine	Coffee & tobacco related compounds	Stimulants	2181		$C_{10}H_{14}N_2$	NS00100868	1.00	0.960	84.1
Caffeine	Coffee & tobacco related compounds	Stimulants	2519		$C_8H_{10}N_4O_2$	NS00000273	-0.10	8.70	5.61
Cotinine	Coffee & tobacco related compounds	Stimulants	854019		$C_{10}H_{12}N_2O$	NS00075577	-0.30	0.940	52.0
Hydroxy-cotinine	Coffee & tobacco related compounds	Stimulants	107963		$C_{10}H_{12}N_2O_2$	NS00010478	-0.90	2.06	2.50
Nicotine	Coffee & tobacco related compounds	Stimulants	89594		$C_{10}H_{14}N_2$	NS00010445	1.20	0.550	36.3
Theobromine	Coffee & tobacco related compounds	Stimulants	5429		$C_7H_8N_4O_2$	NS00009946	-0.80	10.0	513
Theophylline	Coffee & tobacco related compounds	Stimulants	2153		$C_7H_8N_4O_2$	NS00010258	0.00	10.0	51.3
Acesulfame	Food additives	Artificial sweeteners	36573		$C_4H_5NO_4S$	NS00000381	-0.30	7.24	196

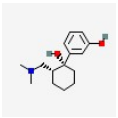
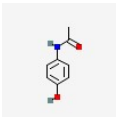
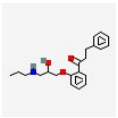
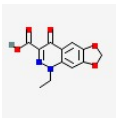
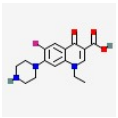
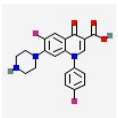
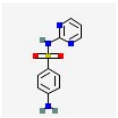
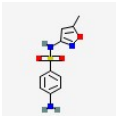
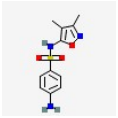
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Saccharin	Food additives	Artificial sweeteners	5143		$C_7H_5NO_3S$	NS00007781	0.90	18.3	93.4
2-amino-benzothiazole	Industrial chemicals	Corrosion inhibitors	8706		$C_7H_6N_2S$	NS00010260	1.90	0.100	3.86
5-methyl-benzotriazole	Industrial chemicals	Corrosion inhibitors	8705		$C_7H_7N_3$	NS00008943	1.40	15.0	705
Benzothiazole-2-sulfonic acid	Industrial chemicals	Corrosion inhibitors	30647		$C_7H_5NO_3S_2$	NS00010634	1.50	1.00	32.6
Mercaptobenzothiazole	Industrial chemicals	Corrosion inhibitors	697993		$C_7H_5NS_2$	NS00000568	2.40	0.0800	42.6
N.N-dimethylaniline	Industrial chemicals	Dyes	949		$C_8H_{11}N$	NS00010833	2.30	4.40	529
1-naphthol	Industrial chemicals	Manufacturing agents	7005		$C_{10}H_8O$	NS00005331	2.80	0.280	76.0
4-iodophenoxyacetic acid	Industrial chemicals	Manufacturing agents	74658		$C_8H_7IO_3$	NS00026148	2.70	0.73	70.5
4-nitrophenol	Industrial chemicals	Manufacturing agents	980		$C_6H_5NO_3$	NS00010495	1.90	0.500	65.9

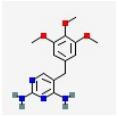
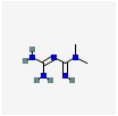
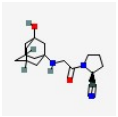
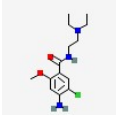
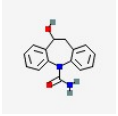
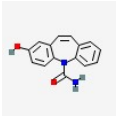
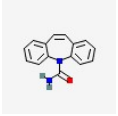
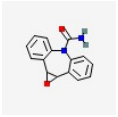
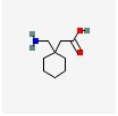
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Bisphenol AF	Industrial chemicals	Manufacturing agents	73864		$C_{15}H_{10}F_6O_2$	NS00011437	4.50	0.100	346
Bisphenol S	Industrial chemicals	Manufacturing agents	6626		$C_{12}H_{10}O_4S$	NS00010610	1.90	27.0	353
Ethylparaben	Industrial chemicals	Parabens	8434		$C_9H_{10}O_3$	NS00008316	2.50	1.00	128
Isopropylparaben	Industrial chemicals	Parabens	20161		$C_{10}H_{12}O_3$	NS00002618	2.80	1.13	72.2
Methylparaben	Industrial chemicals	Parabens	7456		$C_8H_8O_3$	NS00001849	2.00	0.400	21.9
Propylparaben	Industrial chemicals	Parabens	7175		$C_{10}H_{12}O_3$	NS00002126	3.00	0.640	116
2.3.3.3-tetrafluoro-2-(heptafluoropropoxy)propanoic acid (HFPO-DA on GenX)	Industrial chemicals	PFAS	114481		$C_6HF_{11}O_3$	NS00011372	3.60	0.140	29.5
4.8-dioxa-3H-perfluorononanoic acid (ADONA)	Industrial chemicals	PFAS	52915299		$C_7H_2F_{12}O_4$	NS00011374	4.10	0.170	86.2
6:2 fluorotelomer sulfonic acid (6:2 FTS)	Industrial chemicals	PFAS	119688		$C_8H_5F_{13}O_3S$	NS00010579	3.90	0.0620	30.1

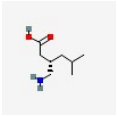
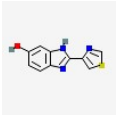
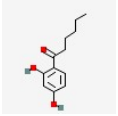
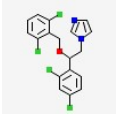
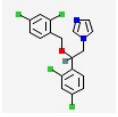
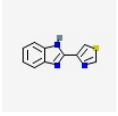
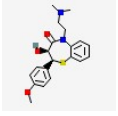
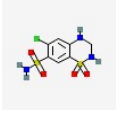
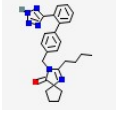
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Perfluoro-4-oxapentanoic acid (PFMPA or PF4OPeA)	Industrial chemicals	PFAS	120228		$C_4HF_7O_3$	NS00002613	2.30	0.460	17.7
Perfluorobutanesulfonic acid (PFBS)	Industrial chemicals	PFAS	67815		$C_4HF_9O_3S$	NS00010276	2.30	37.2	2,166
Perfluorobutanoic acid (PFBA)	Industrial chemicals	PFAS	9777		$C_4HF_7O_2$	NS00000364	2.20	2.78	166
Perfluorododecanoic acid (PFDoA)	Industrial chemicals	PFAS	67545		$C_{12}HF_{23}O_2$	NS00009617	7.60	0.0110	485
Perfluoroheptanesulfonic acid (PFHpS)	Industrial chemicals	PFAS	67820		$C_7HF_{15}O_3S$	NS00011291	4.30	0.0480	30.0
Perfluorohexadecanoic acid (PFHxDA)	Industrial chemicals	PFAS	106027		$C_{16}HF_{31}O_2$	NS00011276	10.30	0.00780	583
Perfluorohexanesulfonic acid (PFHxS)	Industrial chemicals	PFAS	67734		$C_6HF_{13}O_3S$	NS00010279	3.70	0.0870	101
Perfluorohexanoic acid (PFHxA)	Industrial chemicals	PFAS	67542		$C_6HF_{11}O_2$	NS00000366	3.60	14.0	7,602
Perfluorooctanesulfonic acid (PFOS)	Industrial chemicals	PFAS	74483		$C_8HF_{17}O_3S$	NS00010280	5.00	2.50	0.00670

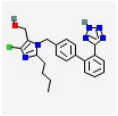
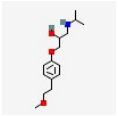
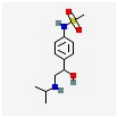
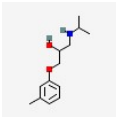
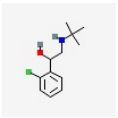
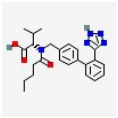
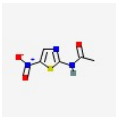
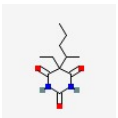
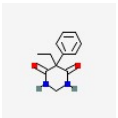
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Perfluorooctanoic acid (PFOA)	Industrial chemicals	PFAS	9554		$C_8HF_{15}O_2$	NS00009389	4.90	0.0180	6.04
Perfluoropentanoic acid (PFPeA)	Industrial chemicals	PFAS	75921		$C_5HF_9O_2$	NS00000365	2.90	0.390	24.8
Perfluorotetradecanoic acid (PFTeDA)	Industrial chemicals	PFAS	67822		$C_{14}HF_{27}O_2$	NS00011273	9.00	0.00830	954
Di-(2-ethylhexyl) phthalate (DEHP)	Industrial chemicals	Plasticizers	8343		$C_{24}H_{38}O_4$	NS00010909	7.40	1.30	0.180
Diethyl phthalate (DEP)	Industrial chemicals	Plasticizers	6781		$C_{12}H_{14}O_4$	NS00009893	2.50	1.20	530
Dimethyl phthalate (DMP)	Industrial chemicals	Plasticizers	8554		$C_{10}H_{10}O_4$	NS00010268	1.60	19.2	1.00
N-butylbenzenesulfonamide	Industrial chemicals	Plasticizers	19241		$C_{10}H_{15}NO_2S$	NS00007746	2.10	3.70	124
Triphenyl phosphate (TPHP)	Industrial chemicals	Plasticizers	8289		$C_{18}H_{15}O_4P$	NS00010271	4.60	0.0740	14.8
1.3-diphenylguanidine	Industrial chemicals	Rubber vulcanizers	7594		$C_{13}H_{13}N_3$	NS00011462	2.40	3.00	12.3

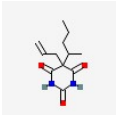
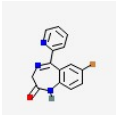
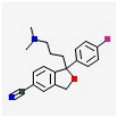
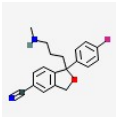
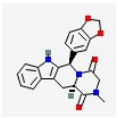
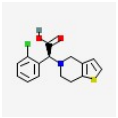
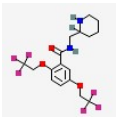
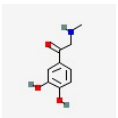
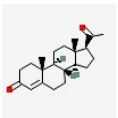
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
3.5-dibromo-4-hydroxy-benzoic acid	Personal care products	Cosmetics preservatives	76857		$C_7H_4Br_2O_3$	NS00000325	3.30	0.480	92.5
Lauramidopropylbetaine	Personal care products	Skin cleansers	20281		$C_{19}H_{39}N_2O_3^+$	NS00010635	4.70	1.35	1,584
Lauryl diethanolamide	Personal care products	Skin cleansers	8430		$C_{16}H_{33}NO_3$	NS00010591	3.50	0.700	65.0
Oxybenzone (3-benzophenone)	Personal care products	UV filters	4632		$C_{14}H_{12}O_3$	NS00000222	3.60	0.0670	35.2
Carbuterol	Pharmaceuticals & TPs	Adrenergics	36976		$C_{13}H_{21}N_3O_3$	NS00009938	-0.10	1.07	2.57
Ipratropium	Pharmaceuticals & TPs	Adrenergics	657309		$C_{20}H_{30}NO_3^+$	NS00099720	2.60	0.360	479
Methylephedrine	Pharmaceuticals & TPs	Adrenergics	4374		$C_{11}H_{17}NO$	NS00002861	1.70	2.38	231
Memantine	Pharmaceuticals & TPs	Alzheimer's disease medications	4054		$C_{12}H_{21}N$	NS00000622	3.30	0.180	450
Lidocaine	Pharmaceuticals & TPs	Analgesics	3676		$C_{14}H_{22}N_2O$	NS00000027	2.30	60.0	10,755

