SUPPORTING INFORMATION FOR:

Suspect screening and regulatory databases: A powerful combination to identify emerging micropollutants

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This Supporting Information document (SI) consists of 31 pages and contains 5 tables and 2 figures.

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CONTENT

SI-1: Chemical and reagents

For the characterization of the wastewater regarding the presence of well-known micropollutants (MPs), 74 substances were evaluated including 49 pharmaceuticals of major consumption in Sweden belonging to different therapeutic groups (viz. antibiotics, antiepileptics, NSAIDs, antilipidemics, antiepileptics, antidiabetics, β-blocking agents, antifungals, analgesics, antihypertensives, diuretics, antiulcers, anesthetics, benzodiazepines, and antidepressants); 14 per- and polyfluoroalkyl substances (PFASs) and other substances including personal care products, pesticides, artificial sweeteners and illicit drugs. Target analyte names, CAS numbers and molecular formulas are shown in Table SI-1.

Table SI-1: CAS numbers and molecular formulas of 74 target analytes.

Category	Compound	CAS number	Molecular formula
Pharmaceuticals (antibiotics)	Amoxicillin	26787-78-0	$C_{16}H_{19}N_3O_5S$
	Azithromycin	83905-01-5	$C_{38}H_{72}N_2O_{12}$
	Ciprofloxacin	85721-33-1	$C_{17}H_{18}FN_3O_3$
	Clarithromycin	81103-11-9	$C_{38}H_{69}NO_{13}$
	Erythromycin	114-07-8	$C_{37}H_{67}NO_{13}$
	Metronidazole	443-48-1	$C_6H_9N_3O_3$
	Norfloxacin	70458-96-7	$C_{16}H_{18}FN_3O_3$
	Ofloxacin	82419-36-1	$C_{18}H_{20}FN_3O_4$
	Roxithromycin	80214-83-1	$C_{41}H_{76}N_2O_{15}$
	Sulfamethoxazole	723-46-6	$C_{10}H_{11}N_3O_3S$
	Trimethoprim	738-70-5	$C_{14}H_{18}N_4O_3$
Pharmaceuticals (analgesics)	Acetaminophen (Paracetamol)	103-90-2	$C_8H_9NO_2$
	Tramadol	27203-92-5	$C_{16}H_{25}NO_2$
Pharmaceuticals (anesthetics)	Lidocaine	137-58-7	$C_{14}H_{22}N_2O$
Pharmaceuticals (antidepressants)	Amitriptylline	50-48-7	$C_{20}H_{23}N$
	Citalopram	59729-33-9	$C_{20}H_{21}FN_2O$
	Desvenlafaxine	93413-62-8	$C_{16}H_{25}NO_2$
	Fluoxetine	54910-89-4	$C_{17}H_{18}F_3NO$
	Sertraline	79617-96-3	$C_{17}H_{17}Cl_2N$
	Venlafaxine	93413-69-6	$C_{17}H_{27}NO_2$
Pharmaceuticals (antiepileptics)	Carbamazepine	298-46-5	$C_{15}H_{12}N_2O$
	Lamotrigine	84057-84-2	$C_9H_7Cl_2N_5$
	Valproic acid	99-66-2	$C_8H_{16}O_2$
Pharmaceuticals (antidiabetics)	Metformin	657-24-9	$C_4H_{11}N_5$
Pharmaceuticals (antihipertensives)	Atenolol	29122-68-7	$C_{14}H_{22}N_2O_3$
	Diltiazem	42399-41-7	$C_{22}H_{26}N_2O_4S$

	Irbesartan	138402-11-6	$C_{25}H_{28}N_6O$
	Losartan	114798-26-4	$C_{22}H_{23}ClN_6O$
	Metoprolol	51384-51-1	$C_{15}H_{25}NO_3$
	Valsartan	137862-53-4	$C_{24}H_{29}N_5O_3$
Pharmaceuticals (antilipidemic agents)	Atorvastatin	134523-00-5	$C_{33}H_{35}FN_2O_5$
Pharmaceuticals (antiulcers drugs)	Omeprazole	73590-58-6	$C_{17}H_{19}N_3O_3S$
	Ranitidine	66357-35-5	$C_{13}H_{22}N_4O_3S$
Pharmaceuticals (antifungal)	Climbazole	38083-17-9	$C_{15}H_{17}ClN_2O_2$
	Fluconazole	86386-73-4	$C_{13}H_{12}F_2N_6O$
Pharmaceuticals (benzodiazepines)	Diazepam	439-14-6	$C_{16}H_{13}ClN_2O$
	Oxazepam	604-75-2	$C_{15}H_{11}ClN_2O_2$
Pharmaceuticals (beta blocking agents)	Propranolol	525-66-6	$C_{16}H_{21}NO_2$
	Sotalol	3930-20-9	$C_{12}H_{20}N_2O_3S$
Pharmaceuticals (diuretics)	Furosemide	54-31-9	$C_{12}H_{11}ClN_2O_5S$
	Hydrochlorothiazide	58-93-5	$C_7H_8ClN_3O_4S_2$
Pharmaceuticals (lipid lowering agent)	Bezafibrate	41859-67-0	$C_{19}H_{20}ClNO_4$
Pharmaceuticals (NSAIDs)	Diclofenac	15307-86-5	$C_{14}H_{11}Cl_2NO_2$
	Ibuprofen	15687-27-1	$C_{13}H_{18}O_2$
	Meclofenamic acid	644-62-2	$C_{14}H_{11}Cl_2NO_2$
	Mefenamic Acid	61-68-7	$C_{15}H_{15}NO_2$
	Niflumic acid	4394-00-7	$C_{13}H_9F_3N_2O_2$
Artificial sweetener	Sucralose	56038-13-2	$C_{12}H_{19}Cl_3O_8$
Illicit drugs	Cocaine (COC)	50-36-3	$C_{17}H_{21}NO_4$
Personal care products (insect repellents)	DEET (diethyltoluamide)	134-62-3	$C_{12}H_{17}NO$
Personal care products (parabens)	Ethylparaben	120-47-8	$C_9H_{10}O_3$
	Methylparaben	99-76-3	$C_8H_8O_3$
	Propylparaben	94-13-3	$C_{10}H_{12}O_3$
Personal care products (sunscreens)	Octocrylene	6197-30-4	$C_{24}H_{27}NO_2$
Pesticides	Isoproturon	34123-59-6	$C_{12}H_{18}N_2O$
	Terbutryn	886-50-0	$C_{10}H_{19}N_5S$
	BAM (Dichlorobenzamide)	2008-58-4	$C_7H_5Cl_2NO$
PFASs	Perfluorobutane sulfonic acid (PFBS)	375-73-5	$C_4HF_9O_3S$
	Perfluorobutanoic acid (PFBA)	375-22-4	$C_4HF_7O_2$
	Perfluorodecanoic acid (PFDA)	335-76-2	$C_{10}HF_{19}O_2$
	Perfluorododecanoic acid (PFDoDA)	307-55-1	$C_{12}HF_{23}O_2$
	Perfluoroheptanoic acid (PFHpA)	375-85-9	$C_7HF_{13}O_2$
	Perfluorohexane sulfonic acid (PFHxS)	355-46-4	$C_6HF_{13}O_3S$

	Perfluorohexanoic acid (PFHxA)	307-24-4	$C_6HF_{11}O_2$
	Perfluorononanoic acid (PFNA)	375-95-1	$C_9HF_{17}O_2$
	Perfluorooctane sulfonamide (FOSA)	754-91-6	$C_8H_2F_{17}NO_2S$
	Perfluorooctane sulfonic acid (PFOS)	1763-23-1	$C_8HF_{17}O_3S$
	Perfluorooctanoic acid (PFOA)	335-67-1	$C_8HF_{15}O_2$
	Perfluoropentanoic acid (PFPeA)	2706-90-3	$C_5HF_9O_2$
	Perfluorotetradecanoic acid (PFTeDA)	376-06-7	$C_{14}HF_{27}O_2$
	Perfluoroundecanoic acid (PFUnDA)	2058-94-8	$C_{11}HF_{21}O_2$
Opiates, opioids and metabolites	Codeine (COD)	76-57-4	$C_{18}H_{21}NO_3$
	Oxycodone (OC)	76-42-7	$C_{18}H_{21}NO_4$
Stimulants	Caffeine	8/2/1958	$C_8H_{10}N_4O_2$

All analytical standards used for quantification were of high purity grade (>95%) and purchased from Sigma- Aldrich (Sweden) except pesticides, which were acquired from Teknolab AB (Kungsbacka, Sweden). Isotopically labeled standards (IS) for PFASs, pesticides and pharmaceuticals and personal care products (PPCPs) were purchased from Wellington Laboratories (Canada), Teknolab AB (Kungsbacka, Sweden), and Sigma-Aldrich and Toronto Research Chemicals (Toronto, Canada), respectively.

For the confirmation of suspect compounds, 1,2,3-benzotriazole, 2,2'-dimorpholinyldiethyl-ether, 2-dodecylbenzenesulfonic acid, acesulfame, benzoic acid, benzylamine, dazomet, di-(2-ethylhexyl)phosphoric acid, dibutyl phosphate, diethyl thiourea, laureth 5, laurilsulfate, mono-n-butylphosphoric acid, N-butyldiethanolamine, natammycin, nicotinamide, N,N-dimethyl-1-tetradecanamineoleic acid, panthenol, pyridoxine, ricinoleic acid, sebacic acid, stearic acid, sulisobenzone, tetraethyleneglycol, triisopropanolamine, tris(2-butoxyethyl) phosphate were purchased from Sigma-Aldrich (Steinheim, Germany).

For chemical analysis, gradient grade methanol, acetonitrile and ethyl acetate were purchased from Merck (Darmstadt, Germany), whereas formic acid 98%, ammonium formate, 25% ammonia solution and ammonium acetate were acquired from Sigma-Aldrich (Sweden). Ultrapure water was produced by a Milli-Q Advantage Ultrapure Water purification system (Millipore, Billercia, MA) and filtered through a 0.22 µm Millipak Express membrane. Regarding the consumables for the sample preparation, the empty solid phase extraction polypropylene tubes (6 mL), as well as the cartridge sorbent materials Sepra ZT (Strata-X), Sepra ZT-WCX (Strata-X-CW) and ZT-WAX (Strata-X-AW) were obtained from Phenomenex (Torrance, USA). The Isolute ENV+ sorbent material and the frits (20 µm, 6 mL) were from Biotage (Ystrad Mynach, UK). Glass fiber filters (GFF, pore size 0.7 µm) used in wastewater filtration were obtained from Millipore (Cork, Ireland). Regenerated cellulose syringe filters (RC) of 15 mm diameter and 0.2 µm pore size were obtained from Phenomenex (Torrance, CA, USA).

SI-2: Instrumental analysis

The instrumental analysis was conducted with an Acquity Ultra-Performance Liquid Chromatography (UPLC) system (Waters Corporation, USA) coupled to a quadrupole-time-of-flight (QTOF) mass spectrometer (QTOF Xevo G2S, Waters Corporation, Manchester, UK). Extracts were analyzed in positive (PI) and negative (NI) electrospray ionisation mode. The chromatographic separation was carried out on an Acquity HSS T3 column (100 mm x 2.1 mm, 1.8 µm) in PI mode and on an Acquity BEH C18 column (50 mm x 2.1 mm, 1.7 µm) in NI mode which were both purchased from Waters Corporation (Manchester, UK). For PI mode, the aqueous phase consisted of 5 mM ammonium formate buffer with 0.01% formic acid and the organic phase with acetonitrile and 0.01% formic acid. For NI mode, the aqueous phase was composed of 5 mM ammonium acetate buffer with 0.01% ammonia and the organic phase consisting of acetonitrile with 0.01% ammonia.

The adopted elution gradient for both ionization modes started with 5% of organic phase for 0.5 minutes, increasing to 95% by 16 min, and then to 99% in the following 0.1 min. These almost pure organic conditions were kept constant for 3 min, and then initial conditions were restored and kept for 2 min. The total run time was 21 min in both modes. The chromatographic flow rate was 0.5 mL min^{-1} and the injection volume was 5 µL. The column temperature was set to 40 °C and the sample manager temperature was 15 °C. The resolution of the TOF mass spectrometer was 30 000 at full width and half maximum (FWHM) at m/z 556. MS data were acquired over an m/z range of 100-1200 in a scan time of 0.25 s. Capillary voltages of 0.35 kV were used in PI and 0.4 kV in NI. A cone voltage of 30 V was applied, the desolvation gas flow rate was set at 700 L h^{-1} and the cone gas flow was set to 25 L h^{-1}. The desolvation temperature was set to 450 °C and the source temperature to 120 °C. Two acquisition functions with different collision energies were created: the low energy (LE) function with a collision energy of 4 eV, and the high energy (HE) function with a collision energy ramp ranging from 10 to 45 eV. Calibration of the mass axis from m/z 100 to 1200 was conducted daily with a 0.5 mM sodium formate solution prepared in 90:10 (v/v) 2-propanolol/water. For automated accurate mass measurement, the lock spray probe was employed (10 µL min^{-1}), using a lock mass leucine encephalin solution (2 mg mL^{-1}) in ACN/water (50:50) with 0.1% formic acid.

