

Supplementary material

Prioritizing Emerging Organic Pollutants in Rivers of Thailand Using Suspect Screening Analysis with High-Resolution Mass Spectrometry

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Text S1 The general water parameters of the raw water in each water source

The water quality parameters measured across the four rivers (CPR, PhR, PIR, and UTR) revealed notable differences in their physicochemical characteristics (**Table S1**). UTR exhibited the highest turbidity (58.9 NTU), suggesting significant particulate matter or runoff influence, while PhR recorded the lowest turbidity (10.75 NTU), indicating clearer water. PhR also had the highest dissolved organic carbon (DOC) level at 5.27 mg/L, though its SUVA value was the lowest (1.42 L/mg·m), implying the presence of more aliphatic or hydrophilic organic matter. In contrast, PIR demonstrated the highest SUVA value (2.61 L/mg·m), pointing to more aromatic and potentially reactive compounds, despite its relatively low DOC concentration. The pH values of all rivers ranged from 6.53 to 6.81, remaining within a slightly acidic to neutral range suitable for most aquatic life. Dissolved oxygen (DO) levels varied, with PhR showing the highest (6.5 mg/L) and UTR the lowest (4.83 mg/L), potentially reflecting differences in biological activity or pollutant load. Additionally, CPR recorded the highest electrical conductivity (316 μ S/cm), suggesting a greater concentration of dissolved ions, possibly from industrial or urban sources. These findings underscore the distinct environmental conditions of each river and highlight the importance of region-specific water quality monitoring and management.

Text S2 Identification compounds with varying degrees of confidence

To identify suspect peak compounds, each peak was analyzed as described in Section 2.4. Quality assurance and quality control procedures included the use of blank samples to monitor potential contamination. The blanks consisted of 100 % methanol and were inserted after every four samples. Procedural blanks were analyzed to identify and correct any contamination introduced during sampling or laboratory processing. The method's performance was validated by confirming that blank intensities in each run remained consistent, with variations within 5 %. After validation, background subtraction was applied to the sample data. Features were retained only when the peak area in the sample exceeded five times the corresponding area in the blank.

After background subtraction, these MS/MS spectra enabled identification with varying degrees of confidence, following the criteria described in previous studies ^{1,2}. Profiles with well-supported structural assignments were classified under confidence level 2. Tentative structural assignments corresponded to a confidence level of 3. When only molecular formulae could be determined, the profiles were assigned to confidence level 4. In cases where only exact masses were available, profiles were classified under confidence level 5.

Text S3 PNEC Calculation Methodology

The Predicted No-Effect Concentration (PNEC) was calculated using established risk assessment frameworks recommended by regulatory authorities, such as the European Chemicals Agency (ECHA). PNEC values are used to estimate concentrations below which adverse effects on the aquatic environment are not expected.

When experimental ecotoxicological data were available, the PNEC was calculated from the lowest relevant toxicity value, such as the No Observed Effect Concentration (NOEC), Lethal Concentration for 50% of the test organisms (LC₅₀), or Effective Concentration for 50% (EC₅₀). An assessment factor (AF) was then applied to address uncertainty related to interspecies variability and data limitations. The general formula is:

$$\text{PNEC} = \frac{\text{Toxicity Endpoint (e.g., LC}_{50}, \text{EC}_{50}, \text{NOEC})}{\text{AF}}$$

Assessment factors were chosen based on the quality and type of toxicity data as follows:³

	Available Data	AFs
PNEC _{water}	1) At least one short-term L(E)C50 from each of three trophic levels	1000
	2) One long-term EC10 or NOEC from one trophic level	100
	3) Two long-term results (e.g., EC10 or NOECs) from species representing two trophic levels	50
	4) Long-term results (e.g., EC10 or NOECs) from at least three species representing three trophic levels	10
	5) Species sensitivity distribution (SSD) method	1–5
	6) Field data or model ecosystems	Case by case

In the absence of experimental data, Quantitative Structure Activity Relationship (QSAR) models were used to estimate ecotoxicity values. These were sourced from public databases such as ECOTOX by the U.S. Environmental Protection Agency (EPA) (<https://cfpub.epa.gov/ecotox/>)

and the ECHA REACH database (<https://echa.europa.eu/information-on-chemicals/registered-substances>). The derived PNECs were then used in a preliminary risk assessment to prioritize contaminants of emerging organic pollutants (EOPs) for further monitoring.

Text S4 Check chromatographic profiles to identify the retention time of the compound

Compound Discoverer™ 3.3 identified a major ion with m/z 216.09998 at a retention time (RT) of 9.8 minutes (**Fig. S2**). This ion was detected in all sample files using triplicate injections analyzed in positive ion mode at the MS1-only level (**Fig. 1a**). The software also identified three corresponding ^{13}C isotopic ions, highlighted by green boxes, which confirmed that their measured masses and intensities were within the expected range. In addition, Compound Discoverer™ 3.3 detected a sodium adduct ion (m/z 238.07672) and a water neutral loss ion (m/z 198.11952), both of which were likely formed during ionization. Detection of the neutral loss was predefined in the acquisition settings (**Fig. 1a**). Using the major ion (m/z 216.09998), the software calculated the ion intensity across the chromatographic separation time for each submitted file analyzed in MS1-only mode. It then generated the corresponding chromatographic peak shape and determined the area under the curve (**Fig. S2**). The chromatogram showed clear baseline resolution, indicating distinct start and end points for the peak associated with this ion. Finally, within the specified tolerance limits in the **section 2.4** settings, Compound Discoverer™ 3.3 confirmed the presence of the m/z 216.09998 ion at RT = 9.8 minutes in sample files (**Fig. 1a** and **S2**). Thus, only ions exhibiting well-defined chromatographic peak shapes were selected for subsequent identification at various confidence levels.

Text S5 Check MS2 from ChemSpider and PubChem for profiles identified with a confidence level of 3

Compounds were assigned a confidence level of 3 when probable structures and molecular formulae could be determined.^{1,2} However, these compounds did not show exact MS/MS matches in the mzCloud spectral library. To improve annotation, product ion matches involving two or more ions were examined in ChemSpider and PubChem.⁴ The details of these profiles are provided below.