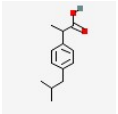
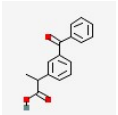
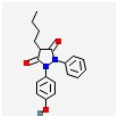
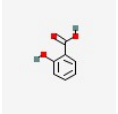
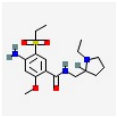
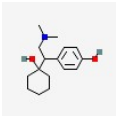
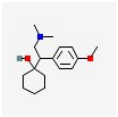
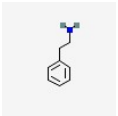
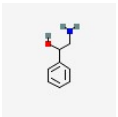
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
O-desmethyltramadol	Pharmaceuticals & TPs	Analgesics	9838803		$C_{15}H_{23}NO_2$	NS00101143	2.30	0.910	14.7
Paracetamol	Pharmaceuticals & TPs	Analgesics	1983		$C_8H_9NO_2$	NS00006214	0.50	1.41	2.28
Propafenone	Pharmaceuticals & TPs	Antiarrhythmics	4932		$C_{21}H_{27}NO_3$	NS00010400	3.30	0.0850	307
Cinoxacin	Pharmaceuticals & TPs	Antibiotics	2762		$C_{12}H_{10}N_2O_5$	NS00006827	2.10	0.370	150
Norfloxacin	Pharmaceuticals & TPs	Antibiotics	4539		$C_{16}H_{18}FN_3O_3$	NS00000224	-1.00	0.0500	8.34
Sarafloxacin	Pharmaceuticals & TPs	Antibiotics	56208		$C_{20}H_{17}F_2N_3O_3$	NS00000677	0.30	0.190	234
Sulfadiazine	Pharmaceuticals & TPs	Antibiotics	5215		$C_{10}H_{10}N_4O_2S$	NS00000198	-0.10	4.60	7.28
Sulfamethoxazole	Pharmaceuticals & TPs	Antibiotics	5329		$C_{10}H_{11}N_3O_3S$	NS00000268	0.90	0.0600	3.67
Sulfisoxazole (Sulfafurazole)	Pharmaceuticals & TPs	Antibiotics	5344		$C_{11}H_{13}N_3O_3S$	NS00002072	1.00	0.460	53.2

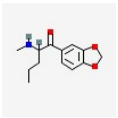
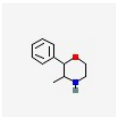
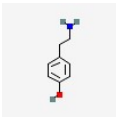
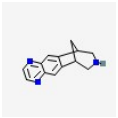
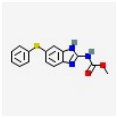
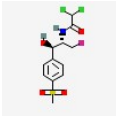
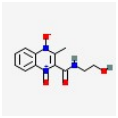
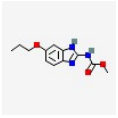
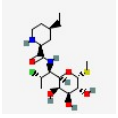
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Trimethoprim	Pharmaceuticals & TPs	Antibiotics	5578		$C_{14}H_{18}N_4O_3$	NS00000211	0.90	10.0	3.64
Metformin	Pharmaceuticals & TPs	Antidiabetics	4091		$C_4H_{11}N_5$	NS00000333	-1.30	16.0	331
Vildagliptin	Pharmaceuticals & TPs	Antidiabetics	6918537		$C_{17}H_{25}N_3O_2$	NS00010516	0.90	56.0	80.8
Metoclopramide	Pharmaceuticals & TPs	Antiemetics	4168		$C_{14}H_{22}ClN_3O_2$	NS00000392	2.60	0.130	22.9
10-hydroxycarbamazepine	Pharmaceuticals & TPs	Antiepileptics	114709		$C_{15}H_{14}N_2O_2$	NS00010437	1.40	10.0	3,548
2-hydroxycarbamazepine	Pharmaceuticals & TPs	Antiepileptics	129274		$C_{15}H_{12}N_2O_2$	NS00009902	2.10	0.200	73.6
Carbamazepine	Pharmaceuticals & TPs	Antiepileptics	2554		$C_{15}H_{12}N_2O$	NS00000207	2.50	0.250	56.9
Carbamazepine-10.11-epoxide	Pharmaceuticals & TPs	Antiepileptics	2555		$C_{15}H_{12}N_2O_2$	NS00000327	1.30	0.260	116
Gabapentin	Pharmaceuticals & TPs	Antiepileptics	3446		$C_9H_{17}NO_2$	NS00000335	-1.10	100	7,872

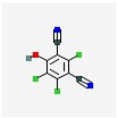
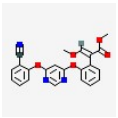
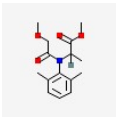
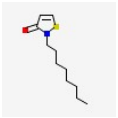
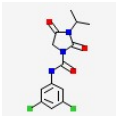
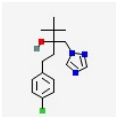
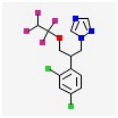
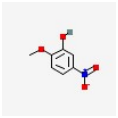
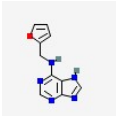
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Pregabalin	Pharmaceuticals & TPs	Antiepileptics	5486971		$C_8H_{17}NO_2$	NS00000537	-1.60	10.0	534
5-hydroxy-thiabendazole	Pharmaceuticals & TPs	Antifungals	108227		$C_{10}H_7N_3OS$	NS00006865	2.10	0.0630	71.5
Caproylresorcinol	Pharmaceuticals & TPs	Antifungals	76596		$C_{12}H_{16}O_3$	NS00006278	3.40	0.0950	2.84
Isoconazole	Pharmaceuticals & TPs	Antifungals	3760		$C_{18}H_{14}Cl_4N_2O$	NS00006034	5.30	0.00450	0.790
Miconazole	Pharmaceuticals & TPs	Antifungals	4189		$C_{18}H_{14}Cl_4N_2O$	NS00004552	5.30	0.0025	0.690
Thiabendazole	Pharmaceuticals & TPs	Antifungals	5430		$C_{10}H_7N_3S$	NS00007958	2.50	0.120	105
Deacetyldiltiazem	Pharmaceuticals & TPs	Antihypertensives	91638		$C_{20}H_{24}N_2O_3S$	NS00006884	2.50	0.0360	22.6
Hydrochlorothiazide	Pharmaceuticals & TPs	Antihypertensives	3639		$C_7H_8ClN_3O_4S_2$	NS00000343	-0.10	10.0	420
Irbesartan	Pharmaceuticals & TPs	Antihypertensives	3749		$C_{25}H_{28}N_6O$	NS00000387	4.10	70.0	744,185

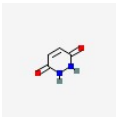
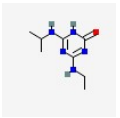
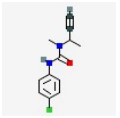
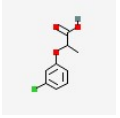
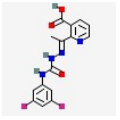
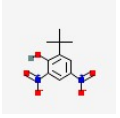
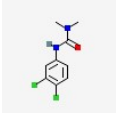
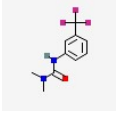
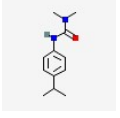
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Losartan	Pharmaceuticals & TPs	Antihypertensives	3961		$C_{22}H_{23}ClN_6O$	NS00008822	4.30	24.5	52,103
Metoprolol	Pharmaceuticals & TPs	Antihypertensives	4171		$C_{15}H_{25}NO_3$	NS00000197	1.90	0.860	557
Sotalol	Pharmaceuticals & TPs	Antihypertensives	5253		$C_{12}H_{20}N_2O_3S$	NS00000195	0.20	0.650	41.7
Toliprolol	Pharmaceuticals & TPs	Antihypertensives	18047		$C_{13}H_{21}NO_2$	NS00010648	1.90	1.24	2.73
Tulobuterol	Pharmaceuticals & TPs	Antihypertensives	5606		$C_{12}H_{18}ClNO$	NS00002191	2.30	0.530	30.7
Valsartan	Pharmaceuticals & TPs	Antihypertensives	60846		$C_{24}H_{29}N_5O_3$	NS00000341	4.40	56.0	1,017
2-acetamido-5-nitrothiazole (Aminitrozole)	Pharmaceuticals & TPs	Antiprotozoans	8798		$C_5H_5N_3O_3S$	NS00024548	1.30	1.27	122
Pentobarbital	Pharmaceuticals & TPs	Barbiturates	4737		$C_{11}H_{18}N_2O_3$	NS00008670	2.10	4.95	392
Primidone	Pharmaceuticals & TPs	Barbiturates	4909		$C_{12}H_{14}N_2O_2$	NS00000208	0.90	0.910	50.0

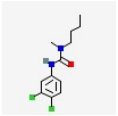
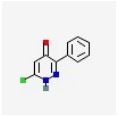
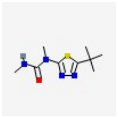
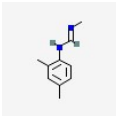
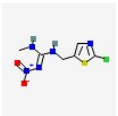
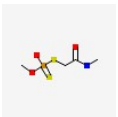
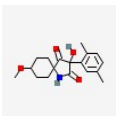
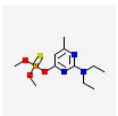
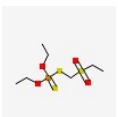
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Secobarbital	Pharmaceuticals & TPs	Barbiturates	5193		$C_{12}H_{18}N_2O_3$	NS00010411	2.00	0.420	25.9
Bromazepam	Pharmaceuticals & TPs	Benzodiazepines	2441		$C_{14}H_{10}BrN_3O$	NS00008673	1.70	0.0590	12.5
Citalopram	Pharmaceuticals & TPs	Benzodiazepines	2771		$C_{20}H_{21}FN_2O$	NS00000035	3.20	1.60	1,923
Norcitalopram	Pharmaceuticals & TPs	Benzodiazepines	162180		$C_{19}H_{19}FN_2O$	NS00006900	2.80	0.0500	24.0
Tadalafil	Pharmaceuticals & TPs	Erectile dysfunction medications	110635		$C_{22}H_{19}N_3O_4$	NS00006532	2.30	4.80	145,366
Clopidogrel carboxylic acid	Pharmaceuticals & TPs	Heart medications	9861403		$C_{15}H_{14}ClNO_2S$	NS00000417	1.10	0.0650	28.2
Flecainide	Pharmaceuticals & TPs	Heart medications	3356		$C_{17}H_{20}F_6N_2O_3$	NS00010512	3.80	0.0640	63.1
Adrenalone	Pharmaceuticals & TPs	Hormones	7436		$C_9H_{11}NO_3$	NS00003497	0.50	4.56	409
Progesterone	Pharmaceuticals & TPs	Hormones	5994		$C_{21}H_{30}O_2$	NS00010899	3.90	0.100	27,806