SI-3: Prioritization

Table SI-2: Prioritized suspect analyte names, molecular formulas, and corresponding SMILES

Compound name	SMILE	Formula
Diethyl thiourea	CCNC(=S)NCC	$C_5H_{12}N_2S$
N-[3-(Dimethylnitroryl) propyl]tetradecanamide	CCCCCCCCCCCCCC(=O)NCCC[N+](C)(C)[O-]	$C_{19}H_{40}N_2O_2$
UNII:G00MDQ58TB	CC(C)C(C)(C)C(C)(C)C(C)(C)S	$C_{12}H_{26}S$
Octyl hydrogen sulfate	CCCCCCCCOS(=O)(=O)O	$C_8H_{18}O_4S$
Nonyl hydrogen sulfate	CCCCCCCCCOS(=O)(=O)O	$C_{10}H_{22}O_4S$
Decyl hydrogen sulfate	CCCCCCCCCCOS(=O)(=O)O	$C_9H_{20}O_4S$
Laurilsulfate	CCCCCCCCCCCCOS(=O)(=O)O	$C_{12}H_{26}O_4S$

Tridecyl hydrogen sulfate	CCCCCCCCCCCCCOS(=O)(=O)O	$C_{13}H_{28}O_4S$
Tetradecyl hydrogen sulfate	CCCCCCCCCCCCCCOS(=O)(=O)O	$C_{14}H_{30}O_4S$
Pentadecyl hydrogen sulfate	CCCCCCCCCCCCCCCOS(=O)(=O)O	$C_{15}H_{32}O_4S$
Hexadecyl hydrogen sulfate	CCCCCCCCCCCCCCCCOS(=O)(=O)O	$C_{16}H_{34}O_4S$
Triethoxy(vinyl)silane	CCO[Si](OCC)(OCC)C=C	$C_8H_{18}O_3Si$
Helvetolide	CCC(=O)OCC(C)(C)OC(C)C1CCCC(C)(C)C1	$C_{17}H_{32}O_3$
1-Hexadecylpyridinium	CCCCCCCCCCCCCCCC[n+]1ccccc1	$C_{21}H_{38}N$
2,2-Bis(hydroxymethyl) propionic acid	CC(CO)(CO)C(=O)O	$C_5H_{10}O_4$
Phenethyl isobutyrate	CC(C)C(=O)OCCc1ccccc1	$C_{12}H_{16}O_2$
N-[3-(4-Morpholinyl)propyl] octadecanamide	CCCCCCCCCCCCCCCCCC(=O)NCCCN1CCOCC1	$C_{25}H_{50}N_2O_2$
Propyl (2S)-2-[(2-methyl-2-butanyl)oxy]propanoate	CCCOC(=O)[C@H](C)OC(C)(C)CC	$C_{11}H_{22}O_3$
2-(Dodecyloxy)ethyl hydrogen sulfate	CCCCCCCCCCCCOCCOS(=O)(=O)O	$C_{14}H_{30}O_5S$
2-[(11-Methyldodecyl)oxy]ethanol	CC(C)CCCCCCCCCCOCCO	$C_{15}H_{32}O_2$
3,3'-{[3-(Decyloxy)propyl]imino} dipropanoic acid	CCCCCCCCCCOCCCN(CCC(=O)O)CCC(=O)O	$C_{19}H_{37}NO_5$
Oleic acid	CCCCCCCC/C=C\CCCCCCCC(=O)O	$C_{18}H_{34}O_2$
Mono-n-butylphosphoric acid	CCCCOP(=O)(O)O	$C_4H_{11}O_4P$
8-Methylnonyl dihydrogen phosphate	CC(C)CCCCCCCOP(=O)(O)O	$C_{10}H_{23}O_4P$
Dipentyl hydrogen phosphate	CCCCCOP(=O)(O)OCCCCC	$C_{10}H_{23}O_4P$
Dibutyl phosphate	CCCCOP(=O)(O)OCCCC	$C_8H_{19}O_4P$
{[(2-hydroxyethyl)imino] dimethanediyl}bis(phosphonic acid)	OCCN(CP(=O)(O)O)CP(=O)(O)O	$C_4H_{13}NO_7P_2$
{1,2-Ethanediylbis[nitrilobis (methylene)]}tetrakis(phosphonic acid)	C(CN(CP(=O)(O)O)CP(=O)(O)O)N(CP(=O)(O)O)CP(=O)(O)O	$C_6H_{20}N_2O_{12}P_4$
Etidronic acid	P(C(C)(O)P(O)(O)=O)(O)(O)=O	$C_2H_8O_7P_2$
(Hydroxymethyl)phosphonic acid	OCP(=O)(O)O	CH_5O_4P
Bis((dimethylamino)methyl)phenol	CN(C)Cc1cccc(O)c1CN(C)C	$C_{12}H_{20}N_2O$
Metoquinone	CNc1ccc(cc1)O	C_7H_9NO
Diisobutyl glutarate	CC(C)COC(=O)CCCC(=O)OCC(C)C	$C_{13}H_{24}O_4$
6,9-Bis[2-(2-hydroxyethoxy) propyl]-4,11-dimethyl-3,12-dioxa-6,9-diazatetradecane-1,14-diol	OCCOC(C)CN(CCN(CC(C)OCCO)CC(C)OCCO)CC(C)OCCO	$C_{22}H_{48}N_2O_8$
Caprylic acid	CCCCCCCC(=O)O	$C_8H_{16}O_2$
2-Methyloctanoic acid	CCCCCCC(C)C(=O)O	$C_9H_{18}O_2$
Octaneperoxoic acid	CCCCCCCC(=O)OO	$C_8H_{16}O_3$

Stearic acid	CCCCCCCCCCCCCCCCCC(=O)O	$C_{18}H_{36}O_2$
UNII:L98N90X0NI	CCCCCCCCCCCCCCCCCC(=O)OC(C)C(=O)OC(C)C(=O)O	$C_{24}H_{44}O_6$
N-[3-(Dimethylamino) propyl]octadecanamid	CCCCCCCCCCCCCCCCCC(=O)NCCCN(C)C	$C_{23}H_{48}N_2O$
9-Oxononanoic acid	C(CCCC=O)CCCC(=O)O	$C_9H_{16}O_3$
UNII:197M6VFC1W	CCCCCCCCCC(=O)OCC(CO)O	$C_{13}H_{26}O_4$
Naphthalenesulfonic acid, dinonyl-	CCCCCCCCCc1cc2c(cccc2)c(c1CCCCCCCCC)S(=O)(=O)O	$C_{28}H_{44}O_3S$
2,3-Diisobutyl-1-naphthalenesulfonic acid	CC(C)Cc1cc2ccccc2c(c1CC(C)C)S(=O)(=O)	$C_{18}H_{24}O_3S$
Ricinoleic acid	CCCCCC[C@H](C/C=C\CCCCCCCC(=O)O)O	$C_{18}H_{34}O_3$
a-Hydroxycyclohexylphenyl-ketone	OC1(CCCCC1)C(=O)c1ccccc1	$C_{13}H_{16}O_2$
2,2',2''-{Nitrilotris[2,1-ethanediylnitrilo (E)methylylidene]}triphenol	c1cc(c(cc1)O)/C=N/CCN(CC/N=C/c2c(cccc2)O)CC/N=C/c3c(cccc3)O	$C_{27}H_{30}N_4O_3$
L-(+)-Glutamic acid	N[C@](C(=O)O)(CCC(=O)O)[H]	$C_5H_9NO_4$
N,N-Bis(carboxymethyl) glutamic acid	C(CC(=O)O)C(C(=O)O)N(CC(=O)O)CC(=O)O	$C_9H_{13}NO_8$
N-Dodecanoyl-L-glutamic acid	CCCCCCCCCCCC(=O)N[C@@H](CCC(=O)O)C(=O)O	$C_{17}H_{31}NO_5$
6-O-Palmitoylhex-1-enofuranos-3-ulose	CCCCCCCCCCCCCCCC(=O)OCC(O)C1OC(=C(O)C1=O)O	$C_{22}H_{38}O_7$
DL-Arginine	NC(CCCN=C(N)N)C(=O)O	$C_6H_{14}N_4O_2$
1,2,3-Benzotriazole	c1ccc2c(c1)[nH]nn2	$C_6H_5N_3$
7-Methyloctanoic acid	CC(C)CCCCCC(=O)O	$C_9H_{18}O_2$
Adipic acid	C(CCC(=O)O)CC(=O)O	$C_6H_{10}O_4$
N-Heptanoic acid	CCCCCCC(=O)O	C7H14O2
N-Laurylsarcosine	CCCCCCCCCCCCN(C)CC(=O)O	$C_{15}H_{31}NO_2$
Pentetic acid	C(CN(CC(=O)O)CC(=O)O)N(CCN(CC(=O)O)CC(=O)O)CC(=O)O	$C_{14}H_{23}N_3O_{10}$
EDDA	C(CNCC(=O)O)NCC(=O)O	$C_6H_{12}N_2O_4$
Ethylenediaminetriacetic acid	C(CN(CC(=O)O)CC(=O)O)NCC(=O)O	$C_8H_{14}N_2O_6$
HIDA	C(CO)N(CC(=O)O)CC(=O)O	$C_6H_{11}NO_5$
Capryloylglycine	CCCCCCCC(=O)NCC(=O)O	$C_{10}H_{19}NO_3$
N-10-Undecenoylglycine	OC(=O)CNC(=O)CCCCCCCCC=C	$C_{13}H_{23}NO_3$
6-Hydroxy-5-nitroso-2-naphthalenesulfonic acid	c1cc(c(c2c1cc(cc2)S(=O)(=O)O)N=O)O	$C_{10}H_7NO_5S$
Musk ketone	CC(=O)c1c(C)c(c(c(c1C)[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-]	$C_{14}H_{18}N_2O_5$
2-Propoxyethanol	CCCOCCO	$C_5H_{12}O_2$

2-{2-[2-(Tridecyloxy)ethoxy] ethoxy}ethyl hydrogen sulfate	CCCCCCCCCCCCCOCCOCCOCCOS(=O)(=O)O	$C_{19}H_{40}O_7S$
2-[2-(2-Propyn-1-yloxy)ethoxy]ethanol	OCCOCCOCC#C	$C_7H_{12}O_3$
2,2'-{[(5-Methyl-1H-benzotriazol-1-yl)methyl]imino}diethanol	Cc1cc2c(cc1)n(CN(CCO)CCO)nn2	$C_{12}H_{18}N_4O_2$
N-Methyldiethanolamine	CN(CCO)CCO	$C_5H_{13}NO_2$
N-Butyldiethanolamine	CCCCN(CCO)CCO	$C_8H_{19}NO_2$
N-Methyltaurine	CNCCS(=O)(=O)O	$C_3H_9NO_3S$
2-{[4-(Diethylamino)phenyl] [4-(Diethyliminio)-2,5-cyclohexadien-1-ylidene] methyl}-4-hydroxy-5-sulfobenzenesulfonate	CCN(CC)c1ccc(cc1)C(=C2C=CC(=[N+](CC)CC)C=C2)c3cc(c(cc3S(=O)(=O)[O-])S(=O)(=O)O)O	$C_{27}H_{32}N_2O_7S_2$
N-{2-[(2-Hydroxyethyl) amino]ethyl}dodecanamide	CCCCCCCCCCCC(=O)NCCNCCO	$C_{16}H_{34}N_2O_2$
Chlorhexidine	c1cc(ccc1NC(=N)NC(=N)NCCCCCCNC(=N)NC(=N)Nc2ccc(cc2)Cl)Cl	$C_{22}H_{30}Cl_2N_{10}$
Sebacic acid	C(CCCCC(=O)O)CCCC(=O)O	$C_{10}H_{18}O_4$
N,N-Dimethyldecanamide	CCCCCCCCCC(=O)N(C)C	$C_{12}H_{25}NO$
UNII:6T6Z1Z1NC4	CC1CCC(C(O)C1)C(C)(C)O	$C_{10}H_{20}O_2$
Cis-p-Menthan-8-yl acetate	C[C@H]1CC[C@H](CC1)C(OC(=O)C)(C)C	$C_{12}H_{22}O_2$
Isophorone diisocyanate	CC1(C)CC(CC(C)(CN=C=O)C1)N=C=O	$C_{12}H_{18}N_2O_2$
1,1'-Methylenebis(4-isocyanatocyclohexane)	C1CC(CCC1CC2CCC(CC2)N=C=O)N=C=O	$C_{15}H_{22}N_2O_2$
[18-(2-Carboxyethyl)-20-(carboxymethyl)-7-ethyl-3,8,13,17-tetramethyl-12-vinyl-17,18-dihydro-2-porphyrincarboxylato(2-)-κ2N,N']copper	CCC1=C(/c/2c/c3c(c(c/4n3[Cu]n\5/c(c\c1n2)/c(c(/c5c(/c6n/c(c4)/C(C6CCC(=O)O)C)\CC(=O)O)C(=O)O)C)C=C)C	$C_{34}H_{34}CuN_4O_6$
Glutaric acid	OC(=O)CCCC(=O)O	$C_5H_8O_4$
Ethylenediaminetetraacetic acid	C(CN(CC(=O)O)CC(=O)O)N(CC(=O)O)CC(=O)O	$C_{10}H_{16}N_2O_8$
Ethyl acetoacetate	CCOC(=O)CC(=O)C	$C_6H_{10}O_3$
2-Sulfosuccinic acid	C(C(C(=O)O)S(=O)(=O)O)C(=O)O	$C_4H_6O_7S$
(±)-Malic Acid	OC(CC(=O)O)C(=O)O	$C_4H_6O_5$
UNII:660854YI1A	C=CCCCCCCC(CC(=O)O)C(=O)O	$C_{12}H_{20}O_4$
Panthenol	CC(C)(CO)C(O)C(=O)NCCCO	$C_9H_{19}NO_4$
Benzylamine	c1ccc(cc1)CN	C_7H_9N
Mercaptobenztiazyl Ether	S(Sc1nc2c(s1)cccc2)c1nc2c(s1)cccc2	$C_{14}H_8N_2S_4$
Benzoic acid	c1ccc(cc1)C(=O)O	$C_7H_6O_2$