For tentative compound annotations with a confidence level of 3, we consulted MS2 spectral information from publicly accessible chemical databases to support structural elucidation. Compound identities were queried in ChemSpider, a chemically diverse resource hosting contributed and aggregated spectral data, including MS2 spectra when available. Spectra linked to candidate structures were carefully examined to compare experimental fragment patterns with reference data, bearing in mind the variability and limited standardization of spectra in this resource. In addition, the website will display related publications, and you can check any that contain MS2 data for comparison.⁵

Similarly, PubChem was used to retrieve MS2 spectra from curated spectral libraries integrated within its platform, such as those provided by the NIST Mass Spectrometry Data Center. MS2 spectral data for each candidate were accessed under the "Spectral Properties" section of the respective compound records. Key spectral parameters including ionization mode, collision energy, and fragment ion m/z values were considered to confirm or refine tentative identifications (<https://pubchem.ncbi.nlm.nih.gov/docs/spectral-information>). However, the intensity of product ions is not often the same as in our data, since the value of collision energy differs across measurements and experiments. This difference results in variations in product ion intensity.

Therefore, we compared only the m/z values of product ions. If at least two or more product ions match, the compound is classified as level 3.⁴

Although compounds assigned to confidence level 3 were identified based on probable structures and molecular formulas, they lacked confirmatory MS/MS fragment matches in the mzCloud spectral library. Therefore, these features were not included in the semi-quantification step, which focused on level 2 identifications with higher structural certainty. However, the presence of level 3 compounds still provides valuable qualitative information about potential contaminants in the studied rivers. Although their concentrations were not estimated, their detection suggests possible environmental exposure pathways. These compounds should be regarded as potential candidates for future targeted analysis once reference standards become available. Future work will include quantitative validation of these features to better assess their environmental risk.

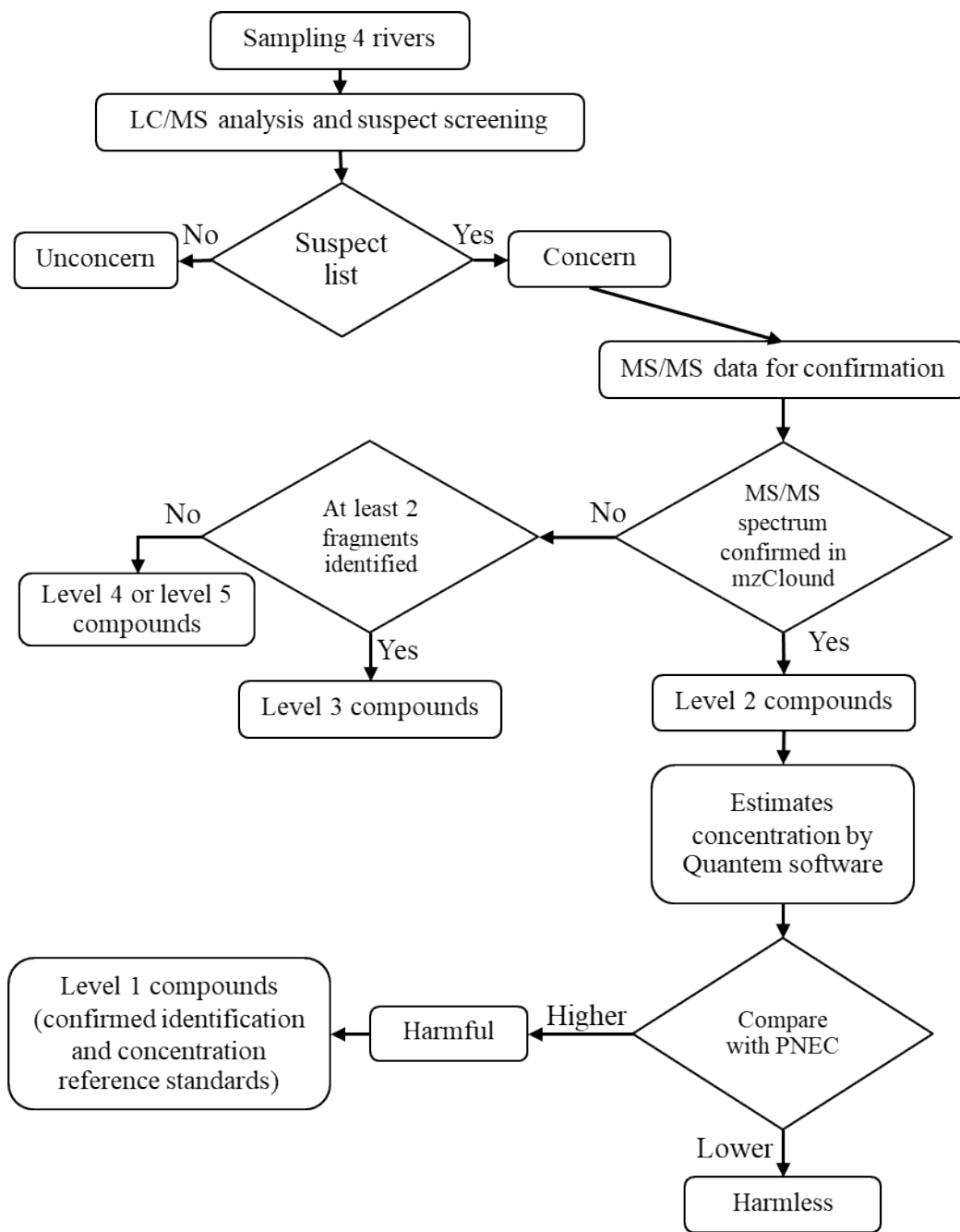


Fig. S1. Flowchart of the strategy and method used to select the EOP compounds found in positive and negative ionization modes

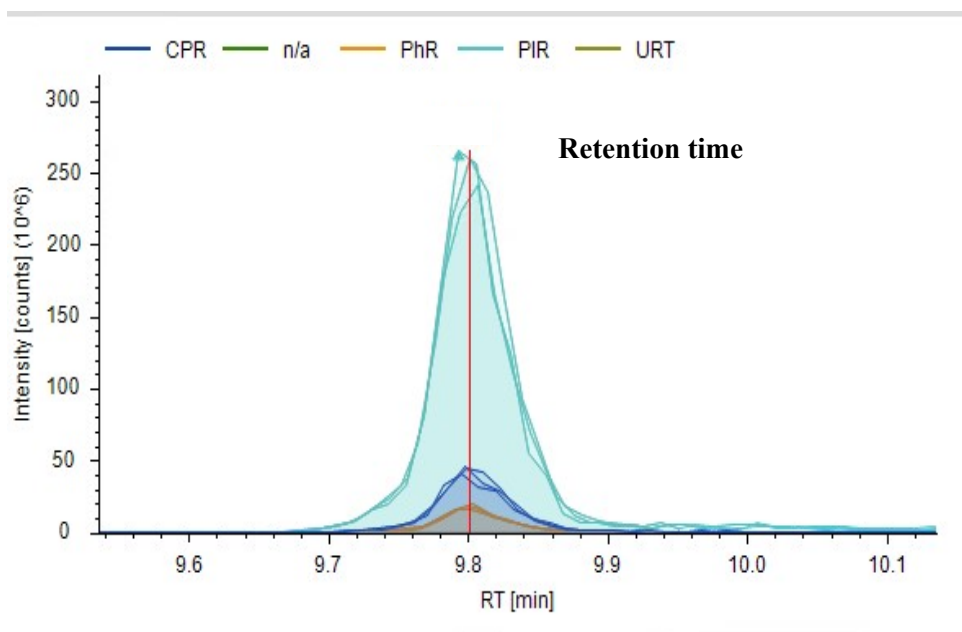


Fig. S2 Chromatographic representation of the m/z 216.09998 ion from all sample files