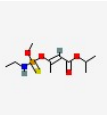
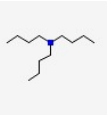
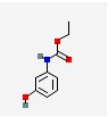
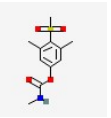
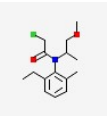
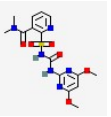
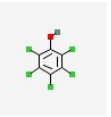
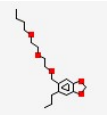
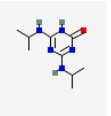
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Ibuprofen	Pharmaceuticals & TPs	NSAIDs	3672		$C_{13}H_{18}O_2$	NS00000214	3.50	0.00110	0.0930
Ketoprofen	Pharmaceuticals & TPs	NSAIDs	3825		$C_{16}H_{14}O_3$	NS00000216	3.10	0.210	75.4
Oxyphenbutazone	Pharmaceuticals & TPs	NSAIDs	4641		$C_{19}H_{20}N_2O_3$	NS00009020	2.70	0.0870	82.8
Salicylic acid	Pharmaceuticals & TPs	NSAIDs	338		$C_7H_6O_3$	NS00010274	2.30	17.1	62.0
Amisulpiride	Pharmaceuticals & TPs	Psychoactive substances	2159		$C_{17}H_{27}N_3O_4S$	NS00000416	1.50	14.0	9,079
O-desmethylvenlafaxine (Desvenlafaxine)	Pharmaceuticals & TPs	Psychoactive substances	125017		$C_{16}H_{25}NO_2$	NS00069030	2.60	0.710	109
Venlafaxine	Pharmaceuticals & TPs	Psychoactive substances	5656		$C_{17}H_{27}NO_2$	NS00000031	2.90	0.0880	29.8
2-phenethylamine	Pharmaceuticals & TPs	Stimulants	1001		$C_8H_{11}N$	NS00010853	1.40	1.60	57.7
Apophedrin (Phenylethanolamine)	Pharmaceuticals & TPs	Stimulants	1000		$C_8H_{11}NO$	NS00014647	0.10	5.44	205

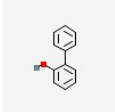
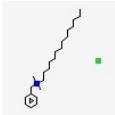
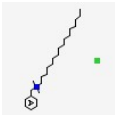
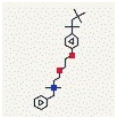
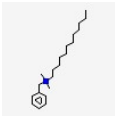
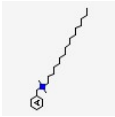
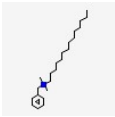
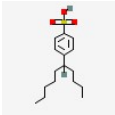
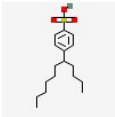
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Pentylone	Pharmaceuticals & TPs	Stimulants	60208608		$C_{13}H_{17}NO_3$	NS00015478	2.30	0.590	2.76
Phenmetrazine	Pharmaceuticals & TPs	Stimulants	4762		$C_{11}H_{15}NO$	NS00002554	1.40	3.95	276
Tyramine	Pharmaceuticals & TPs	Stimulants	5610		$C_8H_{11}NO$	NS00000072	1.10	5.96	229
Vareniclin	Pharmaceuticals & TPs	Stimulants	170361		$C_{13}H_{13}N_3$	NS00000682	0.80	0.0300	39.8
Fenbendazole	Pharmaceuticals & TPs	Veterinary drugs	3334		$C_{15}H_{13}N_3O_2S$	NS00010603	3.60	0.00630	8.41
Florfenicol	Pharmaceuticals & TPs	Veterinary drugs	114811		$C_{12}H_{14}Cl_2FNO_4S$	NS00009622	0.80	2.10	8.14
Olaquindox	Pharmaceuticals & TPs	Veterinary drugs	71905		$C_{12}H_{13}N_3O_4$	NS00001828	-0.20	1.12	2.56
Oxibendazole	Pharmaceuticals & TPs	Veterinary drugs	4622		$C_{12}H_{15}N_3O_3$	NS00003293	2.40	0.130	29.7
Pirlimycin	Pharmaceuticals & TPs	Veterinary drugs	157385		$C_{17}H_{31}ClN_2O_5S$	NS00011647	1.70	0.160	2.71

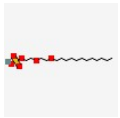
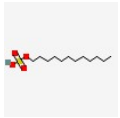
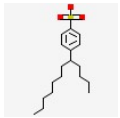
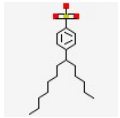
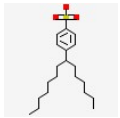
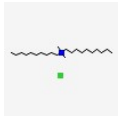
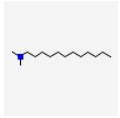
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
4-hydroxy-chlorothalonil	Plant protection products & TPs	Fungicides	34217		$C_8HCl_3N_2O$	NS00005725	2.50	0.00350	3.20
Azoxystrobin	Plant protection products & TPs	Fungicides	3034285		$C_{22}H_{17}N_3O_5$	NS00009778	3.70	0.0200	11.5
Metalaxyl	Plant protection products & TPs	Fungicides	42586		$C_{15}H_{21}NO_4$	NS00098478	1.60	10.0	343
Octhilinone	Plant protection products & TPs	Fungicides	33528		$C_{11}H_{19}NOS$	NS00000270	3.50	0.000710	0.260
RP 30228	Plant protection products & TPs	Fungicides	149013		$C_{13}H_{13}Cl_2N_3O_3$	NS00002123	2.50	0.0860	26.9
Tebuconazole	Plant protection products & TPs	Fungicides	86102		$C_{16}H_{22}ClN_3O$	NS00000280	3.70	0.0240	5.48
Tetraconazole	Plant protection products & TPs	Fungicides	80277		$C_{13}H_{11}Cl_2F_4N_3O$	NS00000709	4.40	1.90	733
5-nitroguaiacol	Plant protection products & TPs	Growth regulators	69471		$C_7H_7NO_4$	NS00035528	1.30	0.220	25.1
Kinetin	Plant protection products & TPs	Growth regulators	3830		$C_{10}H_9N_5O$	NS00013804	1.00	0.0890	4.72

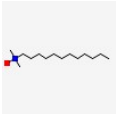
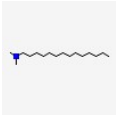
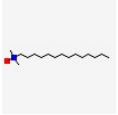
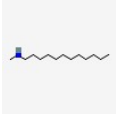
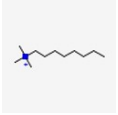
Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Maleic hydrazide	Plant protection products & TPs	Growth regulators	21954		$C_4H_4N_2O_2$	NS00005908	-0.80	8.03	140
2-hydroxy-atrazine	Plant protection products & TPs	Herbicides	135398733		$C_8H_{15}N_5O$	NS00000255	0.10	1.00	69.8
Buturon	Plant protection products & TPs	Herbicides	19587		$C_{12}H_{13}ClN_2O$	NS00006372	3.00	0.330	21.1
Cloprop	Plant protection products & TPs	Herbicides	7542		$C_9H_9ClO_3$	NS00015265	2.30	0.990	43.3
Diflufenzopyr	Plant protection products & TPs	Herbicides	6125184		$C_{15}H_{12}F_2N_4O_3$	NS00003816	1.80	0.130	41.0
Dinoterb	Plant protection products & TPs	Herbicides	14994		$C_{10}H_{12}N_2O_5$	NS00009297	3.40	0.00300	3.78
Diuron	Plant protection products & TPs	Herbicides	3120		$C_9H_{10}Cl_2N_2O$	NS00000265	2.70	0.00490	0.690
Fluometuron	Plant protection products & TPs	Herbicides	16562		$C_{10}H_{11}F_3N_2O$	NS00010278	2.40	0.0320	1.77
Isoproturon	Plant protection products & TPs	Herbicides	36679		$C_{12}H_{18}N_2O$	NS00000260	2.90	0.300	1.97

Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Neburon	Plant protection products & TPs	Herbicides	11145		$C_{12}H_{16}Cl_2N_2O$	NS00005770	3.80	0.0360	45.2
Pyridafol	Plant protection products & TPs	Herbicides	92316		$C_{10}H_7ClN_2O$	NS00007024	2.40	0.100	5.85
Tebuthiuron	Plant protection products & TPs	Herbicides	5383		$C_9H_{16}N_4OS$	NS00005719	1.60	0.320	16.0
2.4-dimethylphenyl-N-methylformamidine	Plant protection products & TPs	Insecticides	36326		$C_{10}H_{14}N_2$	NS00067117	1.70	1.03	78.4
Clothianidin	Plant protection products & TPs	Insecticides	86287519		$C_6H_8ClN_5O_2S$	NS00009180	1.30	0.00100	0.0190
Desmethyl-dimethoate	Plant protection products & TPs	Insecticides	3080588		$C_4H_{10}NO_3PS_2$	NS00067291	0.20	0.290	6.81
Keto-hydroxy-spirotetramate	Plant protection products & TPs	Insecticides	71312325		$C_{18}H_{23}NO_4$	NS00002790	1.90	1.09	71.6
Methyl-pirimiphos	Plant protection products & TPs	Insecticides	34526		$C_{11}H_{20}N_3O_3PS$	NS00010883	4.20	0.0000500	0.0250
Phorate-sulfone	Plant protection products & TPs	Insecticides	17425		$C_7H_{17}O_4PS_3$	NS00010171	3.70	0.000130	0.0460

Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
Propetamphos	Plant protection products & TPs	Insecticides	5372405		$C_{10}H_{20}NO_4PS$	NS00004990	2.80	0.00490	0.510
Tributylamine	Plant protection products & TPs	Insecticides	7622		$C_{12}H_{27}N$	NS00000551	4.00	0.360	1,803
Ethyl-N-(3-hydroxyphenyl)-carbamate	Plant protection products & TPs	Pesticides	23548		$C_9H_{11}NO_3$	NS00005873	1.90	1.25	70.0
Methiocarb-sulfone	Plant protection products & TPs	Pesticides	16589		$C_{11}H_{15}NO_4S$	NS00002491	1.60	2.68	181
Metolachlor	Plant protection products & TPs	Pesticides	4169		$C_{15}H_{22}ClNO_2$	NS00000248	3.10	0.0200	3.17
Nicosulfuron	Plant protection products & TPs	Pesticides	73281		$C_{15}H_{18}N_6O_6S$	NS00008411	0.60	0.000870	0.0270
Pentachlorophenol (PCP)	Plant protection products & TPs	Pesticides	992		C_6HCl_5O	NS00009449	5.10	0.400	0.400
Piperonylbutoxide	Plant protection products & TPs	Pesticides	5794		$C_{19}H_{30}O_5$	NS00011484	3.70	0.100	148
Propazine-2-hydroxy (Prometon-hydroxy)	Plant protection products & TPs	Pesticides	135461611		$C_9H_{17}N_5O$	NS00000456	0.60	0.00700	0.290

Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
2-phenylphenol	Surfactants	Antiseptics & disinfectants	7017		$C_{12}H_{10}O$	NS00010901	3.10	0.0180	5.91
BAC 14	Surfactants	Antiseptics & disinfectants	8755		$C_{23}H_{42}ClN$	NS00075629	8.40	0.00500	35.7
BAC 16	Surfactants	Antiseptics & disinfectants	31202		$C_{25}H_{46}ClN$	NS00079326	4.90	0.00300	0.0485
Benzethonium	Surfactants	Antiseptics & disinfectants	2335		$C_{27}H_{42}NO_2^+$	NS00010384	6.70	0.000440	3.03
Benzododecinium	Surfactants	Antiseptics & disinfectants	8754		$C_{21}H_{38}N^+$	NS00007281	7.40	0.0370	49.4
Benzyldimethylhexadecylammonium	Surfactants	Antiseptics & disinfectants	31203		$C_{25}H_{46}N^+$	NS00004120	9.50	0.00340	16.8
Benzyldimethyltetradecylammonium	Surfactants	Antiseptics & disinfectants	8756		$C_{23}H_{42}N^+$	NS00010630	8.40	0.0290	210
C10-LAS	Surfactants	Antiseptics & disinfectants	51834		$C_{16}H_{26}O_3S$	NS00000998	5.60	0.0330	41.4
C11-LAS	Surfactants	Antiseptics & disinfectants	15593874		$C_{17}H_{28}O_3S$	NS00000999	6.10	0.0180	20.7

Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
C12-AE2S	Surfactants	Antiseptics & disinfectants	18336		$C_{16}H_{34}O_6S$	NS00005253	4.40	8.61	13.9
C12-AEO2	Surfactants	Antiseptics & disinfectants	76457		$C_{16}H_{34}O_3$	NS00013814	4.90	0.0600	67.7
C12-AEO3	Surfactants	Antiseptics & disinfectants	76458		$C_{18}H_{38}O_4$	NS00013815	4.80	0.0680	238
C12DEA	Surfactants	Antiseptics & disinfectants	8778		$C_{12}H_{26}O_4S$	NS00010587	4.70	0.380	239
C12-LAS	Surfactants	Antiseptics & disinfectants	15593880		$C_{18}H_{30}O_3S$	NS00101192	6.70	0.00860	0.139
C13-LAS	Surfactants	Antiseptics & disinfectants	15593889		$C_{19}H_{32}O_3S$	NS00014615	7.20	0.0130	56.2
C14-LAS	Surfactants	Antiseptics & disinfectants	92041852		$C_{20}H_{34}O_3S$	NS00094978	7.80	0.00450	0.0727
DDAC-C10	Surfactants	Antiseptics & disinfectants	23558		$C_{22}H_{48}ClN$	NS00075672	2.59	0.200	143
N.N-dimethyldodecylamine	Surfactants	Antiseptics & disinfectants	8168		$C_{14}H_{31}N$	NS00006542	5.90	0.0110	15.0

Analyte Name	Chemical Classification	Sub - class	PubChem CID	Chemical Structure	Formula	Norman SusDat ID	XLogP*	Seawater PNEC** (µg/L)	Sediment PNEC** (µg/kg d.w.)
N.N-dimethyldodecylamine-N-oxide	Surfactants	Antiseptics & disinfectants	15433		$C_{14}H_{31}NO$	NS00001592	5.30	0.920	1,526
N.N-dimethyltetradecylamine	Surfactants	Antiseptics & disinfectants	8211		$C_{16}H_{35}N$	NS00001314	6.90	0.0300	6.11
N.N-dimethyltetradecylamine-N-oxide	Surfactants	Antiseptics & disinfectants	18739		$C_{16}H_{35}NO$	NS00001390	6.40	3.35	353
N-methyldodecylamine	Surfactants	Antiseptics & disinfectants	81746		$C_{13}H_{29}N$	NS00044167	5.40	0.0100	9.03
Trimethyloctylammonium	Surfactants	Antiseptics & disinfectants	24950		$C_{11}H_{26}N^{+}$	NS00014217	4.20	0.690	186

223 * PubChem database (last accessed in March 2025). **NORMAN ecotoxicology database (last accessed in March 2025).

6. Results

6.1. ECs and PPs in seawater samples

A total of 128 analytes were identified and quantified in tested seawater samples from sampling stations S1, S7, S8, S11 and S1-biol, S7-biol sewage effluent from the Thriassio and Psyttalia WWTPs, respectively. Calculated concentrations per sampling depth are provided in **Table S6**, along with the determined limits of detection and quantification. All concentration levels and LOD-LOQ values are expressed as ng L^{-1} of seawater.

231 **Table S6:** Concentrations of determined ECs and PPs in seawater samples per sampling depth, expressed as ng L^{-1}.