Cyclohexyl salicylate	c1ccc(c(c1)C(=O)OC2CCCCC2)O	$C_{13}H_{16}O_3$
2-Phenylethyl salicylate	Oc1c(cccc1)C(=O)OCCc1ccccc1	$C_{15}H_{14}O_3$
2-Methylbutyl salicylate	CCC(C)COC(=O)c1c(O)cccc1	$C_{12}H_{16}O_3$
Octisalate	CCCCC(CC)COC(=O)c1c(O)cccc1	$C_{15}H_{22}O_3$
4-Icosylbenzenesulfonic acid	CCCCCCCCCCCCCCCCCCCCc1ccc(cc1)S(=O)(=O)O	$C_{26}H_{46}O_3S$
Dodecyl benzenesulfonic acid	CCCCCCCCCCCCOS(=O)(=O)c1ccccc1	$C_{18}H_{30}O_3S$
2,2'-Dimorpholinyldiethyl-ether	C1COCCN1CCOCCN2CCOCC2	$C_{12}H_{24}N_2O_3$
2-Decyl-6-(2-sulfophenoxy) benzenesulfonic acid	CCCCCCCCCCc1cccc(c1S(=O)(=O)O)Oc2ccccc2S(=O)(=O)O	$C_{22}H_{30}O_7S_2$
Sulisobenzone	COc1cc(c(cc1S(=O)(=O)O)C(=O)c2ccccc2)O	$C_{14}H_{12}O_6S$
4-[(2Z)-2-(2-Oxo-1(2H)-naphthalenylidene)hydrazino]benzenesulfonic acid	c1ccc\2c(c1)C=CC(=O)/C2=N\Nc3ccc(cc3)S(=O)(=O)O	$C_{16}H_{12}N_2O_4S$
2,2'-(E)-Ethene-1,2-diylbis[5-({4-anilino-6-[(2-hydroxyethyl)(methyl) amino]-1,3,5-triazin-2-yl}amino)benzenesulfonic acid]	CN(CCO)c1nc(nc(n1)Nc2ccc(c(c2)S(=O)(=O)O)/C=C/c3ccc(cc3S(=O)(=O)O)Nc4nc(nc(n4)N(C)CCO)Nc5ccccc5)Nc6ccccc6	$C_{38}H_{40}N_{12}O_8S_2$
[[4-[Bis[4-[(sulfophenyl)amino]-phenyl] methylene]-2,5-cyclohexadien-1-ylidene]amino]benzenesulfonic acid	c1ccc(c(c1)Nc2ccc(cc2)C(=C3C=CC(=Nc4ccccc4S(=O)(=O)O)C=C3)c5ccc(cc5)Nc6ccccc6S(=O)(=O)O)S(=O)(=O)O	$C_{37}H_{29}N_3O_9S_3$
Tetraethyleneglycol	C(COCCOCCOCCO)O	$C_8H_{18}O_5$
Octadecylbenzyldimethylammonium	CCCCCCCCCCCCCCCCCC[N+](C)(C)Cc1ccccc1	$C_{27}H_{50}N$
1,3-Bis(2-isocyanato-2-propanyl)benzene	CC(C)(N=C=O)c1cc(ccc1)C(C)(C)N=C=O	$C_{14}H_{16}N_2O_2$
Musk xylene	Cc1c(c(c(c(C)c1[N+](=O)[O-])[N+](=O)[O-])C(C)(C)C)[N+](=O)[O-]	$C_{12}H_{15}N_3O_6$
4-Methoxybenzaldehyde	COc1ccc(C=O)cc1	$C_8H_8O_2$
Ethylvanillin	CCOc1cc(C=O)ccc1O	$C_9H_{10}O_3$
10,10-Dimethyl-1-undecanamine	CC(C)(C)CCCCCCCCCN	$C_{13}H_{29}N$
N,N-Bis(2-hydroxyethyl)octanamide	CCCCCCCC(=O)N(CCO)CCO	$C_{12}H_{25}NO_3$
Phenethyl acetate	CC(=O)OCCc1ccccc1	$C_{10}H_{12}O_2$
2-(Dimethylamino)ethyl acetate	CN(C)CCOC(=O)C	$C_6H_{13}NO_2$
UNII:152RJL554H	NC(=O)C(Br)C#N	$C_3H_3BrN_2O$
Ricinoleic Acid	CCCCCC[C@@H](O)C/C=C\CCCCCCCC(=O)O	$C_{18}H_{34}O_3$
(9E,12E)-N,N-Bis(2-hydroxyethyl)-9,12-octadecadienamide	CCCCC/C=C/C/C=C/CCCCCCCC(=O)N(CCO)CCO	$C_{22}H_{41}NO_3$
Nicotinamide	NC(=O)c1cnccc1	$C_6H_6N_2O$
4-((2,4-Dimethylphenyl)azo)-2,4-	CC1=NN(C(=O)C1N=Nc1ccc(C)cc1C)c1ccccc1	$C_{18}H_{18}N_4O$

dihydro-5-methyl-2-phenyl-3H-pyrazol-3-one		
2,5,8,11,14-Pentaoxahexadecan-16-ol	COCCOCCOCCOCCOCCO	$C_{11}H_{24}O_6$
Laureth-5	CCCCCCCCCCCCOCCOCCOCCOCCOCCO	C22H46O6
Pyridoxine	Cc1c(c(c(cn1)CO)CO)O	$C_8H_{11}NO_3$
Benzyl cinnamate	O=C(OCc1ccccc1)/C=C/c1ccccc1	$C_{16}H_{14}O_2$
Isobutyl acrylate	CC(C)COC(=O)C=C	$C_7H_{12}O_2$
Allyl methacrylate	CC(=C)C(=O)OCC=C	$C_7H_{10}O_2$
Dipropylene glycol diacrylate	CC(COCC(C)OC(=O)C=C)OC(=O)C=C	$C_{12}H_{18}O_5$
N-Allyl-N,N-dimethyl-2-propen-1-aminium	C[N+](C)(CC=C)CC=C	$C_8H_{16}N$
UNII:W9EN9DLM98	CC(O)CN(CC(C)O)CC(C)O	$C_9H_{21}NO_3$
(5E)-5-[(2-Methoxy-5-methyl-4-sulfophenyl)hydrazono]-6-oxo-5,6-dihydro-2-naphthalenesulfonic acid	CC1=CC(=C(C=C1S(=O)(=O)O)OC)N/N=C\2/C3=C(C=CC2=O)C=C(C=C3)S(=O)(=O)O	$C_{18}H_{16}N_2O_8S_2$
Maleic acid	C(=C\C(=O)O)\C(=O)O	$C_4H_4O_4$
p-Methoxybenzylacetone	COc1ccc(CCC(=O)C)cc1	$C_{11}H_{14}O_2$
1-Amino-9,10-dioxo-4-({4-[(2-oxo propyl)amino]-2-sulfophenyl}amino)-9,10-dihydro-2-anthracene sulfonic acid	CC(=O)CNc1ccc(c(c1)S(=O)(=O)O)Nc2cc(c(c3c2C(=O)c4ccccc4C3=O)N)S(=O)(=O)O	$C_{23}H_{19}N_3O_9S_2$
DCEMH	CCC1(C)N(Cl)C(=O)N(Cl)C1=O	$C_6H_8Cl_2N_2O_2$
1,3-dichloro-5,5-dimethylhydantoin	CC1(C(=O)N(C(=O)N1Cl)Cl)C	$C_5H_6Cl_2N_2O_2$
Piroctone	Cc1cc(n(c(=O)c1)O)CC(C)CC(C)(C)C	$C_{14}H_{23}NO_2$
N,N-Dimethyl-1-tetradecanamine	CCCCCCCCCCCCCCN(C)C	$C_{16}H_{35}N$
2-Methyl-2-(methylamino)-1-propanol	CNC(C)(C)CO	$C_5H_{13}NO$
Helvetolide	CCC(=O)OCC(C)(C)OC(C)C1CCCC(C)(C)C1	$C_{17}H_{32}O_3$
UNII:KY9R9R74G9	C(C(CCl)O)S(=O)(=O)O	$C_3H_7ClO_4S$
{Dimethyl[3-(tetradecanoylamino) propyl]ammonio}acetate	CCCCCCCCCCCCCC(=O)NCCC[N+](C)(C)CC(=O)[O-]	$C_{21}H_{42}N_2O_3$
{Dimethyl[3-(stearoylamino)propyl] ammonio}acetate	CCCCCCCCCCCCCCCCCC(=O)NCCC[N+](C)(C)CC(=O)[O-]	$C_{25}H_{50}N_2O_3$
Pendecamaine	CCCCCCCCCCCCCCCC(=O)NCCC[N+](C)(C)CC(=O)[O-]	$C_{23}H_{46}N_2O_3$
1-[2-(2-Propoxyethoxy) ethoxy]propane	CCCOCCOCCOCCC	$C_{10}H_{22}O_3$
Octylamine	CCCCCCCCN	$C_8H_{19}N$
Hexadecyl dihydrogen phosphate	CCCCCCCCCCCCCCCCOP(=O)(O)O	$C_{16}H_{35}O_4P$

Tiabendazole	c1ccc2c(c1)[nH]c(n2)c3cscn3	$C_{10}H_7N_3S$
N-Ethyl-N,N-dimethyl-1-dodecanaminium	CCCCCCCCCCCC[N+](C)(C)CC	$C_{16}H_{36}N$
N-(3-{[4-(Dimethylamino)benzoyl]amino}propyl)-N,N-dimethyl-1-dodecanaminium	CCCCCCCCCCCC[N+](C)(C)CCCNC(=O)c1ccc(cc1)N(C)C	$C_{26}H_{48}N_3O$
Tolytriazole	Cc1cccc2c1nn[nH]2	$C_7H_7N_3$
N,N,N-Trimethyl-1-docosanaminium	CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C	$C_{25}H_{54}N$
Decyl dimethylamine oxide	CCCCCCCCCC[N+](C)(C)[O-]	$C_{12}H_{27}NO$
UNII:SJ995B41AO	COC(C)CCO	$C_5H_{12}O_2$
Phenothiazine	N1c2c(Sc3c1cccc3)cccc2	$C_{12}H_9NS$
Avobenzone	COc1ccc(cc1)C(=O)CC(=O)c1ccc(cc1)C(C)(C)C	$C_{20}H_{22}O_3$
2-Ethyl-2-(methoxymethyl)-1,3-propanediol	CCC(CO)(CO)COC	$C_7H_{16}O_3$
Dimethylolpropane	CCC(CO)CO	$C_5H_{12}O_2$
Fructone	CCOC(=O)CC1(C)OCCO1	$C_8H_{14}O_4$
Piperonal	O=Cc1cc2c(OCO2)cc1	$C_8H_6O_3$
Tris(2-butoxyethyl) phosphate	CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC	$C_{18}H_{39}O_7P$
Trithiocyanuric acid	c1(=S)[nH]c(=S)[nH]c(=S)[nH]1	$C_3H_3N_3S_3$
1,2-Pentanediol	CCCC(O)CO	$C_5H_{12}O_2$
2-Methyl-1,2-benzothiazol-3(2H)-one	Cn1c(=O)c2ccccc2s1	C_8H_7NOS
Acesulfame	CC1=CC(=NS(=O)(=O)O1)O	$C_4H_5NO_4S$
Ethyl N-acetyl-N-butyl-β-alaninate	CCCCN(CCC(=O)OCC)C(=O)C	$C_{11}H_{21}NO_3$
(8Z,14Z,16Z,18Z,20Z)-22-[(3-amino-3,6-dideoxyhexopyranosyl)oxy]-1,3,26-trihydroxy-12-methyl-10-oxo-6,11,28trioxatricyclo[22.3.1.$0^{5,7}$]octacosa-8,14,16,18,20-pentaene-25-carboxylic acid	CC1OC(OC2CC3OC(O)(CC(O)C3C(=O)O)CC(O)CC3OC3C=CC(=O)OC(C)CC=CC=CC=CC=C2)C(O)C(N)C1O	$C_{33}H_{47}NO_{13}$

SI-4: Quality assurance and quality control

Background contamination in the laboratory represents a frequent problem in the determination of micropollutants. In order to reduce those errors, several measures were taken into account when preparing and processing the samples. All glassware used was previously washed and heated overnight at 450 °C. Furthermore, gloves were worn during sample preparation. Since many of the compounds analyzed may undergo photodegradation and the samples may suffer the exposure to light during the procedure, all samples and stock standard solutions were in amber glass bottles and stored in the dark. Blanks were prepared to avoid a false determination of compounds coming from a different source than the effluent water.