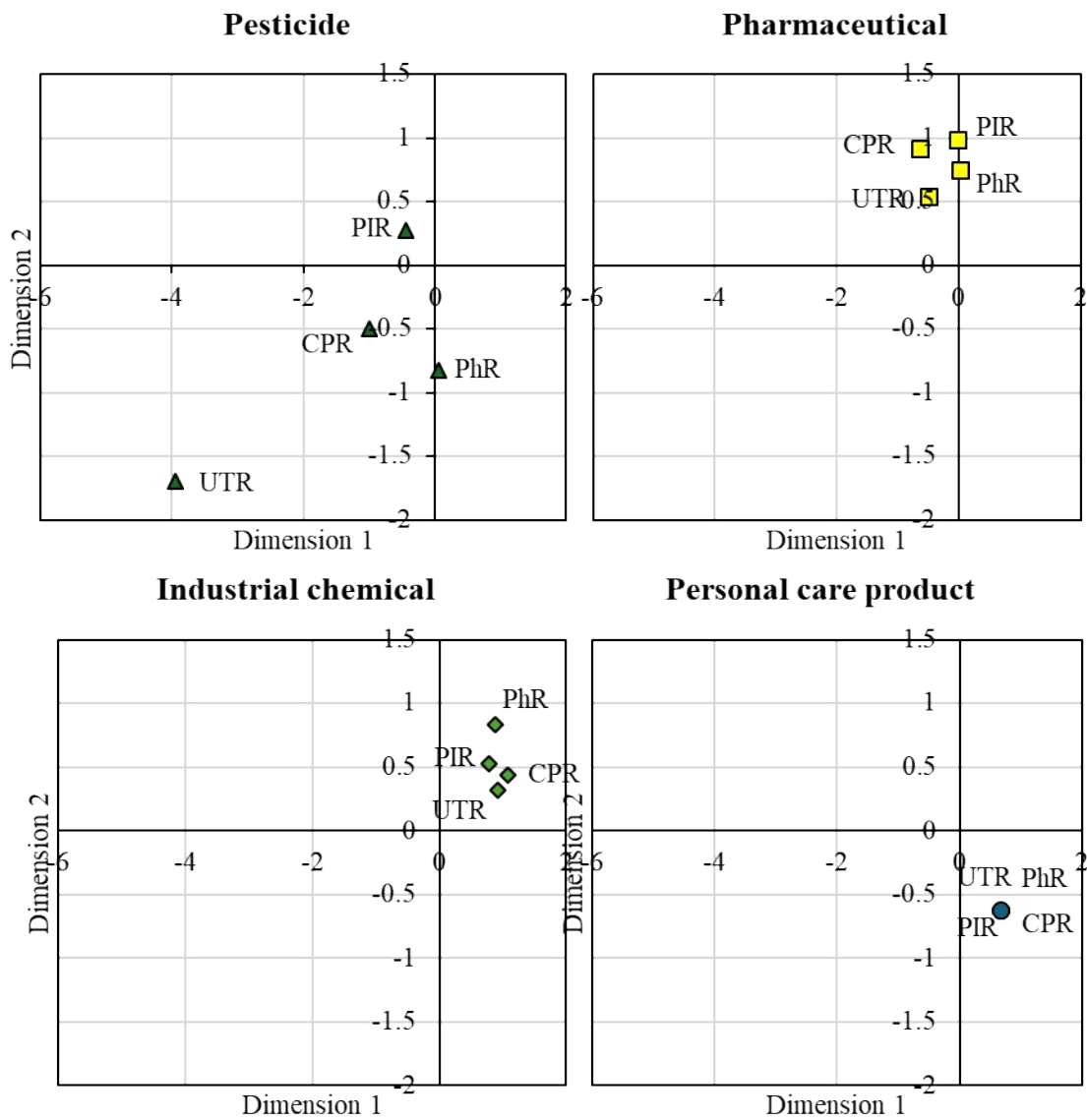


Fig. S3. Multidimensional scaling of EOPs features level 2 in each classification

Classification of common level 2 EOPs

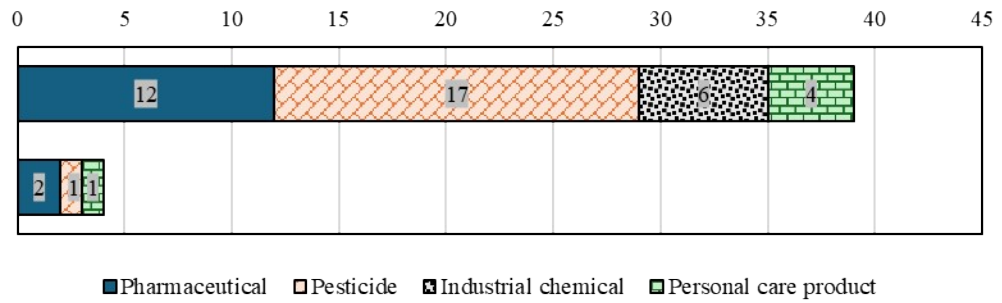


Fig. S4 The classification of common level 2 EOPs identified with predicted no-effect concentrations (PNECs).