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
Caffeine	206	16.8	<LOD	143	34.7	45.7	<LOD	61.3	49.0	58.5	76.6	45.1	59.7	0.410	1.23	85%
Cotinine	580	<LOD	<LOD	163	32.6	216	<LOD	56.7	8.57	35.1	65.1	24.0	73.0	0.513	1.54	77%
Hydroxy-cotinine	5.43	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.853	<LOD	<LOD	<LOD	<LOD	<LOD	0.178	0.533	15%
Nicotine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	68.6	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0413	0.124	8%
Theobromine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	10.0	<LOD	12.1	0.279	0.836	15%
Theophylline	27.8	3.26	17.6	<LOD	42.5	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	6.38	<LOD	0.272	0.816	38%
Acesulfame	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.105	0.316	15%
Saccharin	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.16	0.479	8%
2-amino-benzothiazole	<LOD	<LOD	<LOD	3.61	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	0.149	0.447	15%
5-methyl-benzotriazole	19.9	1.68	3.40	6.46	3.30	5.12	2.73	2.22	4.52	4.18	1.69	3.16	3.21	0.430	1.29	100%
Benzothiazole-2-sulfonic acid	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.255	0.764	15%
Mercaptobenzothiazole	21.3	2.19	<LOD	46.9	5.68	62.2	<LOD	15.7	7.38	9.12	4.05	3.95	7.68	0.332	0.995	85%
N.N-dimethylaniline	5.90	<LOD	<LOD	8.29	BQL	4.94	<LOD	1.25	BQL	BQL	BQL	<LOD	BQL	0.326	0.978	85%
1-naphthol	<LOD	<LOD	350	<LOD	<LOD	<LOD	26.5	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.270	0.807	15%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
4-iodophenoxyacetic acid	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0689	0.207	8%
4-nitrophenol	<LOD	<LOD	11,801	<LOD	<LOD	<LOD	10,220	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.259	0.777	15%
Bisphenol AF	<LOD	<LOD	164	<LOD	<LOD	<LOD	298	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.178	0.533	15%
Bisphenol S	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	78.3	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.249	0.746	8%
Ethylparaben	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.234	0.702	8%
Isopropylparaben	<LOD	<LOD	1.04	<LOD	<LOD	<LOD	1.43	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.220	0.660	15%
Methylparaben	<LOD	<LOD	1.94	<LOD	<LOD	<LOD	2.21	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.207	0.620	15%
Propylparaben	<LOD	<LOD	0.980	<LOD	<LOD	<LOD	1.36	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.195	0.583	15%
2.3.3.3-tetrafluoro-2-(heptafluoropropoxy)propanoic acid (HFPO-DA or GenX)	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.626	<LOD	<LOD	<LOD	<LOD	<LOD	0.174	0.522	8%
4.8-dioxa-3H-perfluorononanoic acid (ADONA)	3.60	2.82	<LOD	83.5	<LOD	160	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.235	0.705	38%
6:2 fluorotelomer sulfonic acid (6:2 FTS)	<LOD	0.321	25.5	<LOD	<LOD	<LOD	22.3	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0237	0.0712	23%
Perfluoro-4-oxapentanoic acid (PFMPA or PF4OPeA)	<LOD	<LOD	<LOD	1.88	<LOD	1.39	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.289	0.867	15%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
Perfluorobutanesulfonic acid (PFBS)	<LOD	<LOD	BQL	BQL	BQL	BQL	<LOD	<LOD	BQL	BQL	BQL	BQL	BQL	0.0309	0.0926	77%
Perfluorobutanoic acid (PFBA)	3.43	1.23	<LOD	1.08	3.73	1.72	<LOD	2.75	1.18	6.32	2.16	2.57	3.92	0.328	0.984	85%
Perfluorododecanoic acid (PFDoA)	3.75	<LOD	<LOD	4.58	6.40	4.31	<LOD	1.45	3.92	5.57	5.90	4.62	5.94	0.0967	0.290	85%
Perfluorohexanesulfonic acid (PFHxS)	<LOD	0.815	0.955	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0849	0.255	15%
Perfluorohexanoic acid (PFHxA)	0.985	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	0.557	BQL	<LOD	0.0511	0.153	54%
Perfluorooctanesulfonic acid (PFOS)	<LOD	BQL	18.4	<LOD	1.07	<LOD	6.57	<LOD	2.09	<LOD	2.98	4.35	2.42	0.150	0.449	77%
Perfluoropentanoic acid (PFPeA)	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	0.0346	0.104	23%
Perfluorotetradecanoic acid (PFTeDA)	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.386	<LOD	0.0173	0.0519	23%
Di-(2-ethylhexyl) phthalate (DEHP)	31.6	1.27	<LOD	24.6	7.87	24.1	<LOD	14.4	7.02	7.49	8.86	7.03	8.45	0.177	0.532	85%
Diethyl phthalate	<LOD	<LOD	2.86	<LOD	<LOD	<LOD	9.07	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0747	0.224	15%
N-butylbenzenesulfonamide	<LOD	<LOD	32.9	<LOD	<LOD	<LOD	53.8	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0561	0.168	15%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
Triphenylphosphate	67.6	<LOD	<LOD	47.5	15.0	59.4	<LOD	30.1	13.2	19.9	33.2	8.02	13.0	0.685	2.06	77%
1.3-diphenylguanidine	<LOD	<LOD	84.5	<LOD	<LOD	<LOD	24.0	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0689	0.207	15%
Lauryl diethanolamide	<LOD	<LOD	4.84	<LOD	<LOD	<LOD	4.48	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0777	0.233	15%
Lauramidopropylbetaine	853	<LOD	161	87.4	9.01	18.4	85.5	<LOD	<LOD	55.5	63.5	38.8	<LOD	0.164	0.492	69%
Oxybenzone (3-benzophenone)	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.30	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0625	0.188	8%
Carbuterol	<LOD	9.90	<LOD	<LOD	7.56	<LOD	<LOD	<LOD	9.07	12.0	<LOD	<LOD	<LOD	0.293	0.879	31%
Ipratropium	<LOD	<LOD	<LOD	<LOD	<LOD	17.4	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.290	0.871	8%
Methylephedrine	17.8	2.91	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0857	0.257	15%
Memantine	<LOD	<LOD	<LOD	16.5	<LOD	<LOD	<LOD	<LOD	<LOD	25.4	62.4	28.9	<LOD	0.530	1.59	31%
Lidocaine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	6.24	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.192	0.577	8%
O-desmethyltramadol	<LOD	<LOD	30.5	<LOD	<LOD	<LOD	4.91	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0571	0.171	15%
Paracetamol	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	35.0	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	2.15	6.45	8%
Sarafloxacin	<LOD	<LOD	<LOD	13.4	<LOD	5.69	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.421	1.26	15%
Sulfadiazine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.91	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.201	0.604	8%
Sulfamethoxazole	<LOD	<LOD	3.34	<LOD	<LOD	<LOD	4.75	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.125	0.374	15%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
Trimethoprim	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	5.07	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.118	0.354	8%
Metformin	78.8	4.26	<LOD	26.8	3.81	6.49	<LOD	4.49	BQL	BQL	BQL	2.84	3.87	0.907	2.72	85%
Vildagliptin	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.97	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.471	1.41	8%
Metoclopramide	2.94	<LOD	<LOD	1.62	BQL	2.26	<LOD	BQL	1.65	BQL	<LOD	<LOD	1.53	0.463	1.39	77%
10-hydroxycarbamazepine	3.28	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.912	2.74	8%
2-hydroxycarbamazepine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.20	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.163	0.489	8%
Carbamazepine	3.77	<LOD	1.46	2.08	<LOD	<LOD	3.30	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0413	0.124	46%
Carbamazepine-10.11-epoxide	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.18	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.295	0.882	8%
Pregabalin	<LOD	<LOD	<LOD	43.8	<LOD	<LOD	<LOD	12.7	<LOD	<LOD	<LOD	<LOD	22.4	0.162	0.485	23%
5-hydroxy-thiabendazole	1.11	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.265	0.796	8%
Caproylresorcinol	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	30.2	<LOD	<LOD	<LOD	<LOD	0.333	0.999	8%
Thiabendazole	29.3	<LOD	<LOD	42.6	<LOD	136	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.977	2.93	23%
Hydrochlorothiazide	2.52	<LOD	<LOD	8.31	<LOD	<LOD	1.51	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.280	0.841	23%
Irbesartan	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	3.66	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.144	0.433	8%
Losartan	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	2.70	<LOD	<LOD	<LOD	<LOD	2.54	0.566	1.70	15%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
Metoprolol	<LOD	<LOD	<LOD	2.46	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.357	1.07	8%
Sotalol	<LOD	<LOD	<LOD	2.83	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.189	0.567	15%
2-acetamido-5-nitrothiazole (Aminitrozole)	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0281	0.0844	8%
Pentobarbital	<LOD	<LOD	<LOD	<LOD	0.0961	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0267	0.0801	8%
Primidone	14.1	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.271	0.812	15%
Secobarbital	<LOD	<LOD	<LOD	6.75	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.250	0.750	8%
Bromazepam	<LOD	<LOD	<LOD	<LOD	<LOD	11.2	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.385	1.16	8%
Citalopram	3.92	<LOD	<LOD	5.00	<LOD	<LOD	4.37	2.19	<LOD	<LOD	<LOD	<LOD	<LOD	0.236	0.707	31%
Norcitalopram	1.72	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0551	0.165	15%
Tadalafil	<LOD	<LOD	<LOD	<LOD	4.76	<LOD	<LOD	<LOD	<LOD	19.7	<LOD	33.9	10.4	0.260	0.780	31%
Clopidogrel carboxylic acid	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.496	1.49	8%
Flecainide	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	5.50	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0401	0.120	8%
Ibuprofen	<LOD	BQL	<LOD	2.18	<LOD	<LOD	<LOD	1.07	<LOD	<LOD	1.35	1.35	4.78	0.0864	0.259	46%
Ketoprofen	1.86	<LOD	<LOD	3.28	5.85	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0607	0.182	31%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
Salicylic acid	60.1	<LOD	<LOD	11.0	76.3	<LOD	<LOD	18.4	43.1	79.1	81.3	52.4	101	0.351	1.05	69%
Amisulpiride	<LOD	<LOD	<LOD	6.93	<LOD	<LOD	8.32	1.48	<LOD	<LOD	<LOD	<LOD	<LOD	0.247	0.741	23%
O-desmethylvenlafaxine (Desvenlafaxine)	10.4	BQL	1.41	7.14	<LOD	<LOD	3.41	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.316	0.948	15%
Venlafaxine	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	4.17	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.228	0.685	8%
Pentylone	<LOD	<LOD	<LOD	<LOD	<LOD	11.4	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0756	0.227	8%
Fenbendazole	<LOD	<LOD	98.9	<LOD	<LOD	<LOD	69.9	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.186	0.558	15%
Florfenicol	3.56	<LOD	BQL	<LOD	<LOD	1.11	0.817	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.195	0.586	31%
4-hydroxy-chlorothalonil	<LOD	BQL	<LOD	0.381	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0292	0.0876	31%
Azoxystrobin	0.743	<LOD	<LOD	<LOD	1.00	<LOD	<LOD	<LOD	<LOD	<LOD	1.96	<LOD	<LOD	0.191	0.572	23%
Metalaxyl	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.04	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.114	0.343	8%
Octhilinone	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	1.15	<LOD	<LOD	1.03	<LOD	<LOD	<LOD	0.214	0.642	15%
Tebuconazole	<LOD	<LOD	<LOD	7.87	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.328	0.983	8%
Tetraconazole	20.3	<LOD	<LOD	2.76	<LOD	6.62	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.418	1.26	23%
5-nitroguaiacol	0.957	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.465	0.949	0.701	<LOD	<LOD	0.0776	0.233	46%
Kinetin	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0259	0.0778	8%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
2-hydroxy-atrazine	<LOD	<LOD	BQL	<LOD	<LOD	2.73	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.337	1.01	15%
Cloprop	0.499	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.119	0.357	8%
Dinoterb	1.48	<LOD	BQL	1.54	<LOD	3.03	BQL	<LOD	<LOD	<LOD	<LOD	BQL	BQL	0.110	0.329	92%
Diuron	<LOD	<LOD	1.81	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0471	0.141	8%
Fluometuron	8.03	0.883	1.21	35.2	BQL	1.65	2.52	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.269	0.808	54%
Tebuthiuron	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	0.0174	0.0521	8%
2.4-dimethylphenyl-N-methylformamidine	BQL	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.321	0.962	15%
Clothianidin	0.829	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.154	0.461	8%
Desmethyl-dimethoate	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	7.32	<LOD	<LOD	<LOD	<LOD	<LOD	0.241	0.724	8%
2-hydroxy-propazine (Hydroxy-prometon)	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.902	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0387	0.117	8%
Ethyl-N-(3-hydroxyphenyl)-carbamate	<LOD	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0617	0.185	8%
Methiocarb-sulfone	<LOD	<LOD	14.1	<LOD	<LOD	<LOD	5.17	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.212	0.635	15%
Metolachlor	2.18	BQL	<LOD	1.93	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0721	0.216	100%
Nicosulfuron	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	26.7	<LOD	<LOD	<LOD	0.489	1.47	8%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
Pentachlorophenol (PCP)	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.968	<LOD	<LOD	<LOD	BQL	<LOD	<LOD	0.0369	0.111	62%
2-phenylphenol	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	43.5	<LOD	<LOD	<LOD	<LOD	0.277	<LOD	0.0486	0.146	15%
BAC 14	<LOD	<LOD	9.78	<LOD	<LOD	<LOD	7.34	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0567	0.170	15%
BAC 16	<LOD	<LOD	3.12	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0618	0.185	8%
Benzododecinium	34.8	12.2	313	47.7	39.3	23.5	158	47.0	40.4	42.3	120	406	43.2	0.509	1.53	100%
Benzyldimethylhexadecylammonium	<LOD	<LOD	3.66	<LOD	<LOD	<LOD	1.42	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0716	0.215	15%
Benzyldimethyltetradecylammonium	9.83	1.71	22.9	11.7	10.0	10.2	16.2	6.49	6.87	9.15	25.5	58.0	5.82	0.173	0.518	100%
C12-AE2S	<LOD	<LOD	32.6	<LOD	<LOD	<LOD	17.6	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0569	0.171	15%
C12DEA	<LOD	<LOD	2.67	<LOD	<LOD	<LOD	2.56	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0565	0.169	15%
C12-LAS	<LOD	<LOD	212	<LOD	<LOD	<LOD	416	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0618	0.185	15%
C13-LAS	<LOD	<LOD	100	<LOD	<LOD	<LOD	148	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0639	0.191	15%
DDAC-C10	<LOD	<LOD	6.34	<LOD	<LOD	<LOD	4.78	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0602	0.180	15%
N.N-dimethyldodecylamine	<LOD	<LOD	33.9	<LOD	<LOD	<LOD	23.8	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0579	0.174	15%
N.N-dimethyldodecylamine-N-	8.39	BQL	180	3.22	4.78	2.78	83.1	3.47	3.49	5.42	5.09	6.55	4.03	0.647	1.94	100%

Analyte Name	S1 2m	S1 18m	S1-biol 10m	S7 2m	S7 50m	S7 69m	S7-biol 63m	S8 2m	S8 50m	S8 90m	S11 2m	S11 50m	S11 73m	LOD	LOQ	%FoD
oxide																
N.N-dimethyltetradecylamine	<LOD	<LOD	9.23	<LOD	<LOD	<LOD	3.82	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0615	0.184	15%
N.N-dimethyltetradecylamine-N-oxide	<LOD	<LOD	45.2	<LOD	<LOD	<LOD	21.7	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.0591	0.177	15%
N-methyldodecylamine	19.5	1.30	43.5	13.1	4.49	<LOD	8.54	9.41	4.88	4.50	7.89	5.48	4.75	0.407	1.22	92%
Trimethyloctylammonium	<LOD	<LOD	<LOD	20.2	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	0.279	0.836	8%

232 * Compounds identified in **confidence level 2a**[9]

233 ** Substances prioritized in the proposal for new EU Directive[16]

Highlighted cells: Concentration levels exceeding PNEC values (risk quotient factor > 1, high risk substances)

6.2. ECs and PPs in sediment samples

A total of 71 analytes were identified and quantified in the tested sediment samples. Calculated concentrations are provided in **Table S7**, along with the determined limits of detection and quantification. All concentration levels and LOD-LOQ values are expressed as μg kg^{-1} d.w.

240 **Table S7:** Concentrations of determined ECs and PPs in sediment samples. expressed as µg kg^{-1} d.w.