The present work followed the same protocol and used the same materials for sample pre-treatment and SPE as other previous studies.[1, 2, 3, 4] These works described extensively the performance of the approach and the good recoveries obtained for a long list of micropollutants with a very wide range of physicochemical properties. Those studies indicate a good performance of the approach and its applicability for the study at hand.

SI-5: Target analysis of micropollutants

Table SI-3: Concentrations (ng L^{-1}) of the target analytes in the investigated effluents of Uppsala, Stockholm and Västerås and method limits of detection (MLOD) and limits of quantification (MLOQ) for individual target analyte.

Target analytes	Wastewater effluents			Average	Range	MLOD	MLOQ
	Uppsala	Stockholm	Västerås				
Acetaminophen	n.d.	n.d.	n.d.	n.d.	n.d.	0.5	1.6
Amitriptyline	16	14	16	15	14-16	0.2	0.5
Amoxicillin	n.d.	n.d.	n.d.	n.d.	n.d.	1.1	3.6
Atenolol	110	110	370	200	110-370	0.001	0.003
Atorvastatin	5.3	19	95	40	5.3-95	0.002	0.006
Azithromycin	13	39	42	31	13-42	0.4	1.2
BAM	n.d.	n.d.	n.d.	n.d.	n.d.	0.6	1.9
Bezafibrate	12	8.4	9.9	10	8.4-10	0.003	0.009
Caffeine	410	200	140	150	140-410	0.3	0.9
Carbamazepine	140	66	100	100	66-140	0.005	0.02
Ciprofloxacin	67	74	42	61	42-67	3	9
Citalopram	100	44	71	71	44-100	0.02	0.05
Clarithromycin	12	36	38	29	12-38	0.04	0.1
Climbazole	37	88	42	56	37-88	0.007	0.02
Cocaine	0.8	5.0	11	5.7	0.8-11	0.005	0.02

Codeine	58	103	170	110	58-170	0.070	0.2
DEET	71	52	51	58	51-71	0.006	0.02
Desvenlafaxine	240	160	290	230	160-290	0.02	0.05
Diazepam	< MLOQ	< MLOQ	0.4	0.4	0.1-0.4	0.1	0.4
Diclofenac	280	200	290	250	200-290	0.6	1.8
Diltiazem	6.3	6.7	7.5	6.8	6.3-7.5	0.003	0.01
Erythromycin	3.9	8.7	7.6	6.8	3.9-8.7	0.08	0.3
Ethylparaben	n.d.	0.01	0.2	0.1	0.01-0.2	0.06	0.2
Fluconazole	190	68	92	120	68-190	0.004	0.02
Fluoxetine	6.9	4.3	4.5	5.3	4.3-6.9	0.3	0.9
FOSA	n.d.	n.d.	n.d.	n.d.	n.d.	0.1	0.4
Furosemide	360	350	470	390	350-470	0.2	0.5
Hydrochlorothiazide	360	< MLOQ	620	440	<0.2-620	0.07	0.2
Ibuprofen	n.d.	46	100	74	46-10	3.3	11
Irbesartan	40	70	42	51	40-70	0.004	0.02
Isoproturon	n.d.	n.d.	n.d.	n.d.	n.d.	0.6	2
Lamotrigine	260	69	110	140	60-260	0.1	0.4
Lidocaine	140	65	92	99	65-140	0.004	0.01
Losartan	77	170	670	300	77-670	0.2	0.5
Meclofenamic acid	5.2	7.1	7.9	6.7	5.2-7.9	0.05	0.17
Mefenamic Acid	3.3	3.4	1.3	2.7	1.3-3.4	0.07	0.24
Metformin	69	440	1400	640	69-1400	0.05	0.2
Methylparaben	1.6	1.5	2.6	1.9	1.5-2.6	0.1	0.4
Metoprolol	1800	1400	1300	1500	1300-1800	0.3	0.9
Metronidazole	5.1	16	21	14	5.1-21	0.02	0.07
Niflumic acid	n.d.	n.d.	n.d.	n.d.	n.d.	0.5	2
Norfloxacin	n.d.	n.d.	n.d.	n.d.	n.d.	3.3	10
Octocrylene	n.d.	n.d.	n.d.	n.d.	n.d.	10	31
Ofloxacin	n.d.	n.d.	n.d.	n.d.	n.d.	3	10
Omeprazole	0.8	1.1	1.8	1.2	0.8-1.8	0.01	0.04
Oxazepam	150	86	180	140	86-180	0.03	0.1
Oxycodone	12	6.2	23	13	6.2-23	0.02	0.06
PFBA	n.d.	n.d.	n.d.	n.d.	n.d.	0.4	1.3
PFBS	< MLOQ	< MLOQ	0.4	0.5	<0.05-0.5	0.02	0.05
PFDA	n.d.	n.d.	n.d.	n.d.	n.d.	0.02	0.07
PFDoDA	n.d.	n.d.	n.d.	n.d.	n.d.	0.08	0.3
PFHpA	n.d.	0.7	< MLOQ	0.	<0.2-0.7	0.06	0.2
PFHxA	3.5	n.d.	n.d.	3.5	3.5	0.1	0.4

PFHxS	< MLOQ	0.8	1.5	1.2	<0.06-1.5	0.02	0.06
PFNA	n.d.	n.d.	n.d.	n.d.	n.d.	0.03	0.1
PFOA	0.7	0.9	1.2	0.9	0.7-1.2	0.05	0.2
PFOS	0.9	< MLOQ	0.8	0.8	<0.06-0.9	0.02	0.06
PFPeA	< MLOQ	n.d.	n.d.	< MLOQ	0.9-3	0.9	3.0
PFTeDA	n.d.	n.d.	n.d.	n.d.	n.d.	0.007	0.03
PFUnDA	n.d.	n.d.	n.d.	n.d.	n.d.	0.06	0.2
Propranolol	69	42	67	60	42-69	0.02	0.06
Propylparaben	n.d.	n.d.	0.4	0.4	0.4	0.03	0.09
Ranitidine	44	47	39	43	39-47	0.03	0.09
Roxithromycin	1.1	0.2	1.9	1.1	0.2-1.9	0.03	0.1
Sertraline	16	14	12	14	12-16	0.01	0.04
Sotalol	150	60	37	80	37-150	0.04	0.1
Sucralose	5200	4800	2900	4300	2900-5200	20	62
Sulfamethoxazole	50	48	130	75	48-130	0.03	0.09
Terbutryn	3.5	3.8	7.0	4.8	3.5-7.0	0.1	0.4
Tramadol	510	210	490	400	210-510	0.01	0.03
Trimethoprim	11	8.0	11	10	8.0-11	0.3	1.1
Valproic acid	n.d.	n.d.	n.d.	n.d.	n.d.	1.3	4.3
Valsartan	48	150	120	110	48-150	0.04	0.1
Venlafaxine	220	77	170	160	77-220	0.1	0.4

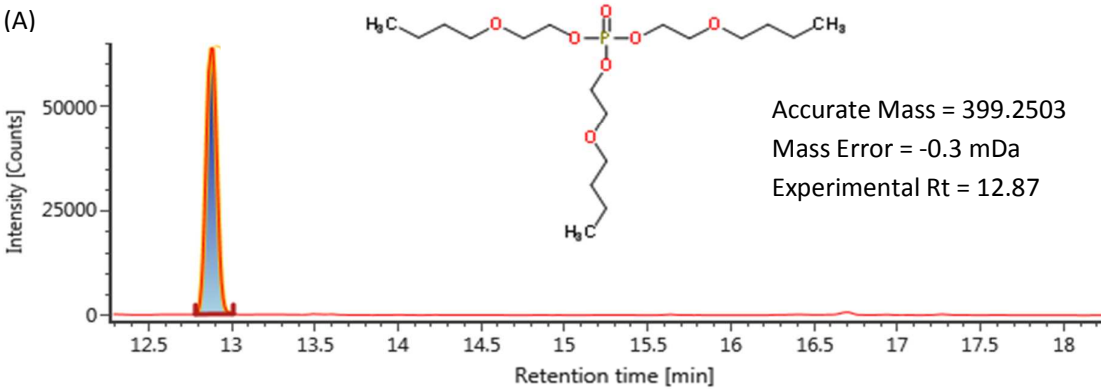
n.d. Not detected
< MLOQ Concentration below the method limit of quantification

SI-6: Identification of suspects

Table SI-4: Suspect analytes accomplishing the reduction of features thresholds but without additional evidences and therefore remaining at a confidence level 4 and 5.

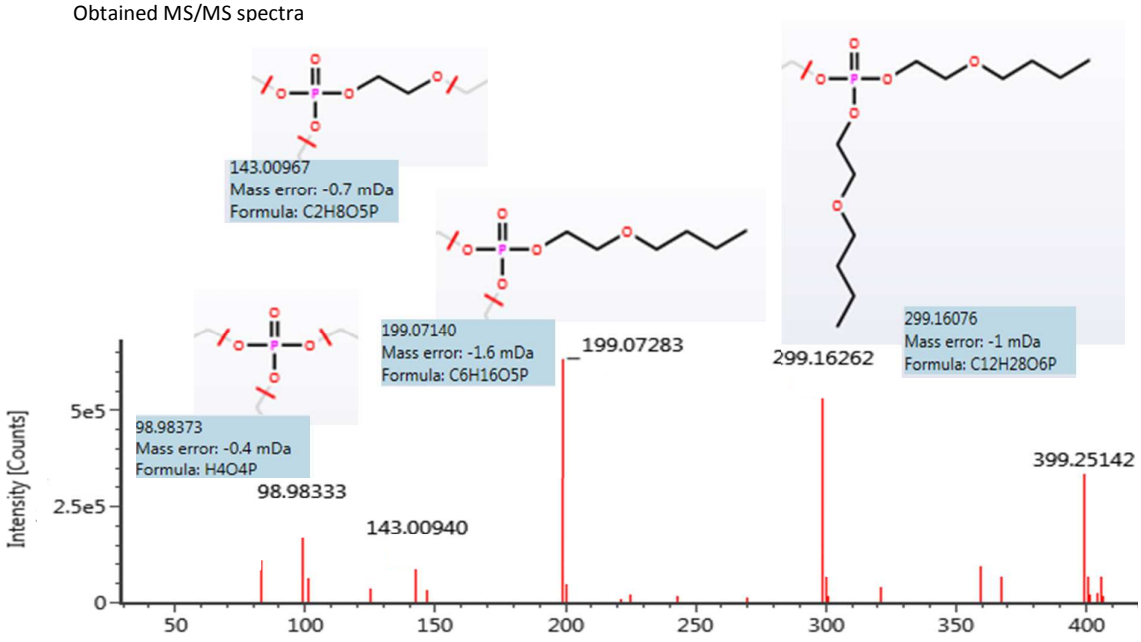
Compound Name	Molecular formula
Naphthalenesulfonic acid	C28H44O3S
Capryloylglycine	*C10H19NO3*
Avobenzone	C20H22O3
UNII:660854YI1A	C12H20O4
2-Methylbutyl salicylate	C12H16O3
Adipic acid	C6H10O4
Dipentyl hydrogen phosphate	C10H23O4P
diethyl hexyl phosphate	C10H23O4P
Diisobutyl phthalate	C16H22O4
2,4,7,9-Tetramethyl-5-Decyn-4,7-Diol	C14H26O2
Butyl glycolate	C6H12O3
Sorbitol	C6H14O6
Ethylvanillin	C9H10O3
5-Isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane	C12H18N2O2
dipropylene glycol diacrylate	C12H18O5
Bis((dimethylamino)methyl)phenol	C12H20N2O
2,2',2''-{Nitrilotris[2,1-ethanediylnitrilo(E)methylylidene]}triphenol	C27H30N4O3
2-(Dimethylamino)ethyl acetate	C6H13NO2
Capryloylglycine	C10H19NO3