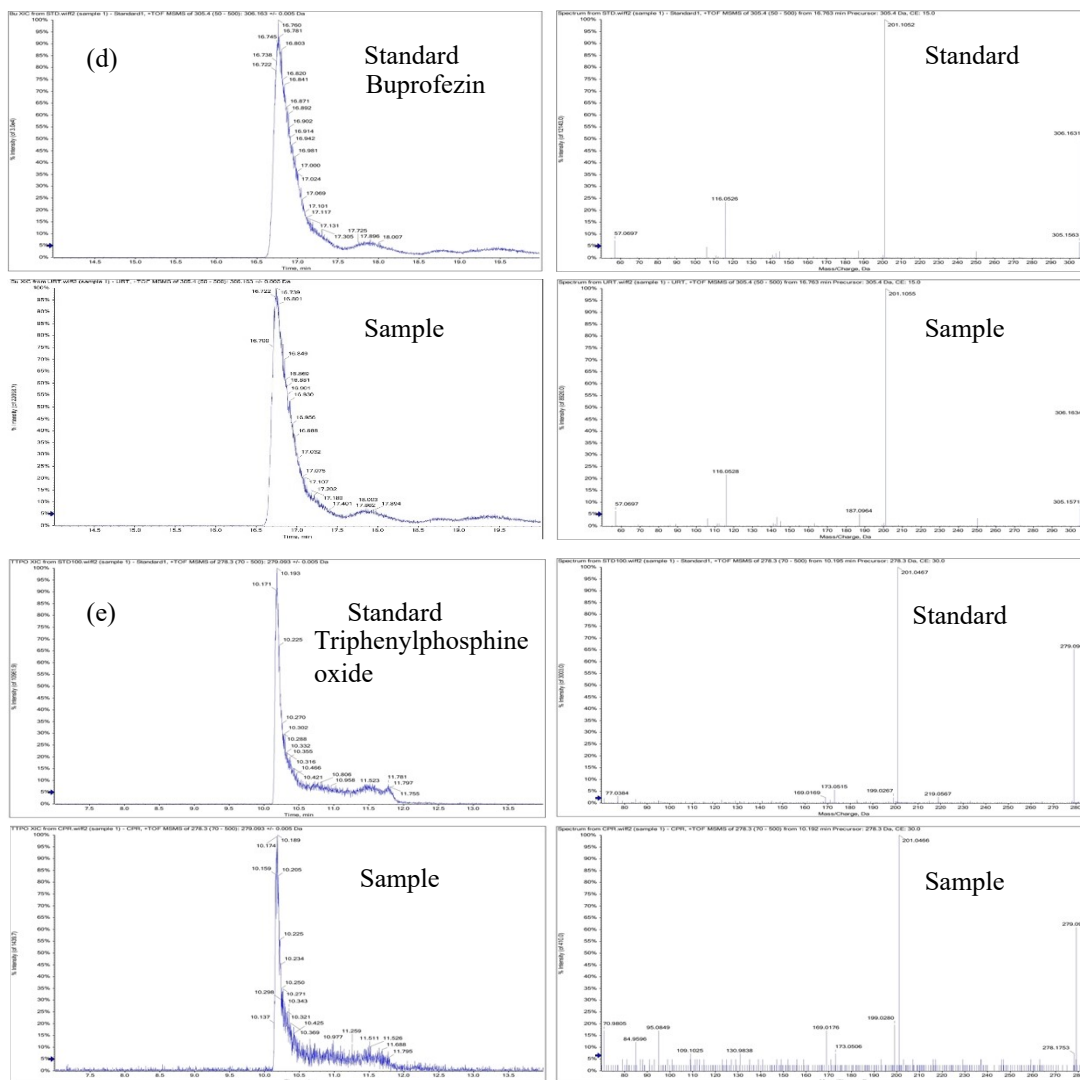
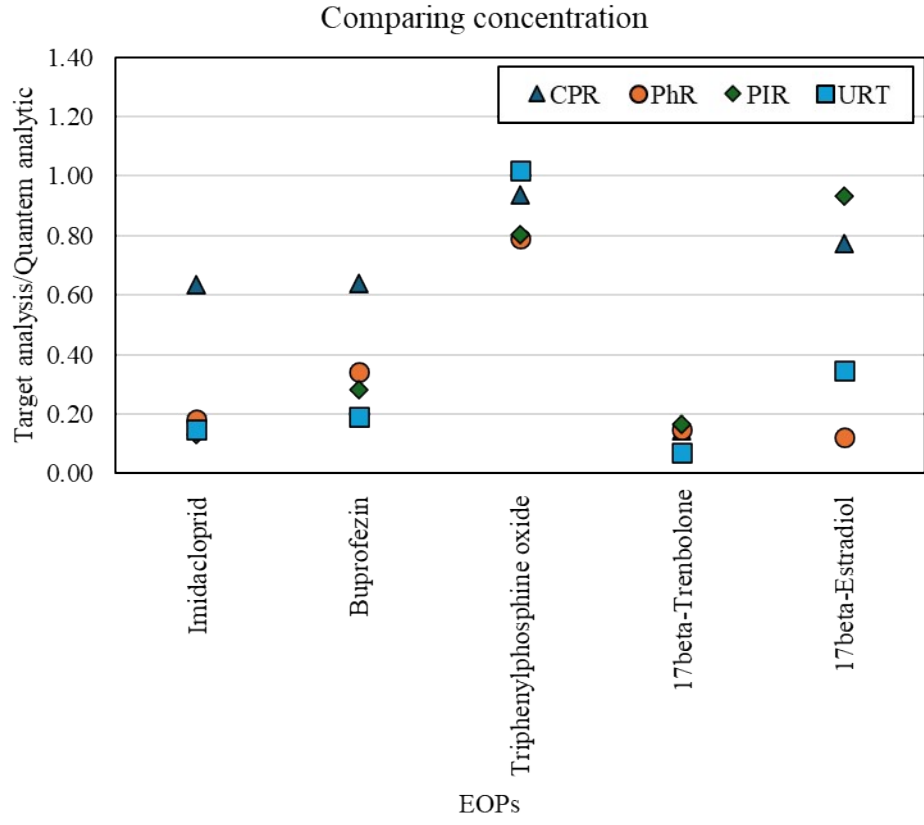


Fig. S5 Extracted ion chromatograms (left) and MS/MS patterns (right) for the reference standards (top) and samples (bottom) of (a) 17 β -estradiol (precursor ion m/z 273.1850, product ions m/z 272.1850, 213.1271, retention time 10.1 min), (b) 17 β -trenbolone (precursor ion m/z 271.1694, product ions m/z 253.1290, 195.1010, retention time 7.4 min), (c) imidacloprid (precursor ion m/z 256.0602, product ions m/z 212.0590, 209.0593, retention time 10.8 min), (d) buprofezin (precursor ion m/z 306.1631, product ion m/z 201.1052, 116.0526, retention time 16.7 min), and (e) triphenylphosphine oxide (precursor ion m/z 279.0940, product ions m/z 201.0467, 173.0515, retention time 10.2 min).



Target analysis/Quantem analytic > 1 : Quantem analytic underestimates
 Target analysis/Quantem analytic =1 : Quantem accurate
 Target analysis/Quantem analytic <1 : Quantem analytic overestimates

Fig. S6 Comparison of concentrations from target analysis and Quantem estimations.