Analyte Name	S1	S7	S8	S11	LOD	LOQ	%FoD
Anabasine	<LOD	42.0	547	<LOD	0.433	1.30	50%
Cotinine	BQL	12.6	35.2	3.14	0.375	1.12	100%
Nicotine	<LOD	50.6	578	<LOD	0.480	1.44	50%
5-methylbenzotriazole	BQL	<LOD	BQL	BQL	0.731	2.19	75%
Mercaptobenzothiazole	0.281	<LOD	<LOD	0.859	0.0851	0.255	50%
Di-(2-ethylhexyl) phthalate (DEHP)	22.3	73.8	84.8	9.25	0.417	1.25	100%
Diethylphthalate (DEP)	0.173	<LOD	<LOD	0.185	0.0340	0.102	50%
Dimethylphthalate (DMP)	0.136	<LOD	<LOD	0.218	0.0378	0.113	50%
6:2 fluorotelomer sulfonic acid (6:2 FTS)	2.37	3.68	3.12	BQL	0.557	1.67	100%
Perfluorooctanesulfonic acid (PFOS)	3.92	1.69	1.41	1.22	0.190	0.571	100%
Perfluorobutanesulfonic acid (PFBS)	<LOD	0.154	<LOD	<LOD	0.0395	0.119	25%
Perfluorobutanoic acid (PFBA)	27.8	<LOD	<LOD	28.4	0.899	2.70	50%
Perfluorododecanoic acid (PFDoA)	0.192	<LOD	<LOD	0.236	0.0377	0.113	50%
Perfluoroheptanesulfonic acid (PFHpS)	<LOD	2.55	<LOD	<LOD	0.531	1.59	25%
Perfluorohexadecanoic acid (PFHxDA)	BQL	BQL	<LOD	<LOD	0.0656	0.197	50%
Perfluorohexanoic acid (PFHxA)	0.675	<LOD	<LOD	BQL	0.0803	0.241	50%
Perfluorooctanoic acid (PFOA)	3.08	<LOD	<LOD	1.19	0.264	0.793	50%
3.5-dibromo-4-hydroxybenzoic acid	9.43	<LOD	<LOD	5.38	0.157	0.471	50%
Propafenone	<LOD	<LOD	0.474	<LOD	0.0607	0.182	25%

Analyte Name	S1	S7	S8	S11	LOD	LOQ	%FoD
Cinoxacin	<LOD	<LOD	<LOD	0.126	0.0351	0.105	25%
Norfloxacin	6.74	6.22	7.65	<LOD	0.798	2.39	75%
Sulfadiazine	<LOD	<LOD	BQL	<LOD	0.252	0.756	25%
Sulfisoxazole (Sulfafurazole)	<LOD	<LOD	0.293	<LOD	0.0888	0.266	25%
Gabapentin	86.9	351	680	<LOD	1.73	5.20	75%
Pregabalin	43.2	415	79.5	4.95	0.589	1.77	100%
Caproyl resorcinol	BQL	<LOD	<LOD	<LOD	0.408	1.22	25%
Isoconazole	<LOD	<LOD	0.205	<LOD	0.0622	0.187	25%
Miconazole	0.829	<LOD	3.03	BQL	0.252	0.757	75%
Octhilinone	0.447	0.508	0.279	0.369	0.0774	0.232	100%
Deacetyldiltiazem	BQL	BQL	0.252	<LOD	0.0317	0.0952	75%
Toliprolol	<LOD	<LOD	2.63	<LOD	0.313	0.939	25%
Tulobuterol	3.45	<LOD	26.4	<LOD	0.328	0.985	50%
Valsartan	BQL	69.2	97.5	<LOD	1.25	3.76	75%
Metoclopramide	0.648	<LOD	<LOD	0.529	0.0766	0.230	50%
Adrenalone	<LOD	<LOD	1.89	<LOD	0.166	0.497	25%
Progesterone	BQL	<LOD	<LOD	BQL	0.364	1.09	50%
Oxyphenbutazone	<LOD	BQL	<LOD	<LOD	0.552	1.66	25%
Amisulpiride	<LOD	<LOD	2.02	<LOD	0.259	0.777	25%

Analyte Name	S1	S7	S8	S11	LOD	LOQ	%FoD
Venlafaxine	45.5	67.5	67.5	<LOD	0.0773	0.232	75%
2-phenethylamine	87.2	76.3	203	34.3	1.24	3.73	100%
Apophedrin (Phenylethanolamine)	22.4	<LOD	71.9	<LOD	0.770	2.31	50%
Phenmetrazine	<LOD	<LOD	2.58	<LOD	0.453	1.36	25%
Tyramine	4.61	<LOD	<LOD	<LOD	0.810	2.43	25%
Vareniclin	<LOD	<LOD	13.8	<LOD	0.383	1.15	25%
Ethyl-N-(3-hydroxyphenyl)-carbamate	<LOD	<LOD	BQL	<LOD	0.0501	0.150	25%
Fenbendazole	13.4	<LOD	<LOD	1.77	0.137	0.412	50%
Olaquindox	0.347	<LOD	<LOD	<LOD	0.0890	0.267	25%
Oxibendazole	<LOD	0.485	3.41	<LOD	0.0951	0.285	50%
Pirlimycin	<LOD	<LOD	0.349	<LOD	0.106	0.317	25%
Azoxystrobin	BQL	BQL	0.806	<LOD	0.0445	0.133	75%
4-hydroxychlorothalonil	0.244	<LOD	<LOD	<LOD	0.0220	0.0660	25%
RP 30228	<LOD	<LOD	BQL	0.260	0.0488	0.146	50%
Maleic hydrazide	3.84	<LOD	4.97	<LOD	0.441	1.32	50%
4-iodophenoxyacetic acid	3.51	<LOD	6.70	3.73	0.433	1.30	75%
Buturon	0.393	<LOD	<LOD	<LOD	0.0468	0.140	25%
Diflufenzopyr	<LOD	<LOD	0.136	0.333	0.0283	0.0848	50%
Isoproturon	<LOD	<LOD	3.45	<LOD	0.348	1.04	25%

Analyte Name	S1	S7	S8	S11	LOD	LOQ	%FoD
Neburon	<LOD	0.293	<LOD	<LOD	0.0361	0.108	25%
Pyridafol	BQL	<LOD	<LOD	<LOD	0.0296	0.0888	25%
2.4-dimethylphenyl-N-methylformamidine	14.2	<LOD	<LOD	18.9	0.555	1.67	50%
Phorate-sulfone	<LOD	<LOD	BQL	<LOD	0.242	0.726	25%
Methylpirimiphos	<LOD	0.216	0.228	<LOD	0.0401	0.120	50%
Propetamphos	<LOD	<LOD	0.150	<LOD	0.0417	0.125	25%
Keto-hydroxyspirotetramate	0.633	<LOD	<LOD	<LOD	0.0918	0.275	25%
Tributylamine	<LOD	<LOD	1.83	<LOD	0.278	0.833	25%
Pentachlorophenol (PCP)	BQL	<LOD	<LOD	BQL	0.0335	0.100	50%
Piperonylbutoxide	BQL	BQL	2.03	<LOD	0.563	1.69	75%
Benzethonium	BQL	<LOD	<LOD	<LOD	0.0311	0.0933	25%
Benzyldimethylhexadecylammonium	<LOD	BQL	1.00	<LOD	0.298	0.894	50%
N.N-dimethyldodecylamine	<LOD	2.45	3.46	<LOD	0.454	1.36	50%
N.N-dimethyltetradecylamine	<LOD	<LOD	0.802	<LOD	0.223	0.669	25%

Highlighted cells: Concentration levels exceeding PNEC values (risk quotient factor > 1, high risk substances)

6.3. ECs and PPs in Thriassio (S1) and Psyttalia (S7) wastewater samples

A total of 214 analytes were identified and quantified through wide-scope target and suspect screening in tested wastewater samples from the Thriassio (S1) and Psyttalia (S7) WWTPs. Calculated concentrations are provided in **Table S8**, along with the determined limits of detection and quantification. All concentration levels and LOD-LOQ values are expressed as ng L^{-1}.

248 **Table S8:** Concentrations of determined ECs and PPs in Thriassio (S1) and Psyttalia (S7) wastewater samples. expressed as ng L^{-1}

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
Anabasine	6,119	<LOD	> 95%	518	17.6	> 95%	0.0589	0.177
Caffeine	49,757	144	> 95%	12,060	106	> 95%	0.0434	0.130
Cotinine	3,431	33.4	> 95%	1,026	8.37	> 95%	0.0106	0.0318
Hydroxycotinine	5,357	<LOD	> 95%	2,654	<LOD	> 95%	0.0103	0.0309
Nicotine	6,391	<LOD	> 95%	539	20.4	> 95%	0.0421	0.126
Theobromine	29,523	<LOD	> 95%	3,891	26.3	> 95%	0.133	0.400
Theophylline	8,143	<LOD	> 95%	1,536	<LOD	> 95%	0.114	0.341
Acesulfame	10,828	56.5	> 95%	25,058	792	> 95%	0.101	0.302
Cyclamic acid	1,940	<LOD	> 95%	1,309	6.62	> 95%	0.0504	0.151
Saccharin	1,718	4.80	> 95%	22,157	2,281	90%	0.0756	0.227
Benzoylecgonine	748	<LOD	> 95%	428	14.0	> 95%	0.0732	0.220
Cocaine	275	<LOD	> 95%	34.8	<LOD	> 95%	0.0470	0.141
Ecgonine methyl ester	<LOD	<LOD	-	70.9	<LOD	> 95%	0.0162	0.0485
Norcocaine	782	<LOD	> 95%	446	<LOD	> 95%	0.0316	0.0947
Codeine	<LOD	<LOD	-	85.2	<LOD	> 95%	0.0244	0.0732
Morphine	<LOD	<LOD	-	134	<LOD	> 95%	0.0395	0.118
Pseudoephedrine	<LOD	<LOD	-	98.3	<LOD	> 95%	0.0434	0.130
1H-benzotriazole	128	205	-60%	12.9	16.6	-29%	0.0422	0.127
5-methyl-Benzotriazole	2,815	5,083	-81%	<LOD	<LOD	-	0.0400	0.120
Benzothiazole-2-sulfonic acid	426	248	42%	70.0	121	-72%	0.0411	0.123
1-methyl-2-pyrrolidinone	<LOD	<LOD	-	920	63.3	93%	0.0493	0.148
2.4-dihydroxyquinoline	<LOD	<LOD	-	41.8	1.40	> 95%	0.0542	0.163
2-piperidone	<LOD	<LOD	-	913	<LOD	> 95%	0.0477	0.143
4-chlorophenol	<LOD	<LOD	-	491	<LOD	> 95%	0.0430	0.129