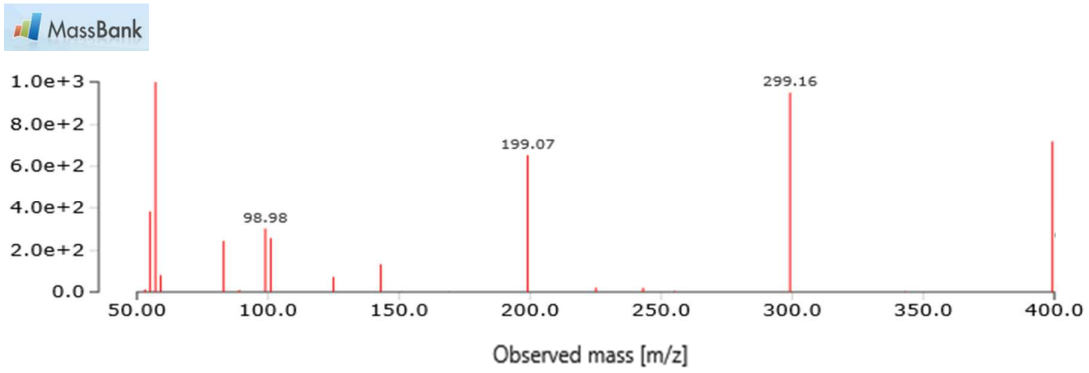
(A)



(B)

Obtained MS/MS spectra





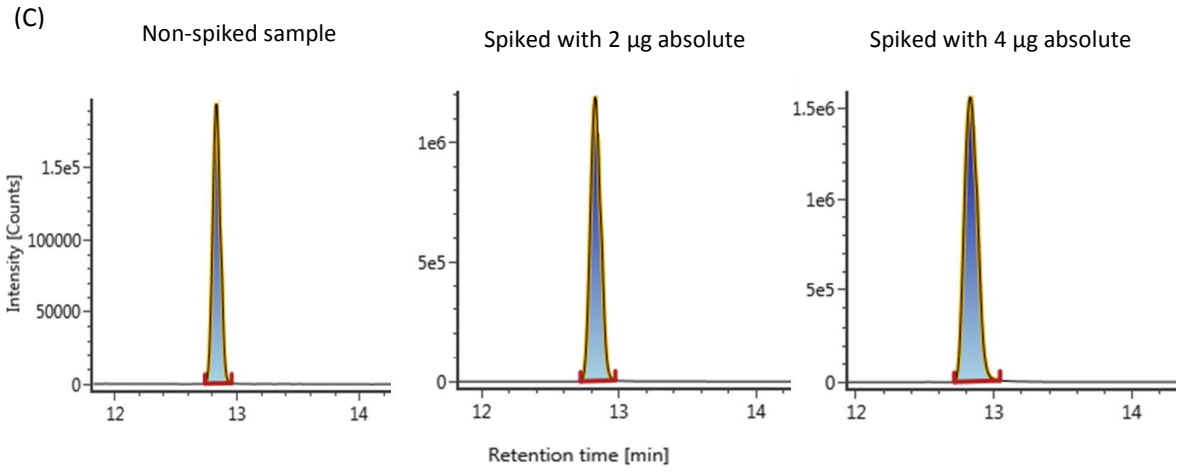
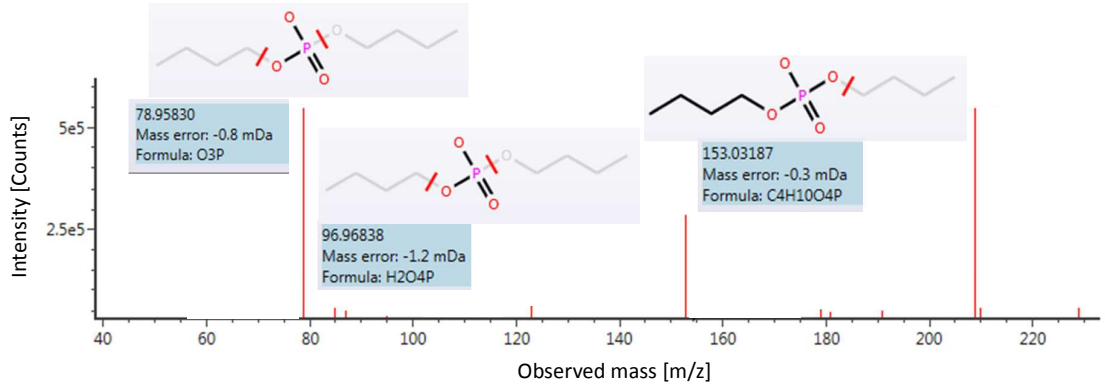
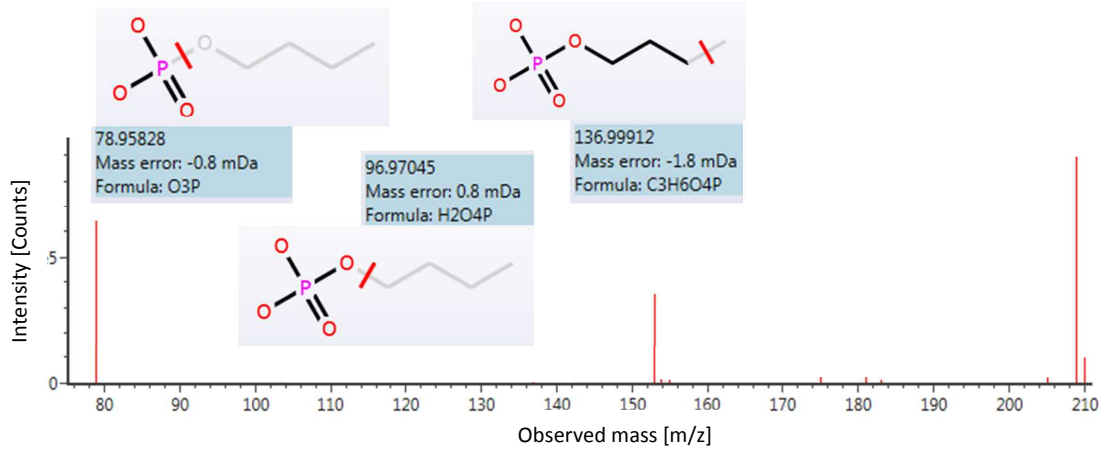


Figure S1: Identification of tris(2-butoxyethyl) phosphate: (A) Full MS chromatogram, (B) experimental spectra with characteristic fragments and MassBank spectra (record SM880602) in order to compare and (C) confirmation step with reference standard.

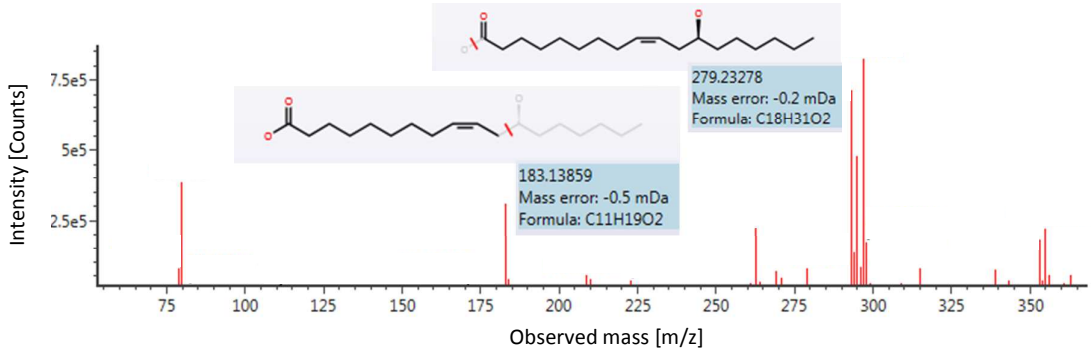
Dibutyl Phosphate [$C_8H_{19}O_4P$]



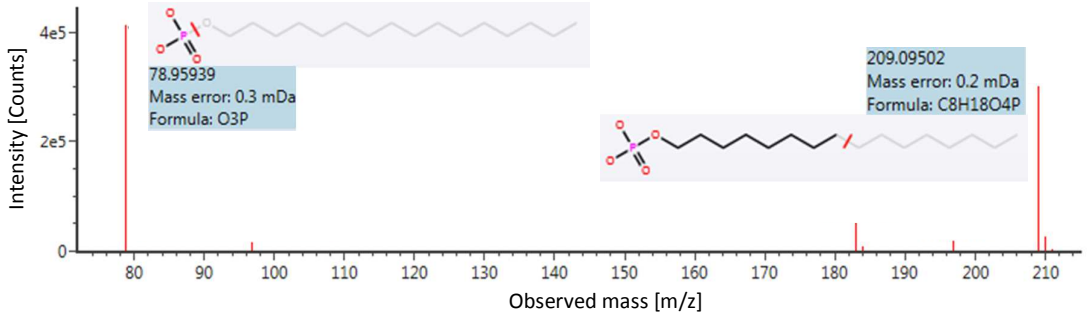
Mono-n-butylphosphoric acid [$C_4H_{11}O_4P$]



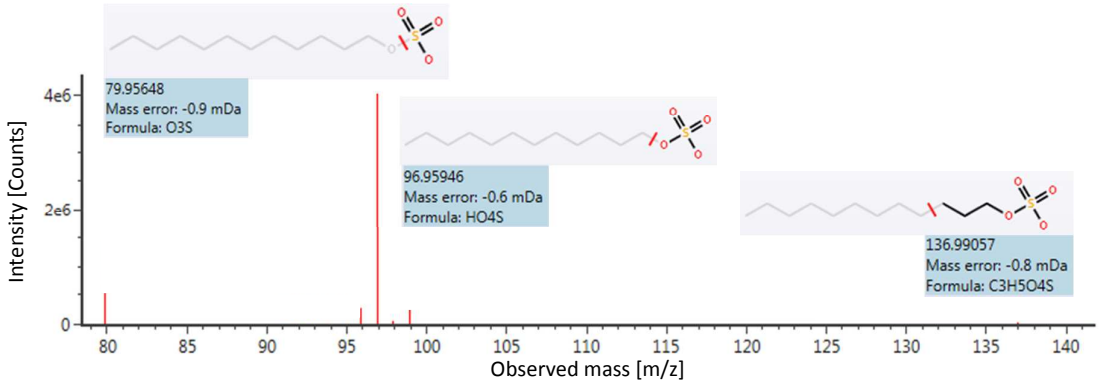
Ricinoleic acid [$C_{18}H_{34}O_3$]



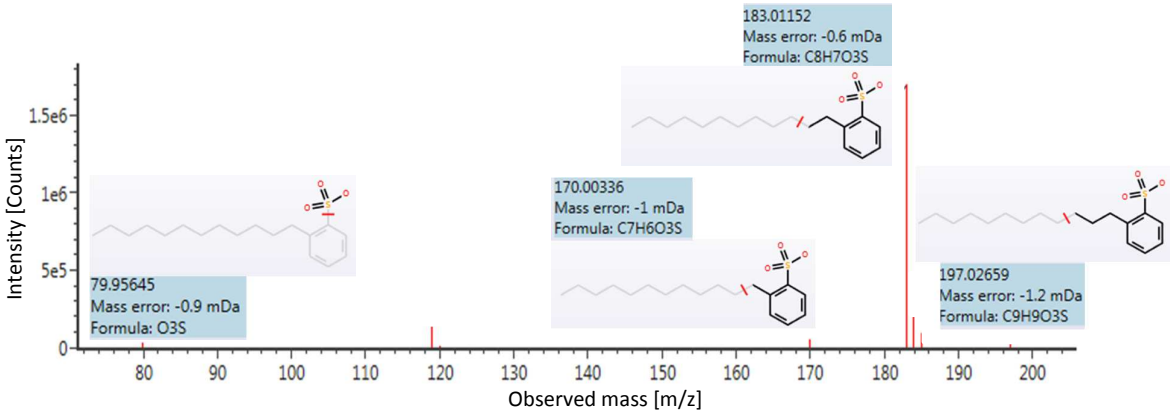
Di-(2-ethylhexyl)phosphoric acid [$C_{16}H_{35}O_4P$]



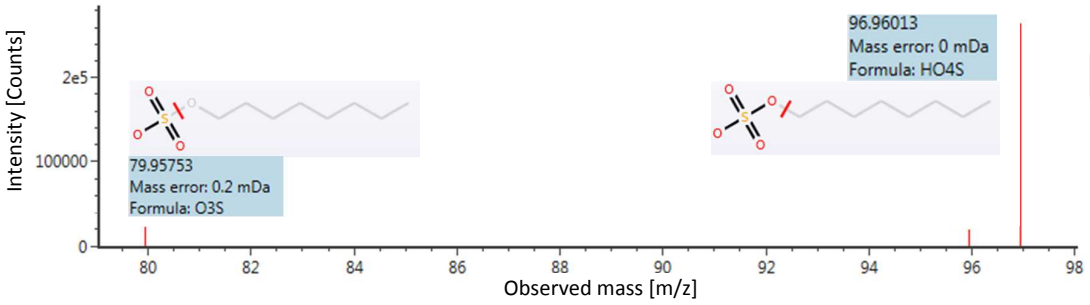
Laurilsulfate [$C_{12}H_{26}O_4S$]