Table S1 General parameters for each river

River	Turbidity (NTU)	DOC (mg/L)	SUVA (L/mg·m)	pH	DO (mg/L)	EC (µS/cm)
CPR	35.5	2.71	2.44	6.81	5.41	316
PhR	10.7	5.27	1.42	6.70	6.50	189
PIR	18.2	2.02	2.61	6.53	6.01	172
UTR	58.9	2.54	1.97	6.80	4.83	202

Sampling Location	Province / Region	Dominant Land Use Types	Mean River Flow (m ³ /day)	Total WTP Discharge (m ³ /day)	Estimated Population in Catchment	Major Potential EOP Sources
Phong River (PhR)	Khon Kaen (Northeast)	Agricultural and peri-urban	$3.2 \times 10^6 \pm 0.4 \times 10^6$	$45,000 \pm 5,000$	~250,000	Agricultural runoff, domestic wastewater, livestock farming, landfill leachate, and limited industrial discharge
Chao Phraya River (CPR)	Bangkok / Central	Urban, industrial, and mixed-use	$1.3 \times 10^6 \pm 1.0 \times 10^6$	$120,000 \pm 20,000$	~5,600,000	Domestic sewage, personal care products, pharmaceuticals, hospital effluents, and industrial discharges from the Chao Phraya watershed
Ping River (PIR)	Chiang Mai (North)	Agricultural, urban, and peri-urban	$4.0 \times 10^6 \pm 0.4 \times 10^6$	$80,000 \pm 10,000$	~200,000	Urban wastewater, household chemicals, tourism activities, veterinary drugs, and agricultural runoff
U-Tapao Canal (UTR)	Songkhla (South)	Agricultural, urban, and industrial	$5.1 \times 10^6 \pm 0.2 \times 10^6$	$30,000 \pm 4,000$	~180,000	Industrial effluents, untreated domestic wastewater, and agricultural inputs

*River flow rate data from <https://www.thaiwater.net/water/dam/large>

*Total WTP discharge = Population served × Water use per capita (L/day)/1000

** Typical Thai urban water use: 200 L/person/day

*Population approximates using provincial or district population densities multiplied by catchment area.

Table S2 Surrogate and internal standards used in this study

Name	Type	Formula	MW(g/mol)
<u>Positive</u>			
Methamidophos-d6	Internal standard	C2H2D6NO2PS	147.17
Methomyl-d3	Internal standard	C5H7D3N2O2S	165.23
Caebendazim-d4	Internal standard	C9H5D4N3O2	195.21
Pirimicarb-d6	Internal standard	C11H12D6N4O2	244.32
Imazail-d5	Internal standard	C14H9C12D5N2O	302.21
Etofenprox-d5	Internal standard	C25H23D5O3	381.52
<u>Negative</u>			
2-Ethylhexanoicacid	Surrogate	C8H16O2	144.24
Decanoicacid	Surrogate	C10H20O2	172.26
2,4-Dinitrophenol	Surrogate	C6H4N2O5	184.106
Diuron-D6	Internal standard	C9H4D6Cl2N2O	239.13
Heptadecafluorooctanesulfonic Acid	Surrogate	C8HF17O3S	500.13
Hexabromocyclododecane	Surrogate	C12H18Br6	641.7

Table S3 Parameters of HESI and Orbitrap MS used for acquiring MS/MS data

Parameter	Description	Value in + mode	Value in - mode
Spray voltage (kV)	The nozzle uses voltage to squirt liquid. Molecules are ionized using this voltage.	4.00	4.00
Sheath gas flow rate (AU)	To aid in nebulizing the sample solution into a fine mist at the ESI nozzle's exit, the sheath gas flow rate (nitrogen) at the ESI source is carefully controlled.	40	40
Sweep gas flow rate	The outer-coaxial gas (nitrogen) assists the sheath gas in dispersing the sample and facilitating solvent evaporation.	0	0
Capillary temp. (°C)	The temperature of the heated capillary in an ESI source. It helps to vaporize the solvent from the sample, facilitating the formation of ions for mass spectrometry analysis.	350	350
Aux gas heater temp. (°C)	The temperature of the auxiliary gas used in the ESI process. It helps to further assist in solvent evaporation and ionization by providing additional heating to the sample as it exists the ESI source.	300	300
Injection time (ms)	Duration for ion injection from the C-trap to the mass analyzer.	50	50
Microscan's (s)	Number of micro scans per second.	1	1
Automatic gain control	Quantity or number of ions per scan.	Full MS : 1E6 MS/MS: 2E4	Full MS : 1E6 MS/MS: 2E4