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
4-nitrophenol	25,608	<LOD	> 95%	54,683	1,683	> 95%	0.0859	0.258
Bisphenol S	2,261	<LOD	> 95%	133	<LOD	> 95%	0.0471	0.141
N-butylbenzenesulfonamide	26,141	3.45	> 95%	<LOD	726	-	0.0777	0.233
Isopropylparaben	191	<LOD	> 95%	<LOD	<LOD	-	0.114	0.342
Propylparaben	191	4.54	> 95%	<LOD	<LOD	-	0.0163	0.049
Diethyl phthalate	399	7.28	> 95%	<LOD	<LOD	-	0.0876	0.263
1.3-diphenylguanidine	106	173	-63%	45.2	71.3	-58%	0.0570	0.171
Lauryl diethanolamide	<LOD	<LOD	-	147	<LOD	> 95%	0.0689	0.207
Avobenzone	95.3	3.92	> 95%	<LOD	<LOD	-	0.0551	0.165
Phenylbenzimidazole sulfonic acid	66.6	50.7	24%	27.3	10.7	61%	0.455	1.37
Umbelliferone	<LOD	<LOD	-	149	2.18	> 95%	0.193	0.579
6:2 fluorotelomer sulfonic acid (6:2 FTS)	108	58.7	46%	<LOD	<LOD	-	0.00313	0.00938
Perfluorobutanesulfonic acid (PFBS)	<LOD	1.63	-	2.52	2.53	-1%	0.00174	0.00521
Perfluorobutanoic acid (PFBA)	<LOD	<LOD	-	79.2	183	-131%	0.00196	0.00587
Perfluorodecanoic acid (PFDA)	0.620	0.250	60%	3.00	1.72	43%	0.00208	0.00623
Perfluorododecanoic acid (PFDoA)	<LOD	<LOD	-	<LOD	8.06	-	0.00231	0.00692
Perfluoroheptanoic acid (PFHpA)	41.6	18.3	56%	18.4	63.3	-244%	0.00301	0.00904
Perfluorohexanesulfonic acid (PFHxS)	<LOD	<LOD	-	37.3	69.2	-86%	0.00540	0.0162
Perfluorononanoic acid (PFNA)	5.16	3.54	32%	5.71	3.88	32%	0.00369	0.0111
Perfluorooctanesulfonic acid (PFOS)	375	133	64%	404	168	58%	0.00123	0.00369
Perfluorooctanoic acid (PFOA)	7.90	5.37	32%	19.0	12.8	33%	0.00150	0.00450
Perfluoropentanesulfonic acid (PFPeS)	<LOD	0.721	-	<LOD	<LOD	-	0.00125	0.00375
Perfluoropentanoic acid (PFPeA)	<LOD	0.548	-	<LOD	<LOD	-	0.00532	0.0160
Perfluorotridecanoic acid (PFTrDA)	<LOD	<LOD	-	<LOD	17.4	-	0.00355	0.0106
Perfluoroundecanoic acid (PFUdA)	<LOD	<LOD	-	<LOD	7.40	-	0.00273	0.00819

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
Memantine	83.0	218	-163%	135	216	-60%	0.0287	0.0860
Dinortramadol (N-didesmethyl-tramadol)	<LOD	<LOD	-	<LOD	17.4	-	0.0104	0.0313
Hydromorphone	<LOD	<LOD	-	22.6	<LOD	> 95%	0.0490	0.147
Lidocaine	1,016	2,291	-125%	32.9	73.0	-122%	0.0107	0.0322
Nortramadol	<LOD	<LOD	-	<LOD	73.4	-	0.0491	0.147
O-desmethylnortramadol	<LOD	134	-	113	115	-2%	0.0498	0.149
O-desmethyltramadol	<LOD	499	-	381	174	54%	0.0499	0.150
Paracetamol	2,321	<LOD	> 95%	289	10.1	97%	0.0158	0.0475
Tapentadol	<LOD	<LOD	-	271	103	62%	0.0272	0.0815
Tramadol	405	233	42%	263	88.5	66%	0.0284	0.0851
Mebendazole	<LOD	<LOD	-	12.4	<LOD	> 95%	0.0448	0.134
Azithromycin	269	265	2%	961	39.1	> 95%	0.0450	0.135
Clarithromycin	320	97.2	70%	88.5	34.8	61%	0.0563	0.169
Clindamycin	<LOD	215	-	<LOD	<LOD	-	0.0775	0.232
Linezolid	196	257	-31%	<LOD	<LOD	-	0.0185	0.0556
Rifaximin	<LOD	<LOD	-	295	6.85	> 95%	0.0349	0.105
Sulfamethoxazole	699	<LOD	> 95%	2,447	725	70%	0.0573	0.172
Triclosan	227	<LOD	> 95%	17.2	<LOD	> 95%	0.0380	0.114
Trimethoprim	24.4	13.2	46%	602	50.6	92%	0.0200	0.0601
Butylscopolamine	<LOD	56.5	-	<LOD	<LOD	-	0.0448	0.134
Norорphenadrine (Tofenacin)	<LOD	<LOD	-	123	70.6	43%	0.0448	0.135
Orphenadrine	<LOD	<LOD	-	25.4	7.71	70%	0.0257	0.0770
Rivaroxaban	7.38	14.2	-93%	6.04	<LOD	> 95%	0.0446	0.134
Lacosamide	<LOD	53.0	-	13.9	<LOD	> 95%	0.1204	0.361
Metformin	11,590	339	> 95%	14,910	402	> 95%	0.0158	0.0473

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
Pioglitazone	26.3	<LOD	> 95%	57.8	<LOD	> 95%	0.0453	0.136
Sitagliptin	111	132	-18%	149	38.9	74%	0.0355	0.106
Vildagliptin	145	226	-55%	181	235	-30%	0.0530	0.159
Metoclopramide	27.0	37.3	-39%	6.32	15.7	-148%	0.0236	0.0709
10-hydroxycarbamazepine	27.1	9.78	64%	39.4	3.82	90%	0.0420	0.126
2-hydroxycarbamazepine	61.3	91.6	-49%	55.0	45.9	17%	0.0434	0.130
Carbamazepine	166	294	-77%	177	164	8%	0.0469	0.141
Carbamazepine-10.11-epoxide	58.7	91.6	-56%	49.0	43.9	10%	0.0402	0.121
Gabapentin	496	<LOD	100%	296	<LOD	> 95%	0.2472	0.742
Lamotrigine	206	1,002	-387%	282	485	-72%	0.0509	0.153
Levetiracetam	560	<LOD	100%	691	34.3	> 95%	0.0404	0.121
N-methyl-pregabalin	<LOD	<LOD	-	<LOD	99.8	-	0.0447	0.134
Pregabalin	<LOD	<LOD	-	192	<LOD	> 95%	0.2804	0.841
Topiramate	118	267	-125%	40.3	64.9	-61%	0.0387	0.116
Caproylresorcinol	179	<LOD	> 95%	153	<LOD	> 95%	0.0394	0.118
Climbazole	412	115	72%	31.2	11.1	64%	0.0217	0.0650
Fenbendazole	<LOD	<LOD	-	807	175	78%	0.0404	0.121
Fluconazole	74.1	99.2	-34%	119	88.1	26%	0.0852	0.256
Cetirizine	121	108	11%	86.6	70.2	19%	0.0694	0.208
Doxylamine	<LOD	<LOD	-	6.10	<LOD	> 95%	0.0439	0.132
Xylometazoline	<LOD	51.3	-	75.6	57.8	24%	0.0454	0.136
Atenolol	620	29.8	> 95%	369	<LOD	> 95%	0.0241	0.0724
Atenolol acid (Metoprolol acid)	3,479	193	94%	4,949	249	> 95%	0.0326	0.0978
Atorvastatin	184	<LOD	100%	193	<LOD	> 95%	0.1502	0.451
Bisoprolol	141	94.7	33%	817	33.8	> 95%	0.0199	0.0598

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
Candesartan	<LOD	<LOD	-	31.4	64.7	-106%	0.0502	0.151
D617	62.1	56.2	9%	247	103	58%	0.0511	0.153
Deacetyldiltiazem	<LOD	17.1	-	53.4	42.8	20%	0.0520	0.156
Diltiazem	29.9	32.5	-9%	28.5	14.4	50%	0.00935	0.0281
Irbesartan	1,968	2,171	-10%	1,577	1,451	8%	0.0330	0.0991
Losartan carboxylic acid	27.7	<LOD	> 95%	<LOD	<LOD	-	0.0521	0.156
Metoprolol	900	452	50%	1,664	207	88%	0.0260	0.0779
Practolol	471	16.4	> 95%	349	9.02	> 95%	0.0522	0.157
Propranolol	<LOD	<LOD	-	45.8	12.3	73%	0.0523	0.157
Rosuvastatin	181	<LOD	> 95%	331	<LOD	> 95%	0.2006	0.602
Sotalol	138	145	-5%	122	75.2	38%	0.0461	0.138
Valsartan	2,531	57.3	> 95%	2,720	128	> 95%	0.0164	0.0493
Tinidazole	<LOD	139	-	<LOD	<LOD	-	0.0559	0.168
Cimetidine	<LOD	157	-	<LOD	43.6	-	0.0561	0.168
Aciclovir	<LOD	<LOD	-	19.2	<LOD	> 95%	0.946	2.84
Oseltamivir	29.2	43.0	-48%	<LOD	<LOD	-	0.112	0.337
Rimantadine	86.3	212	-145%	196	200	-10%	0.0766	0.230
Mycophenolic acid	1,647	<LOD	> 95%	1,415	<LOD	-	0.212	0.637
1-hydroxymidazolam	195	155	21%	<LOD	<LOD	-	0.0802	0.241
Alprazolam	<LOD	30.9	-	<LOD	<LOD	-	0.0813	0.244
Citalopram	75.8	367	-385%	69.8	53.7	23%	0.0411	0.123
Citalopram amide	16.8	<LOD	> 95%	<LOD	27.2	-	0.0819	0.246
Midazolam	<LOD	130	-	<LOD	<LOD	-	0.0414	0.124
Norcitalopram	18.7	52.4	-180%	11.5	11.0	4%	0.0829	0.249
Temazepam	<LOD	12.9	-	10.7	<LOD	> 95%	0.0822	0.247

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
Etofylline	<LOD	<LOD	-	<LOD	84.7	-	0.0834	0.250
Terbutaline	<LOD	<LOD	-	88.2	<LOD	> 95%	0.0841	0.252
Capecitabin	<LOD	<LOD	-	46.3	<LOD	> 95%	0.232	0.696
Hydrochlorothiazide	90.3	136	-51%	104	153	-48%	0.139	0.418
Ambroxol	<LOD	130	-	<LOD	<LOD	-	0.0905	0.272
Noscapine	<LOD	<LOD	-	182	200	-10%	0.0914	0.274
Apophedrin (Phenylethanolamine)	854	<LOD	> 95%	<LOD	<LOD	-	0.0923	0.277
Clopidogrel	16.3	6.95	57%	14.8	4.02	73%	0.0301	0.0904
Clopidogrel carboxylic acid	43.3	67.2	-55%	197	184	7%	0.0929	0.279
Fenofibric acid	198	<LOD	> 95%	5,440	<LOD	> 95%	0.0332	0.0996
Flecainide	423	2,008	-375%	8,252	9,806	-19%	0.0117	0.0351
Propafenone	163	134	18%	840	259	69%	0.0123	0.0370
5-aminosalicylic acid	<LOD	<LOD	-	36.0	<LOD	> 95%	0.0886	0.266
Carboxyibuprofen	285	<LOD	> 95%	283	<LOD	> 95%	0.0851	0.255
Diclofenac	33.7	3.72	89%	7,318	6,604	10%	0.0859	0.258
Ibuprofen	2,735	<LOD	> 95%	596	<LOD	> 95%	0.142	0.425
Ketoprofen	198	<LOD	> 95%	58.6	<LOD	> 95%	0.0849	0.255
Mefenamic acid	330	71.1	78%	463	<LOD	> 95%	0.110	0.329
N-acetyl-mesalazine	48.3	<LOD	> 95%	81.4	<LOD	> 95%	0.137	0.410
Naproxen	88.8	<LOD	> 95%	29.4	<LOD	> 95%	0.357	1.07
Niflumic acid	249	137	45%	64.1	65.0	-2%	0.917	2.75
Amantadine	<LOD	<LOD	-	61.5	88.2	-44%	0.0458	0.137
Amisulpiride	255	938	-268%	106	230	-117%	0.119	0.356
Amitriptyline	320	38.1	88%	21.5	4.05	81%	0.120	0.361
Amitriptylinoxide	<LOD	13.0	-	<LOD	4.78	-	0.120	0.359