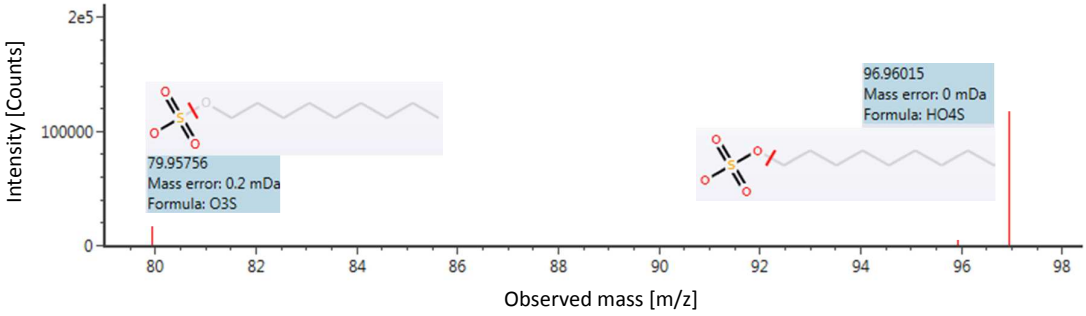
2-Dodecylbenzenesulfonic acid [$C_{18}H_{30}O_3S$]



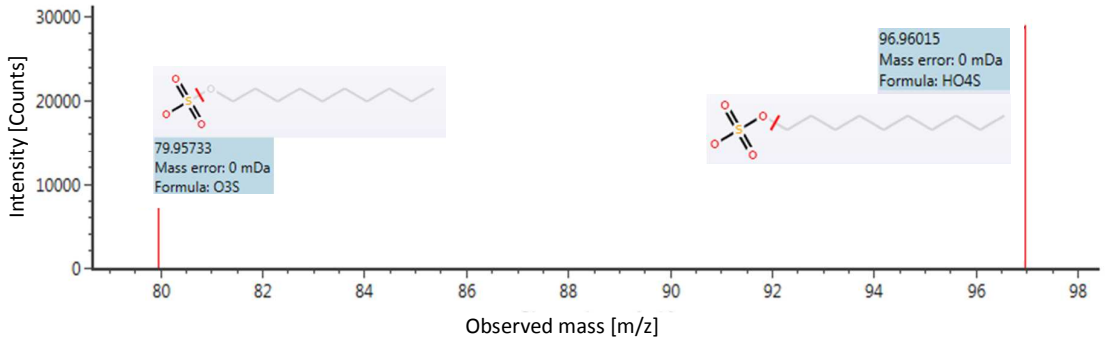
Octyl hydrogen sulfate [$C_8H_{18}O_4S$]



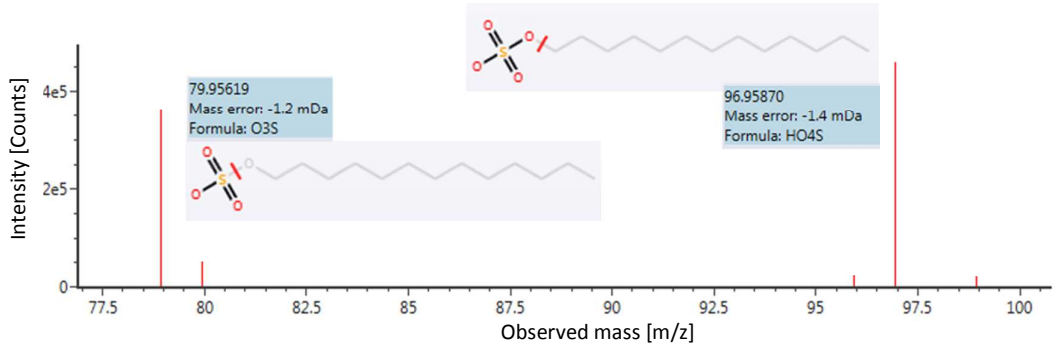
Nonyl hydrogen sulfate [$C_9H_{20}O_4S$]



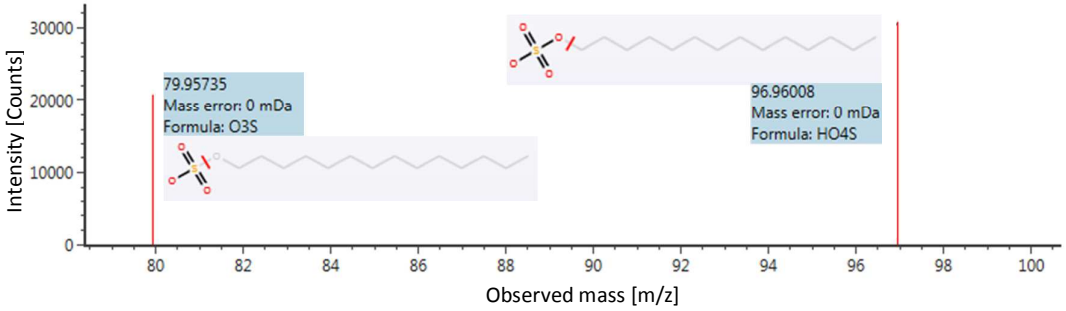
Decyl hydrogen sulfate [$C_{10}H_{22}O_4S$]



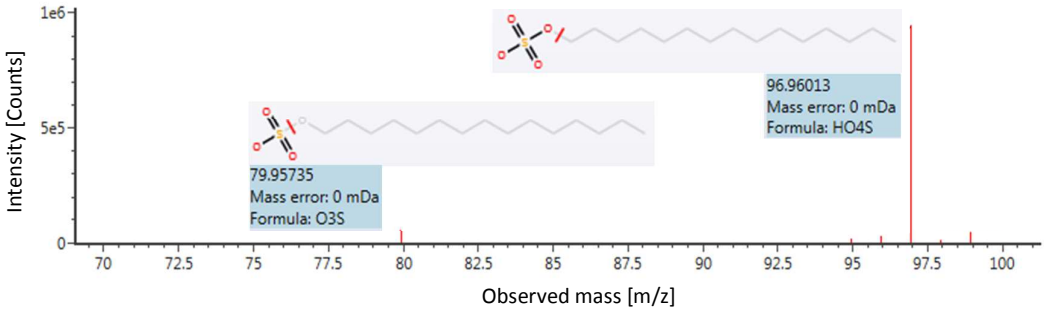
Tridecyl hydrogen sulfate [$C_{13}H_{28}O_4S$]



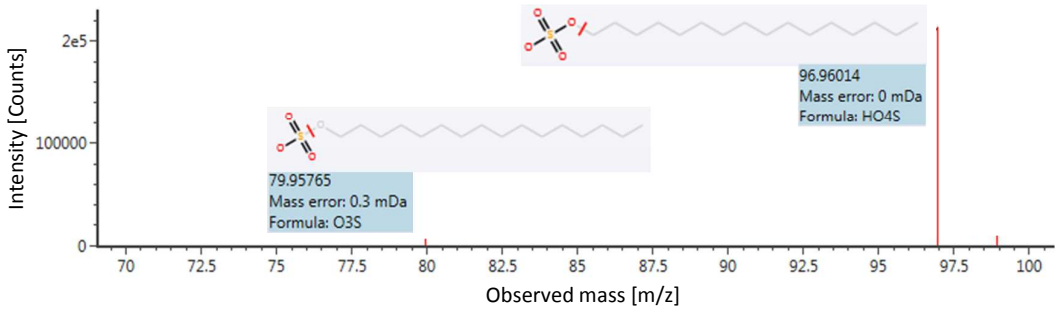
Tetradecyl hydrogen sulfate [$C_{14}H_{30}O_4S$]



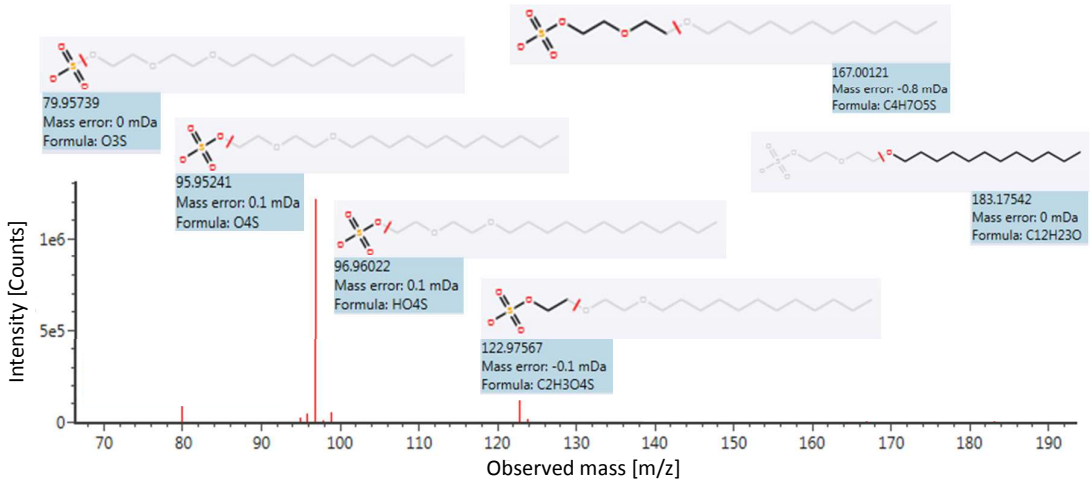
Pentadecyl hydrogen sulfate [$C_{15}H_{32}O_4S$]



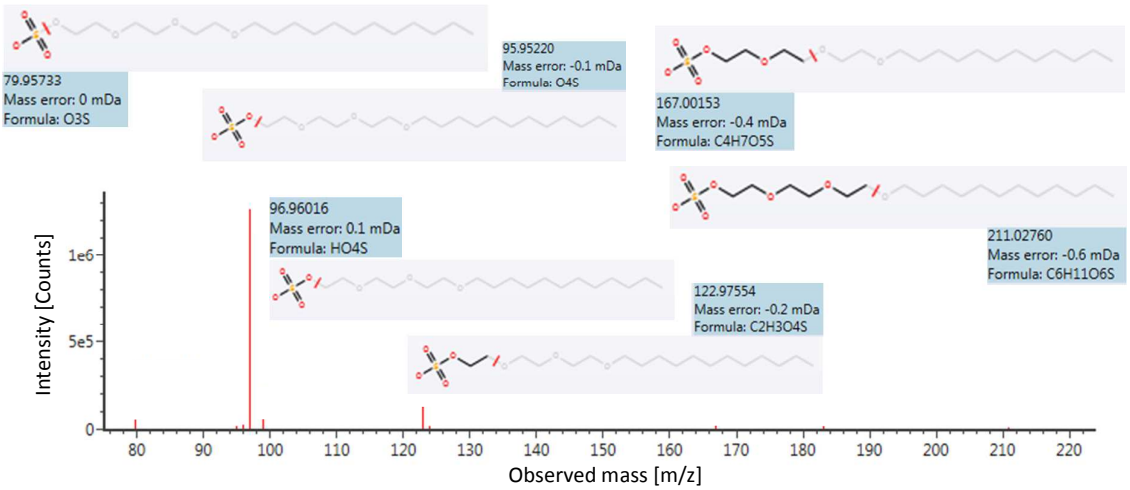
Hexadecyl hydrogen sulfate [$C_{16}H_{34}O_4S$]



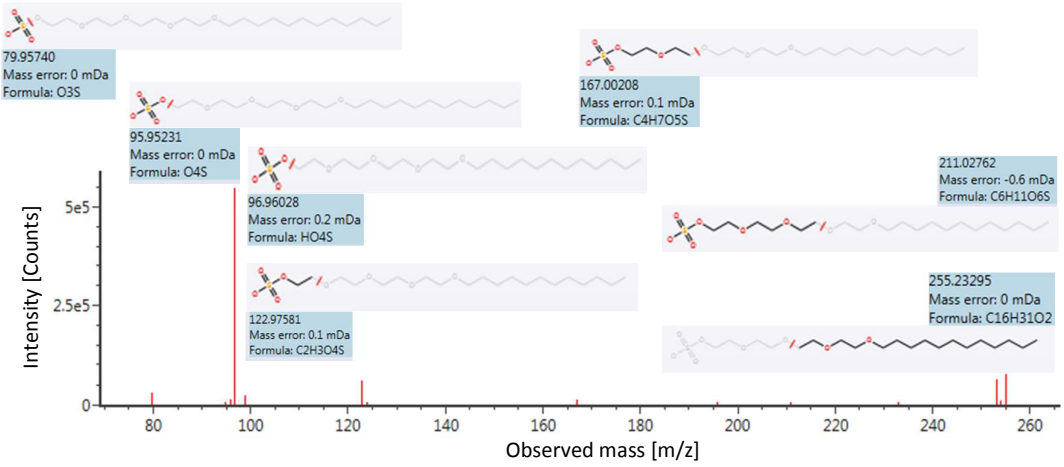
2-[2-(Dodecyloxy)ethoxy]ethyl hydrogen sulfate [$C_{16}H_{34}O_6S$]