Table S4 Details of suspect compounds used for full scan-ddMS2

Number	Name	m/z	mode	Category	Number	Name	m/z	mode	Category	Number	Name	m/z	mode	Category	Number	Name	M/Z	mode	Category
1	Sulpiride	342.1517	[M+H] ⁺	Pharmaceutical	36	Triazophos	314.0729	[M+H] ⁺	Pesticide	72	Cyromazine	167.1048	[M+H] ⁺	Pesticide	108	Chlorpromazine	319.1039	[M+H] ⁺	Pharmaceutical
2	4-Acetamidopyridin	246.1254	[M+H] ⁺	Pharmaceutical	37	Spirotetramat	374.1967	[M+H] ⁺	Pesticide	73	Cotinine	177.1021	[M+H] ⁺	Natural product	109	Metolachlor morpholinone	234.1511	[M+H] ⁺	Pesticide
3	Caffeine	195.0881	[M+H] ⁺	Food additive	38	Tetraconazole	372.0268	[M+H] ⁺	Pesticide	74	Desnitro-imidacloprid	211.0746	[M+H] ⁺	Pesticide	110	Pterosin B	219.1403	[M+H] ⁺	Natural product
3	Thiamethoxam	292.0294	[M+H] ⁺	Pesticide	39	Thifluzamide	526.8494	[M+H] ⁺	Pesticide	75	Desnitro Thiamethoxam	247.041	[M+H] ⁺	Pesticide	111	Azoxystrobin acid	390.1147	[M+H] ⁺	Pesticide
4	Carbendazim	192.0764	[M+H] ⁺	Pesticide	40	Metolachlor	284.1431	[M+H] ⁺	Pesticide	76	2-Aminobenzimidazole	134.0733	[M+H] ⁺	Natural product	112	Deisopropylatrazine	174.0549	[M+H] ⁺	Pesticide
5	Imidacloprid urea	212.0567	[M+H] ⁺	Pesticide	41	Picoxystrobin	368.1109	[M+H] ⁺	Pesticide	77	2,3,4,9-Tetrahydro-6-methoxy-1H-pyrido(3,4-b)indol-1-one	217.0976	[M+H] ⁺	Pharmaceutical	113	4-phenylbutenone	147.082	[M+H] ⁺	Food additive
6	Thiabendazole	202.0447	[M+H] ⁺	Pesticide	42	Flusilazole	316.1067	[M+H] ⁺	Pesticide	78	4-Antipyrinecarboxaldehyde	217.0976	[M+H] ⁺	Pharmaceutical	114	Curcumenol	235.1729	[M+H] ⁺	Pharmaceutical
7	Imidacloprid	256.0586	[M+H] ⁺	Pesticide	43	Loteprednol etabonate	467.1789	[M+H] ⁺	Pharmaceutical	79	Norharman	169.0757	[M+H] ⁺	Natural product	115	Brevilin A	347.1917	[M+H] ⁺	Natural product
8	Antipyrin	189.1021	[M+H] ⁺	Pharmaceutical	44	Chlormadinone acetate	405.1812	[M+H] ⁺	Pharmaceutical	80	5-Carboline	169.0757	[M+H] ⁺	Pharmaceutical	116	Tomatidine	416.3521	[M+H] ⁺	Natural product
9	Clothianidin	250.0181	[M+H] ⁺	Pesticide	45	Benzovindiflupyr	398.0655	[M+H] ⁺	Pesticide	81	4-Aminobenzamide	137.0701	[M+H] ⁺	Industrial chemical	117	Pteleine	230.0833	[M+H] ⁺	Natural product
10	Aldoxycarb	223.074	[M+H] ⁺	Pesticide	46	Tebuconazole	308.1545	[M+H] ⁺	Pesticide	82	1,3-Diphenylguanidine	212.1162	[M+H] ⁺	Industrial chemical	118	Curcumenol	237.1852	[M+H] ⁺	Natural product
11	2-Naphthylamine	144.0802	[M+H] ⁺	Industrial chemical	47	Penconazole	284.0741	[M+H] ⁺	Pesticide	83	Harman	183.093	[M+H] ⁺	Pharmaceutical	119	osthenol	231.1023	[M+H] ⁺	Natural product
12	Tricyclazole	190.043	[M+H] ⁺	Pesticide	48	Progesterone	315.2321	[M+H] ⁺	Pharmaceutical	84	Amantadine	152.1446	[M+H] ⁺	Pharmaceutical	120	Kotanin	439.1411	[M+H] ⁺	Pharmaceutical
13	Monuron	199.0657	[M+H] ⁺	Pesticide	49	Mefenitruconazole	398.09	[M+H] ⁺	Pesticide	85	Isophorone	139.1138	[M+H] ⁺	Industrial chemical	121	N,N-Dimethyltetradecylamine	242.2854	[M+H] ⁺	Industrial chemical
14	Phenolphthalein	319.0966	[M+H] ⁺	Industrial chemical	50	Pyraclostrobin	388.1048	[M+H] ⁺	Pesticide	86	2-Quinolol	146.059	[M+H] ⁺	Natural product	122	Metolachlor OA	280.1565	[M+H] ⁺	Pesticide
15	Etoricoxib	359.0662	[M+H] ⁺	Pharmaceutical	51	Prochloraz	376.0394	[M+H] ⁺	Pesticide	87	3-Methylfoxindole	148.0762	[M+H] ⁺	Natural product	123	Chromone	243.1169	[M+H] ⁺	Pharmaceutical
16	Mesulfenfos	295.0229	[M+H] ⁺	Pesticide	52	(+/-)-Indoxacarb	528.0805	[M+H] ⁺	Pesticide	88	Valgargin	265.1444	[M+H] ⁺	Pharmaceutical	124	Climbazole	293.1037	[M+H] ⁺	Personal care product
17	Phorate sulfone	293.0092	[M+H] ⁺	Pesticide	53	Lopinavir	629.3714	[M+H] ⁺	Pharmaceutical	89	Reynosin	249.1486	[M+H] ⁺	Natural product	125	Triphenylphosphine oxide	279.0925	[M+H] ⁺	Industrial chemical