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
Clozapine	77.0	23.5	70%	<LOD	<LOD	-	0.0150	0.0449
E-10-hydroxyamitriptyline	<LOD	<LOD	-	17.2	3.39	80%	0.121	0.363
Mirtazapine	<LOD	18.5	-	44.6	17.5	61%	0.0308	0.0923
Norvenlafaxine (N-desmethylvenlafaxine)	51.6	22.7	56%	16.3	13.0	20%	0.122	0.365
O-Desmethylvenlafaxine (Desvenlafaxine)	288	171	41%	204	272	-33%	0.124	0.372
Quetiapine	121	<LOD	> 95%	<LOD	<LOD	-	0.0150	0.0449
Sertraline	273	56.9	79%	383	90.7	76%	0.125	0.375
Sulpiride	72.9	41.2	43%	43.6	72.4	-66%	0.0210	0.0631
Trazodone	<LOD	<LOD	-	58.4	<LOD	> 95%	0.126	0.379
Venlafaxine	451	203	55%	380	371	2%	0.0190	0.0570
Methylephedrine	<LOD	<LOD	-	<LOD	138	-	0.127	0.381
Azoxystrobin	6.92	3.91	44%	3.56	2.64	26%	0.126	0.377
Carbendazim	<LOD	<LOD	-	2.82	<LOD	> 95%	0.127	0.382
Fludioxonil	34.7	<LOD	> 95%	28.8	13.3	54%	0.129	0.388
Fluxapyroxad	<LOD	<LOD	-	26.4	16.2	39%	0.131	0.392
Penthiopyrad	<LOD	1.73	-	<LOD	<LOD	-	0.132	0.396
Thiabendazole	<LOD	<LOD	-	3.51	3.51	0%	0.133	0.400
Indole-3-acetic acid	807	<LOD	> 95%	146	<LOD	> 95%	0.0213	0.0640
Indole-3-butyric acid	<LOD	<LOD	-	<LOD	7.15	-	0.116	0.347
Prohexadione	<LOD	<LOD	-	39.3	<LOD	> 95%	0.116	0.347
Amitrole	<LOD	<LOD	-	184	<LOD	> 95%	0.116	0.349
Cycluron	<LOD	40.6	-	<LOD	<LOD	-	0.115	0.344
Dinoterb	3.22	1.16	64%	3.28	0.589	82%	0.115	0.346
Fluometuron	9.19	11.3	-23%	<LOD	<LOD	-	0.116	0.348
Mefluidide	<LOD	<LOD	-	3.58	<LOD	> 95%	0.117	0.352

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
Triclopyr	2.99	<LOD	> 95%	4.47	2.25	50%	0.118	0.354
Acetamiprid	<LOD	<LOD	-	76.5	34.4	55%	0.119	0.358
Aldicarb-sulfone (Aldoxycarb)	<LOD	<LOD	-	164	<LOD	> 95%	0.0840	0.252
Carbofuran-3-hydroxy	<LOD	<LOD	-	1,320	<LOD	> 95%	0.120	0.360
Clothianidin	<LOD	<LOD	-	<LOD	45.4	-	0.121	0.362
Dinotefuran	<LOD	<LOD	-	<LOD	44.7	-	0.121	0.364
Ethiofencarb-sulfone	<LOD	<LOD	-	14,518	1,307	91%	0.119	0.358
Fipronil	1.49	1.07	28%	3.08	1.98	36%	0.0152	0.046
Fipronilsulfone	<LOD	<LOD	-	39.4	20.1	49%	0.118	0.353
Icaridin	<LOD	<LOD	-	577	<LOD	> 95%	0.118	0.354
Imidacloprid	<LOD	<LOD	-	<LOD	29.2	-	0.119	0.356
N.N-Diethyl-m-toluamide (DEET)	401	103	74%	2,781	126	> 95%	0.0362	0.108
Methiocarb-sulfone	2,243	157	93%	29,211	2,119	93%	0.119	0.358
Piperonylbutoxide	219	<LOD	> 95%	206	4.52	> 95%	0.121	0.362
AES-C12. n=0 *	25,832	<LOD	> 95%	<LOD	<LOD	-	0.123	0.368
AES-C14. n=2 *	2,432	49.7	> 95%	<LOD	<LOD	-	0.125	0.375
BAC 18	<LOD	<LOD	-	13.8	6.17	55%	0.126	0.377
Benzododecinium	14,532	2,821	81%	3,107	1,068	66%	0.126	0.379
Benzyldimethylhexadecylammonium	311	8.86	> 95%	50.1	51.1	-2%	0.127	0.381
Benzyldimethyltetradecylammonium	<LOD	<LOD	-	382	250	35%	0.127	0.380
C10-LAS *	<LOD	255	-	21,037	423	> 95%	0.128	0.383
C11-LAS *	<LOD	<LOD	-	46,997	1,256	> 95%	0.128	0.384
C12-AE2S *	13,255	17.3	> 95%	<LOD	<LOD	-	0.128	0.383
C12-AEO2 *	151	13.0	91%	<LOD	<LOD	-	0.123	0.370
C12-AEO3 *	5.232	13.6	> 95%	<LOD	<LOD	-	0.109	0.326

Analyte name	Thriassio influent wastewater	Thriassio effluent wastewater	Thriassio indicative %removal	Psyttalia influent wastewater	Psyttalia effluent wastewater	Psyttalia indicative %removal	LOD	LOQ
C12-LAS *	60,750	<LOD	> 95%	24,210	<LOD	> 95%	0.105	0.315
C13-LAS *	9,784	<LOD	> 95%	8,107	<LOD	> 95%	0.106	0.319
C14-LAS *	3,103	<LOD	> 95%	<LOD	<LOD	-	0.106	0.318
C2DEA *	1,428	899		<LOD	<LOD	-	0.106	0.317
C5DEA *	581	<LOD	> 95%	<LOD	<LOD	-	0.106	0.317
C7DEA *	9,830	25.7	> 95%	<LOD	<LOD	-	0.107	0.322
DDAC-C10	1,167	45.0	> 95%	330	258	22%	0.107	0.321
Hexadecyltrimethylammonium	4,644	<LOD	> 95%	2,015	30.3	> 95%	0.108	0.325
N.N-dimethyldodecylamine	34,134	33.0	> 95%	299	<LOD	> 95%	0.108	0.324
N.N-dimethyldodecylamine N-oxide	<LOD	<LOD	-	253	328	-30%	0.108	0.323
N.N-dimethyltetradecylamine	<LOD	<LOD	-	982	0.591	> 95%	0.110	0.329
N.N-dimethyltetradecylamine-N-oxide	<LOD	<LOD	-	155	208	-35%	0.109	0.328
N-methyldodecylamine	3,549	33.1	> 95%	42.9	16.5	61%	0.111	0.333
NPEO9 *	<LOD	206	-	<LOD	<LOD	-	0.111	0.332
Trimethyloctylammonium	126	<LOD	> 95%	<LOD	<LOD	-	0.112	0.337

* Compounds identified in **confidence level 2a**[9]

250 **Table S9:** Substances determined in seawater samples, which are prioritized by effective
251 Directive 2013/39/EU or the proposal for new EU Directive. along with their AA-EQS.
252 MAC-EQS and RPFs for PFAS

Analyte name	RPF (PFAS)	AA-EQS (ng L^{-1})	MAC-EQS (ng L^{-1})
2.3.3.3-tetrafluoro-2-(heptafluoropropoxy)propanoic acid (HFPO-DA or GenX)	0.06		
4.8-dioxa-3H-perfluorononanoic acid (ADONA)	0.03		
Perfluorobutanesulfonic acid (PFBS)	0.001		
Perfluorobutanoic acid (PFBA)	0.05	∑ PFOA equivalents = 4.40	N/A
Perfluorododecanoic acid (PFDoA)	3		
Perfluorohexanesulfonic acid (PFHxS)	0.6		
Perfluorohexanoic acid (PFHxA)	0.01		
Perfluorooctanesulfonic acid (PFOS)	2		
Perfluoropentanoic acid (PFPeA)	0.03		
Perfluorotetradecanoic acid (PFTeDA)	0.3		
Di-(2-ethylhexyl) phthalate (DEHP)		1,300	N/A
Carbamazepine		250	160,000
Ibuprofen		22.0	N/A
Clothianidin		1.00	34.0
Pentachlorophenol (PCP)		400	1,000

253

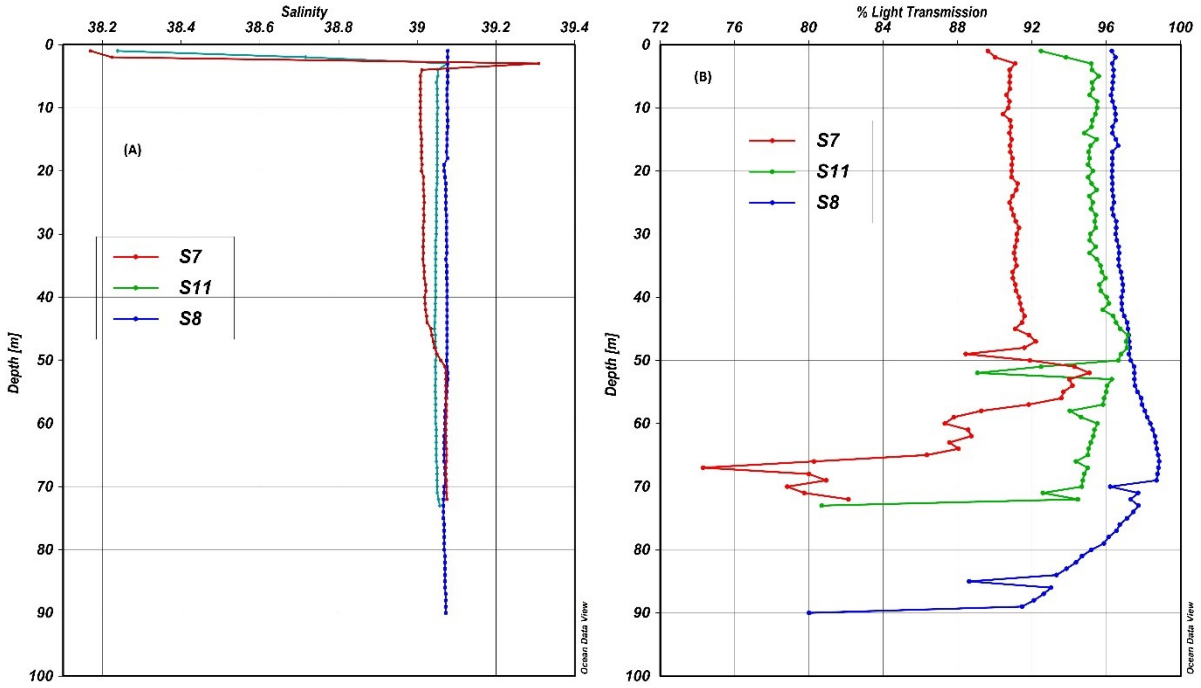


Figure S1: Salinity and % Light Transmission profiles at stations S7, S8 and S11

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