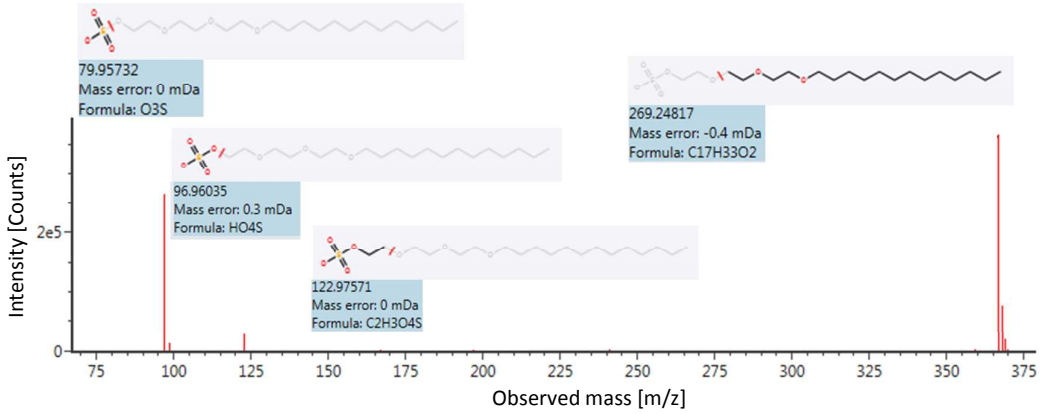
2-{2-[2-(Dodecyloxy)ethoxy]ethoxy}ethyl hydrogen sulfate [$C_{18}H_{38}O_7S$]



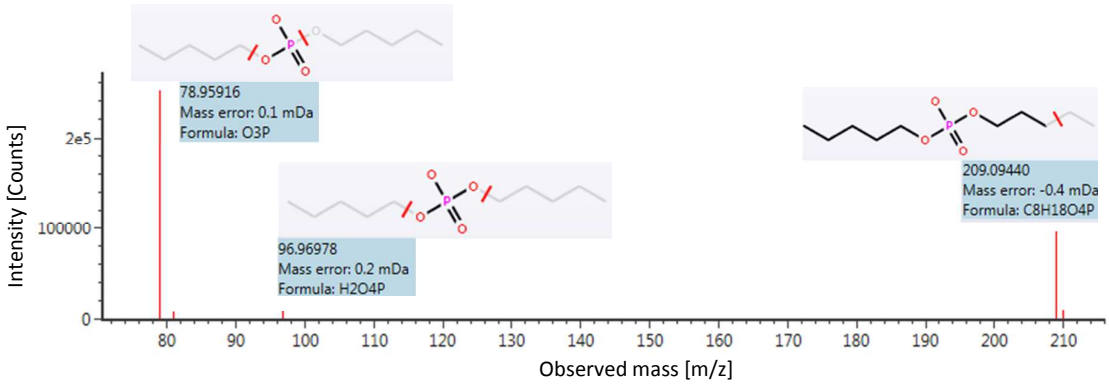
3,6,9,12-Tetraoxatetracos-1-yl hydrogen sulfate [$C_{20}H_{42}O_8S$]



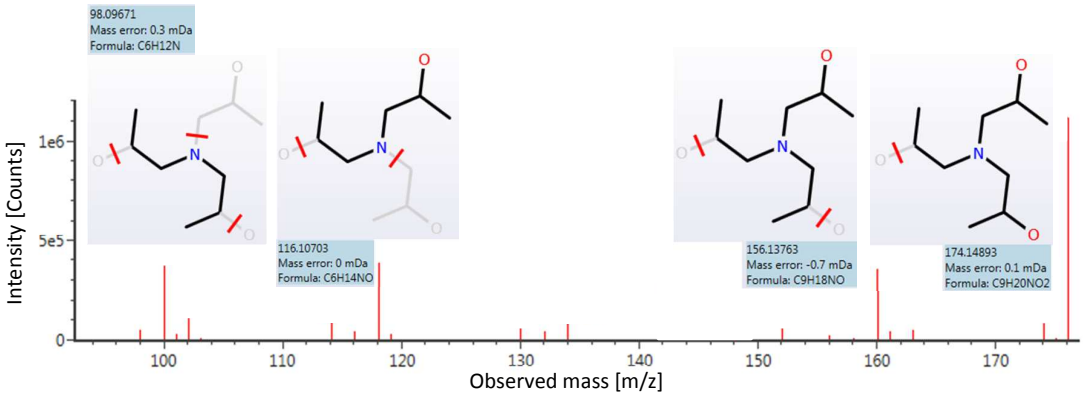
2-{2-[2-(Tridecyloxy)ethoxy]ethoxy}ethyl hydrogen sulfate [$C_{19}H_{40}O_7S$]



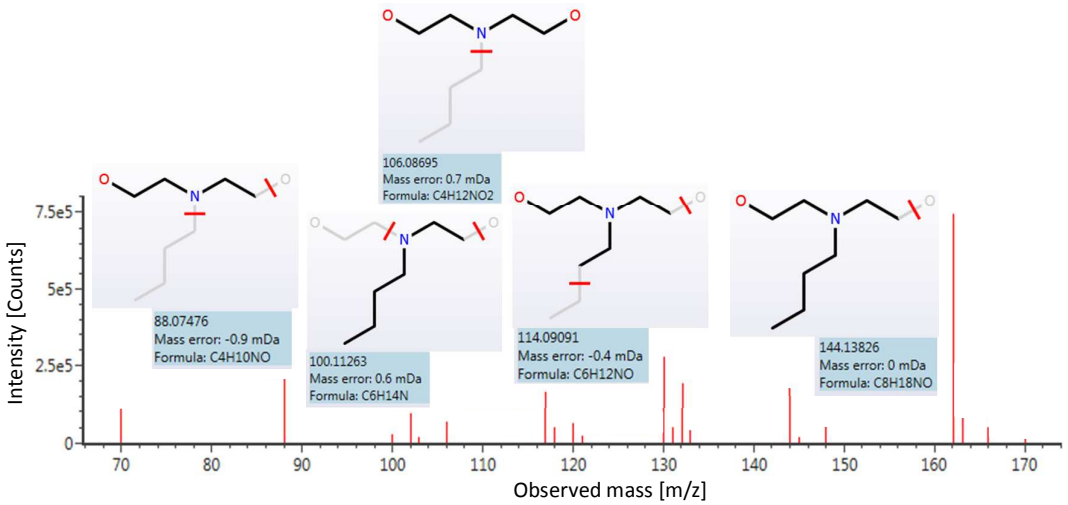
Diethyl hexyl phosphate [$C_{10}H_{23}O_4P$]



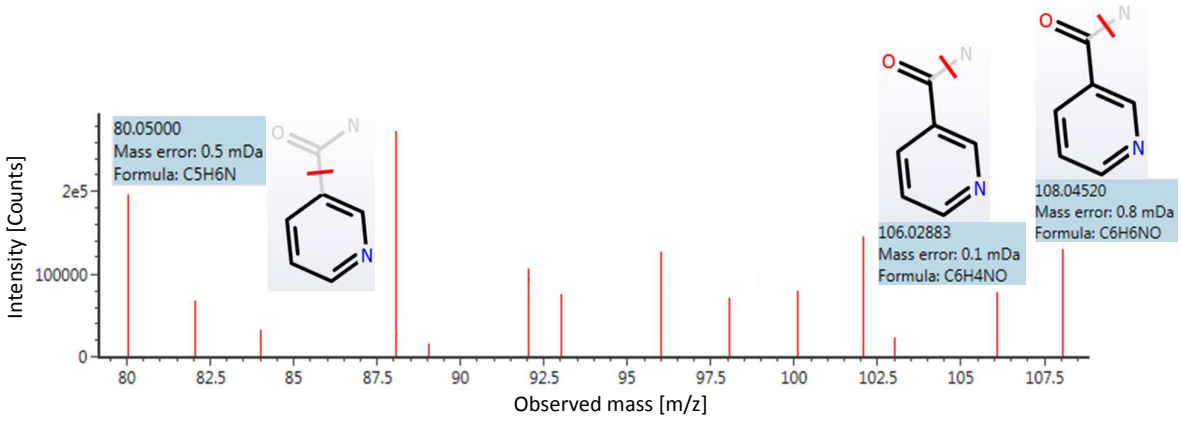
Triisopropanolamine [$C_9H_{21}NO_3$]



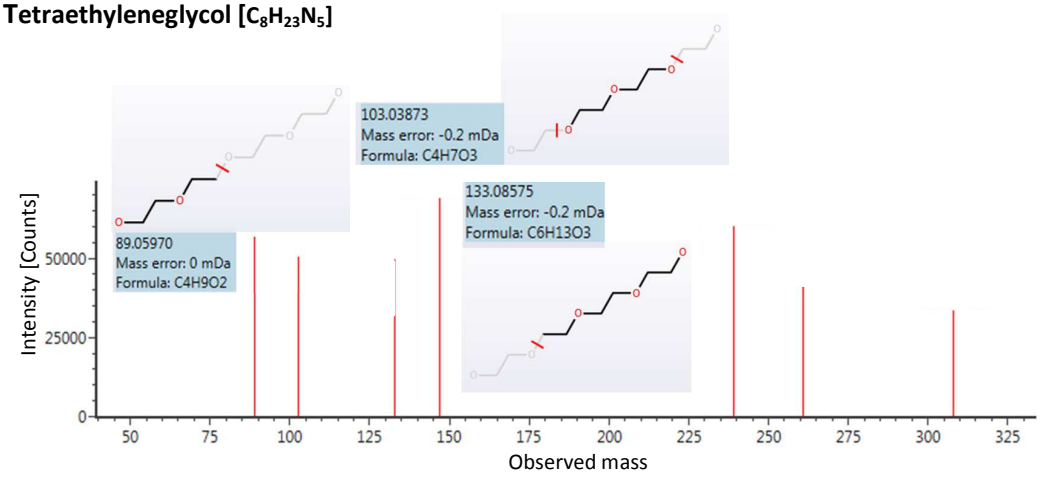
N-Butyldiethanolamine [$C_8H_{19}NO_2$]



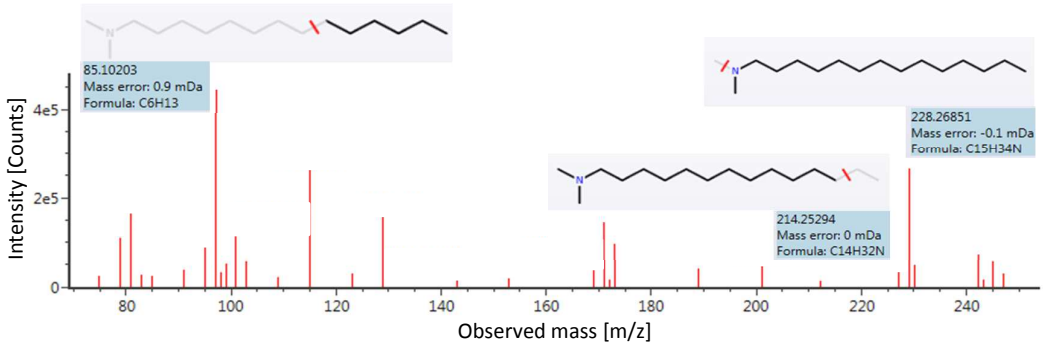
Nicotinamide [$C_6H_6N_2O$]



Tetraethyleneglycol [$C_8H_{23}N_5$]



N,N-Dimethyl-1-tetradecanamine [$C_{16}H_{35}N$]



Pentaethylene glycol monododecyl ether / Laureth 5 [$C_{22}H_{46}O_6$]

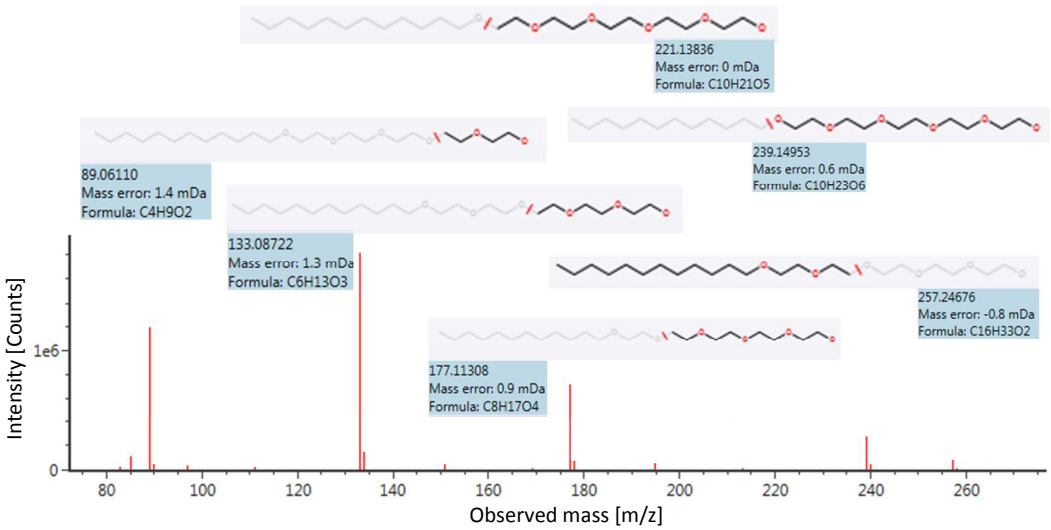


Figure S2: MS/MS spectra of compounds for which this information is not available in Massbank.