18	Atrazine	216.1009	[M+H] ⁺	Pesticide	54	Benzyl butyl phthalate	313.1454	[M+H] ⁺	Industrial chemical	90	Albendazole sulfone	298.0917	[M+H] ⁺	Pharmaceutical	126	3-(4-hydroxy-5-oxo-3-phenyl-2H-furan-2-yl)propanoic acid	249.0776	[M+H] ⁺	Pharmaceutical
19	Metalaxyl	280.1531	[M+H] ⁺	Pesticide	55	Tributyl phosphate	267.1739	[M+H] ⁺	Industrial chemical	91	Tryptophol	162.0914	[M+H] ⁺	Natural product	127	N,N-Dimethyldodecan-1-amine	214.2522	[M+H] ⁺	Industrial chemical
20	Buturon	237.0781	[M+H] ⁺	Pesticide	56	Methylparaben	153.0545	[M+H] ⁺	Food additive	92	1-(4-Methoxyphenyl)pent-1-en-3-one	191.105	[M+H] ⁺	Food additive	128	Traversianal	317.2099	[M+H] ⁺	Pesticide
21	Diuron	233.0254	[M+H] ⁺	Pesticide	57	Metaflumizone	507.121	[M+H] ⁺	Pesticide	93	3,4-Dimethoxycinnamic acid	209.0818	[M+H] ⁺	Food additive	129	N,N-Dimethyldodecylamine-N-oxide	230.2478	[M+H] ⁺	Industrial chemical
22	Flumorph	372.1613	[M+H] ⁺	Pesticide	58	17beta-Estradiol	273.1869	[M+H] ⁺	Pharmaceutical	94	Triethyl phosphate (TEP)	183.0764	[M+H] ⁺	Industrial chemical	130	Terbutylazine	230.1174	[M+H] ⁺	Pesticide
23	Fipronil sulfone	452.9379	[M+H] ⁺	Pesticide	59	Lufenuron	510.9894	[M+H] ⁺	Pesticide	95	laminostilbene	194.0977	[M+H] ⁺	Pharmaceutical	131	Telmisartan	515.2439	[M+H] ⁺	Pharmaceutical
24	Chlorantranilprole	481.9798	[M+H] ⁺	Pesticide	60	Tolfenpyrad	384.1487	[M+H] ⁺	Pesticide	96	N-[2-(2,4,6-trichlorophenoxy)ethyl]propylamine	282.0226	[M+H] ⁺	Pesticide	132	3,4-Dihydrocoumarin	149.0613	[M+H] ⁺	Food additive
25	Ametryn	228.1291	[M+H] ⁺	Pesticide	61	Butachlor	312.1722	[M+H] ⁺	Pesticide	97	Thymol	151.1116	[M+H] ⁺	Personal care product	133	Dimethomorph isomer 1	388.1289	[M+H] ⁺	Pesticide
26	Albendazole	266.0948	[M+H] ⁺	Pharmaceutical	62	Chlorpyrifos	349.9344	[M+H] ⁺	Pesticide	98	d-Carvon	151.1142	[M+H] ⁺	Natural product	134	4-Methylbenzylidene camphor	255.1753	[M+H] ⁺	Personal care product
27	Azoxystrobin	404.1234	[M+H] ⁺	Pesticide	63	Pendimethalin	282.1428	[M+H] ⁺	Pesticide	99	Gabapentin	172.1329	[M+H] ⁺	Pharmaceutical	135	[6]-Gingerol	295.1916	[M+H] ⁺	Natural product
28	Pyrimethanil	200.1183	[M+H] ⁺	Pesticide	64	Dicyclohexyl phthalate	331.1933	[M+H] ⁺	Industrial chemical	100	Eleuthero	245.0833	[M+H] ⁺	Pesticide	136	Tetradecyl sulfate	293.18	[M+H] ⁺	Industrial chemical
29	Boscalid	343.0411	[M+H] ⁺	Pesticide	65	Chlorfluazuron	539.9715	[M+H] ⁺	Pesticide	101	Dexibuprofen	207.1397	[M+H] ⁺	Pharmaceutical	137	Phebalosin	259.0959	[M+H] ⁺	Pharmaceutical
30	Benzylparaben	229.0881	[M+H] ⁺	Personal care product	66	Estradiol benzoate	377.211	[M+H] ⁺	Pharmaceutical	102	Tris(2-chloroethyl) phosphate (TCEP)	284.961	[M+H] ⁺	Industrial chemical	138	Suberosin	245.1185	[M+H] ⁺	Natural product
31	Diazepam	285.0819	[M+H] ⁺	Pharmaceutical	67	Pyridaben	365.1453	[M+H] ⁺	Pesticide	103	2-Methoxycinnamaldelyde;	163.0749	[M+H] ⁺	Food additive	139	Osthole	245.1185	[M+H] ⁺	Natural product
32	Paclotrazol	294.138	[M+H] ⁺	Pesticide	68	4-Aminobenzoic acid	138.054	[M+H] ⁺	Personal care product	104	Isopimpinellin	247.0635	[M+H] ⁺	Pesticide	140	Irbesartan	427.2213	[M+H] ⁺	Pharmaceutical
33	Methoxyfenozide	369.2187	[M+H] ⁺	Pesticide	69	Metformin	130.1088	[M+H] ⁺	Pharmaceutical	105	Ethyl butylacetylaminopropionate	216.1611	[M+H] ⁺	Personal care product	141	Fipronil	434.9294	[M+H] ⁺	Pesticide
34	Fluopicolide	382.9706	[M+H] ⁺	Pesticide	70	Triisopropanolamine	192.1614	[M+H] ⁺	Industrial chemical	106	Hexa(methoxymethyl)melamine	391.2308	[M+H] ⁺	Industrial chemical	142	1-Tetradecanamine	258.2798	[M+H] ⁺	Industrial chemical
35	Prometryn	242.1453	[M+H] ⁺	Pesticide	71	Nicotine	163.1219	[M+H] ⁺	Pharmaceutical	107	1-(2,4-Dichlorophenyl)-2-(1,2,4-triazol-1-yl)ethanol	258.0234	[M+H] ⁺	Pesticides	143	Tebufenozide	351.2079	[M+H] ⁺	Pesticide