SI-7: Toxicity of the identified suspects

Toxicity values for the tentatively identified and confirmed suspect compounds were calculated based on the ecological structure-activity relationships (ECOSAR) predictive model (US EPA 2016). Based on the similarity of structures to chemicals for which the aquatic toxicity has been previously reported, the model predicts the respective aquatic toxicity. The model estimates LC50 (Median concentration in mg/L associated with 50% mortality), EC50 (Median concentration associated with effects on 50% of the organisms) and ChV (Chronic toxicity value) after 96h, respectively 48h of exposure, applied to fish, daphnia magna and green algae representing the entire aquatic environment.

Table SI-5: Toxicity values for the tentatively identified and confirmed suspect compounds estimated based on the ECOSAR prediction model.

Compounds' name	Recipient	Reference unit[1]	Toxicity value [mg/L][2]
(9E)-9-Octadecenamide	Fish	LC50 (96h)	0.053
	Daphnia Magna	LC50 (48h)	0.007
	Green Algae	EC50 (96h)	0.004
	Fish	ChV	0.00129
	Daphnia Magna	ChV	0.008
	Green Algae	ChV	0.027
	High Aquatic Toxicity Concern		
1,2,3-Benzotriazole	Fish	LC50 (96h)	28.321
	Daphnia Magna	LC50 (48h)	66.766
	Green Algae	EC50 (96h)	5.904
	Fish	ChV	4.615
	Daphnia Magna	ChV	3.859
	Green Algae	ChV	2.715
	High Aquatic Toxicity Concern		
2-{2-[2-(Dodecyloxy)ethoxy] ethoxy}ethyl hydrogen sulfate	Fish	LC50 (96h)	750.915
	Daphnia Magna	LC50 (48h)	410.861
	Green Algae	EC50 (96h)	262.568
	Fish	ChV	70.259
	Daphnia Magna	ChV	36.141
	Green Algae	ChV	63.314
	Moderate Aquatic Toxicity Concern		
2-{2-[2-(Tridecyloxy)ethoxy] ethoxy}ethylhydrogen sulfate	Fish	LC50 (96h)	281.550
	Daphnia Magna	LC50 (48h)	161.195
	Green Algae	EC50 (96h)	124.258
	Fish	ChV	27.791
	Daphnia Magna	ChV	16.087
	Green Algae	ChV	33.146
	Moderate Aquatic Toxicity Concern		
2-[2-(Dodecyloxy)ethoxy] ethylhydrogen sulfate	Fish	LC50 (96h)	378.689
	Daphnia Magna	LC50 (48h)	212.515
	Green Algae	EC50 (96h)	150.811

	Fish	ChV	36.507
	Daphnia Magna	ChV	20.059
	Green Algae	ChV	38.476
	Moderate Aquatic Toxicity Concern		
2-(Dodecyloxy)ethylhydrogen sulfate	Fish	LC50 (96h)	188.025
	Daphnia Magna	LC50 (48h)	108.225
	Green Algae	EC50 (96h)	85.283
	Fish	ChV	18.676
	Daphnia Magna	ChV	10.962
	Green Algae	ChV	23.021
	Moderate Aquatic Toxicity Concern		
2,2'-Dimorpholinyldiethyl-ether	Fish	LC50 (96h)	7040.513
	Daphnia Magna	LC50 (48h)	571.003
	Green Algae	EC50 (96h)	1009.315
	Fish	ChV	1325.720
	Daphnia Magna	ChV	32.256
	Green Algae	ChV	253.842
	Moderate Aquatic Toxicity Concern		
2-Dodecylbenzesulfonic acid	Fish	LC50 (96h)	8.469
	Daphnia Magna	LC50 (48h)	6.218
	Green Algae	EC50 (96h)	13.410
	Fish	ChV	1.121
	Daphnia Magna	ChV	1.240
	Green Algae	ChV	6.225
	High Aquatic Toxicity Concern		
3,6,9,12-Tetraoxatetracos-1-yl hydrogen sulfate	Fish	LC50 (96h)	1470.823
	Daphnia Magna	LC50 (48h)	784.622
	Green Algae	EC50 (96h)	451.558
	Fish	ChV	133.566
	Daphnia Magna	ChV	64.319
	Green Algae	ChV	102.912
	Moderate Aquatic Toxicity Concern		
4-(Methylamino) phenolhemisulfate salt (metoquinone)	Fish	LC50 (96h)	177.166
	Daphnia Magna	LC50 (48h)	31.151
	Green Algae	EC50 (96h)	161.118
	Fish	ChV	14.985
	Daphnia Magna	ChV	5.938
	Green Algae	ChV	76.858
	High Aquatic Toxicity Concern		
Acesulfame	Fish	LC50 (96h)	5002.855
	Daphnia Magna	LC50 (48h)	2416.722
	Green Algae	EC50 (96h)	922.806
	Fish	ChV	404.133
	Daphnia Magna	ChV	150.308
	Green Algae	ChV	168.616
	Moderate Aquatic Toxicity Concern		
Benzoic acid	Fish	LC50 (96h)	1300.781
	Daphnia Magna	LC50 (48h)	730.075

	Green Algae	EC50 (96h)	518.374
	Fish	ChV	125.419
	Daphnia Magna	ChV	68.937
	Green Algae	ChV	132.290
	Moderate Aquatic Toxicity Concern		
Butan-2-one O,O',O''-(methylsilanetriyl)oxime	Neutral Organics*		
Di-(2-ethylhexyl) phosphoric acid	Neutral Organics*		
Dibutyl phosphate	Neutral Organics*		
Diethyl hexyl phosphate	Fish	LC50 (96h)	10.349
	Daphnia Magna	LC50 (48h)	19.670
	Green Algae	EC50 (96h)	7.333
	Fish	ChV	0.653
	Daphnia Magna	ChV	10.575
	Green Algae	ChV	2.466
	High Aquatic Toxicity Concern		
Diethyl thiourea	Fish	LC50 (96h)	7650.738
	Daphnia Magna	LC50 (48h)	3.938
	Green Algae	EC50 (96h)	2.155
	Fish	ChV	700.232
	Daphnia Magna	ChV	0.250
	Green Algae	ChV	0.226
	High Aquatic Toxicity Concern		
Dimethyl octadecylphosphonate	Fish	LC50 (96h)	0.0021
	Daphnia Magna	LC50 (48h)	0.023
	Green Algae	EC50 (96h)	0.004
	Fish	ChV	0.000468
	Daphnia Magna	ChV	0.003
	Green Algae	ChV	0.007
	High Aquatic Toxicity Concern		
Decyl hydrogen sulfate	Neutral Organics*		
Hexadecyl hydrogen sulfate	Neutral Organics*		
Laurilsulfate	Fish	LC50 (96h)	0.0021
	Daphnia Magna	LC50 (48h)	0.023
	Green Algae	EC50 (96h)	0.004
	Fish	ChV	0.000468
	Daphnia Magna	ChV	0.003
	Green Algae	ChV	0.007
	High Aquatic Toxicity Concern		
Mono-n-butylphosphoric acid	Neutral Organics*		
N-Butyldiethanolamine	Fish	LC50 (96h)	666.973
	Daphnia Magna	LC50 (48h)	62.797
	Green Algae	EC50 (96h)	82.632
	Fish	ChV	79.705
	Daphnia Magna	ChV	4.101
	Green Algae	ChV	23.141

	High Aquatic Toxicity Concern		
Nicotinamide	Fish	LC50 (96h)	2062.501
	Daphnia Magna	LC50 (48h)	7022.943
	Green Algae	EC50 (96h)	38.229
	Fish	ChV	0.824
	Daphnia Magna	ChV	78.143
	Green Algae	ChV	12.773
	High Aquatic Toxicity Concern		
N,N-Dimethyl-1-tetradecanamine	Fish	LC50 (96h)	0.058
	Daphnia Magna	LC50 (48h)	0.011
	Green Algae	EC50 (96h)	0.003
	Fish	ChV	0.0007
	Daphnia Magna	ChV	0.00156
	Green Algae	ChV	0.00165
	High Aquatic Toxicity Concern		
Nonyl hydrogen sulfate	Neutral Organics		
Octyl hydrogen sulfate	Neutral Organics		
Oleic acid	Neutral Organics		
Panthenol	Fish	LC50 (96h)	39116.633
	Daphnia Magna	LC50 (48h)	2.62e+005
	Green Algae	EC50 (96h)	527.778
	Fish	ChV	6.513
	Daphnia Magna	ChV	1105.093
	Green Algae	ChV	94.777
	High Aquatic Toxicity Concern		
Pentadecyl hydrogen sulfate	Neutral Organics*		
Pentaethylene glycol monododecyl ether / Laureth 5	Neutral Organics*		
Pyridoxine	Fish	LC50 (96h)	2580.650
	Daphnia Magna	LC50 (48h)	248.831
	Green Algae	EC50 (96h)	1467.272
	Fish	ChV	179.145
	Daphnia Magna	ChV	47.533
	Green Algae	ChV	711.990
	Moderate Aquatic Toxicity Concern		
Ricinoleic acid	Neutral Organics*		
Sebacic acid	Neutral Organics*		
Stearic acid	Neutral Organics*		
Sulisobenzone	Fish	LC50 (96h)	9336.408
	Daphnia Magna	LC50 (48h)	1358.373
	Green Algae	EC50 (96h)	7322.173
	Fish	ChV	742.008
	Daphnia Magna	ChV	259.097
	Green Algae	ChV	3511.742
	Moderate Aquatic Toxicity Concern		
Tetradecyl hydrogen sulfate	Neutral Organics*		
Tetraethyleneglycol	Neutral Organics*		

Tolytriazole	Fish	LC50 (96h)	16.386
	Daphnia Magna	LC50 (48h)	36.053
	Green Algae	EC50 (96h)	3.851
	Fish	ChV	2.133
	Daphnia Magna	ChV	1.941
	Green Algae	ChV	1.763
	High Aquatic Toxicity Concern		
Tributyl citrate acetate	Fish	LC50 (96h)	2.488
	Daphnia Magna	LC50 (48h)	4.049
	Green Algae	EC50 (96h)	1.200
	Fish	ChV	0.116
	Daphnia Magna	ChV	1.436
	Green Algae	ChV	0.646
	High Aquatic Toxicity Concern		
Tridecyl hydrogen sulfate	Neutral Organics*		
Triisopropanolamine	Fish	LC50 (96h)	4817.939
	Daphnia Magna	LC50 (48h)	394.807
	Green Algae	EC50 (96h)	683.742
	Fish	ChV	879.077
	Daphnia Magna	ChV	22.528
	Green Algae	ChV	173.246
	Moderate Aquatic Toxicity Concern		
Tris(2-butoxyethyl) phosphate	Fish	LC50 (96h)	13.976
	Daphnia Magna	LC50 (48h)	26.115
	Green Algae	EC50 (96h)	9.494
	Fish	ChV	0.853
	Daphnia Magna	ChV	13.412
	Green Algae	ChV	3.362
	High Aquatic Toxicity Concern		

[1] LC50=Median concentration associated with 50% mortality after the given exposure
EC50=Median concentration associated with effects on 50% of the organisms
ChV=Chronic toxicity value

[2] Acute toxicity concern concentration is the lowest toxicity value divided by an uncertainty factor of 10. Highlighted in red are the toxicity values of high concern corresponds to an estimate < 1mg/L. Highlighted in purple are the toxicity values of moderate concern corresponding to an estimate < 100 mg/L

* Estimates provided below the Neutral Organics QSAR equations which represents the baseline toxicity potential (minimum toxicity) assuming a simple non-polar narcosis model. Without empirical data on structurally similar chemicals, it is uncertain if this substance will present significantly higher toxicity above baseline estimates.

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