Number	Name	M/Z	mode	Category	Number	Name	M/Z	mode	Category	Number	Name	M/Z	mode	Category	Number	Name	M/Z	mode	Category
144	Fipronil sulfide	418.9363	[M+H] ⁺	Pesticide	187	Edifenphos	311.0345	[M+H] ⁺	Pesticide	230	5-Hydroxydamantane-2-one	167.1075	[M+H] ⁺	Industrial chemical	273	5,6-Benzo flavone	273.0888	[M+H] ⁺	Industrial chemical
145	Pterostilbene	257.1204	[M+H] ⁺	Natural product	188	Kaempferol	287.0544	[M+H] ⁺	Pharmaceutical	231	Fenarol	165.1034	[M+H] ⁺	Pesticide	274	BENZYLDIIPHENYLPHOSPHINE OXIDE	293.1107	[M+H] ⁺	Industrial chemical
146	Costunolide	233.1535	[M+H] ⁺	Pharmaceutical	189	Glafefine	373.0974	[M+H] ⁺	Pharmaceutical	232	Terbutylazine-2-Hydroxy	212.152	[M+H] ⁺	Pesticide	275	Normeperidine	234.1511	[M+H] ⁺	Pharmaceutical
147	5-Phenylvaleric acid	179.1062	[M+H] ⁺	Natural product	190	Galaloid	259.2046	[M+H] ⁺	Personal care product	233	Alibamide	252.1254	[M+H] ⁺	Pharmaceutical	276	Xanthone	197.0592	[M+H] ⁺	Natural product
148	Emamectin B1A	886.5359	[M+H] ⁺	Pesticide	191	Gitoxin	781.4387	[M+H] ⁺	Pharmaceutical	234	Cinnamide	148.0787	[M+H] ⁺	Food additive	277	cis-Resveratrol	229.0912	[M+H] ⁺	Natural product
149	Ritonavir	721.3237	[M+H] ⁺	Pharmaceutical	192	Methylprednisolone	375.2186	[M+H] ⁺	Pharmaceutical	235	8-Hydroxyquinolin	146.059	[M+H] ⁺	Industrial chemical	278	Dicyclohexylurea	225.1998	[M+H] ⁺	Industrial chemical
150	Lamotrigine	256.016	[M+H] ⁺	Pharmaceutical	193	Stigmastadienone	411.3658	[M+H] ⁺	Pharmaceutical	236	Quinoline-N-oxide	146.059	[M+H] ⁺	Industrial chemical	279	N-methyldodecylamine	200.237	[M+H] ⁺	Personal care product
151	Propiconazole	342.0755	[M+H] ⁺	Pesticide	194	Butenafine	318.2237	[M+H] ⁺	Pharmaceutical	237	Pteroin G	235.1321	[M+H] ⁺	Natural product	280	5,6,7-Trimethoxycoumarin	237.0781	[M+H] ⁺	Pharmaceutical
152	Costunolide	233.1566	[M+H] ⁺	Natural product	195	Quercitrin	449.1229	[M+H] ⁺	Natural product	238	Tetra(methoxymethyl)melamine (TMMM)	303.1753	[M+H] ⁺	Industrial chemical	281	Tris(2-chloroisopropyl)phosphate (TCPP)	327.0666	[M+H] ⁺	Industrial chemical
153	Hydroxycinnamic acid	165.0535	[M+H] ⁺	Pharmaceutical	196	Oxiglutatione	613.1649	[M+H] ⁺	Pharmaceutical	239	Benzo[g]quinoline	180.0796	[M+H] ⁺	Industrial chemical	282	1,2-Chrysenedione	259.0795	[M+H] ⁺	Industrial chemical
154	3-Hydroxycinnamic Acid	165.0561	[M+H] ⁺	Natural product	197	Nicotiflorin	595.1616	[M+H] ⁺	Natural product	240	(E)-3-(4-Hydroxyphenyl)acrylaldehyde	149.0588	[M+H] ⁺	Natural product	283	Isoprothiolane	291.0721	[M+H] ⁺	Pesticide
155	Methyl 2,4-Dihydroxy-3,6-Dimethylbenzoate	197.0822	[M+H] ⁺	Personal care product	198	Furosemide	331.0146	[M+H] ⁺	Pharmaceutical	241	N-Acetyltryptamine	203.1164	[M+H] ⁺	Pharmaceutical	284	4-Methylcinnamic Acid	163.0749	[M+H] ⁺	Personal care product
156	Eplereone	415.209	[M+H] ⁺	Pharmaceutical	199	cis-3-(2,5-Dimethylphenyl)-4-hydroxy-8-methoxy-1-azaspiro[4.5]decane-2-one	304.195	[M+H] ⁺	Pesticide	242	Benothiazole-2-sulfonic acid	213.9638	[M+H] ⁺	Industrial chemical	285	7-Methoxy-4-methylcoumarin	191.071	[M+H] ⁺	Natural product
157	Pyroquon	174.0927	[M+H] ⁺	Pesticide	200	Lupatine	170.1522	[M+H] ⁺	Pharmaceutical	243	1-HYDROXYPHENAZINE	197.0735	[M+H] ⁺	Natural product	286	Reynoutrin	435.0902	[M+H] ⁺	Natural product
158	Norethynodrel	299.202	[M+H] ⁺	Pharmaceutical	201	Tolnafate	308.115	[M+H] ⁺	Pesticide	244	Ethirimol	210.16	[M+H] ⁺	Pesticide	287	Allylescaline	238.1409	[M+H] ⁺	Pharmaceutical
159	Betaxolol	308.2263	[M+H] ⁺	Pharmaceutical	202	L-Glutamic acid	313.0693	[M+H] ⁺	Food additive	245	6-Methylcoumarin	161.0615	[M+H] ⁺	Natural product	288	Nandrolone	275.2027	[M+H] ⁺	Pharmaceutical
160	Urea, N-propyl-N-[2-(2,4,6-trichlorophenoxy)ethyl]-	325.0265	[M+H] ⁺	Pesticide	203	Solasodine	414.3298	[M+H] ⁺	Natural product	246	6-Methoxyquinoline	160.0763	[M+H] ⁺	Industrial chemical	289	4'-Methyl-alpha-pyrrolidino propiophenone	218.154	[M+H] ⁺	Pharmaceutical
161	Difenoconazole	406.0713	[M+H] ⁺	Pesticide	204	Lithocholic acid	377.3062	[M+H] ⁺	Pharmaceutical	247	Indole-3-acetic acid	176.0689	[M+H] ⁺	Natural product	290	Fipronil-desulfinyl	386.9621	[M+H] ⁺	Pesticide
162	2-Methoxybenzoic acid	153.0545	[M+H] ⁺	Pesticide	205	Permethrin	391.0851	[M+H] ⁺	Pesticide	248	Phentermine	150.1298	[M+H] ⁺	Pharmaceutical	291	BENZO(C)ACRIDINE	230.0988	[M+H] ⁺	Industrial chemical
163	Aspirin	181.0501	[M+H] ⁺	Pharmaceutical	206	Bis-(2-ethylhexyl) phthalate	391.2834	[M+H] ⁺	Industrial chemical	249	4-Isopropylbenzyl alcohol	151.1116	[M+H] ⁺	Food additive	292	Penbotolol	292.2287	[M+H] ⁺	Pharmaceutical
164	Dimethyl phthalate	195.0652	[M+H] ⁺	Industrial chemical	207	4-Methylphthalic anhydride	163.0383	[M+H] ⁺	Pharmaceutical	250	Dihydroxytyrosin	277.1067	[M+H] ⁺	Pharmaceutical	293	cinnamaldehyde	133.066	[M+H] ⁺	Food additive
165	Diethyl phthalate	223.0984	[M+H] ⁺	Personal care product	208	Glycerol 1-monostearate	359.316	[M+H] ⁺	Food additive	251	Indoline	120.0809	[M+H] ⁺	Pharmaceutical	294	BISPHENOL A (2,3-DIHYDROXYPROPYL) GLYCID	359.1841	[M+H] ⁺	Industrial chemical
166	4-Dodecylbenzenesulfonic acid	325.1831	[M+H] ⁺	Industrial chemical	209	Deoxycholic acid	393.3055	[M+H] ⁺	Natural product	252	Mexacarbate	223.1473	[M+H] ⁺	Pesticide	295	Tutin	295.1178	[M+H] ⁺	Natural product
167	Cryptotanshinone	297.1493	[M+H] ⁺	Natural product	210	Dodecylmorph	282.2803	[M+H] ⁺	Pesticide	253	Hexazinone	253.166	[M+H] ⁺	Pesticide	296	Shogaol	277.1816	[M+H] ⁺	Natural product
168	Galaxolidone	273.1869	[M+H] ⁺	Personal care product	211	Erucamide	338.3433	[M+H] ⁺	Industrial chemical	254	Pyracarbolid	218.1162	[M+H] ⁺	Pesticide	297	Butylparaben	193.0857	[M+H] ⁺	Personal care product
169	Phenmedipham	301.1161	[M+H] ⁺	Pesticide	212	Diethanolamine	106.0889	[M+H] ⁺	Personal care product	255	Dimethyl telluride	256.0062	[M+H] ⁺	Industrial chemical	298	Cyprodinil	226.1341	[M+H] ⁺	Pesticide
170	Androstenedione	287.2035	[M+H] ⁺	Pharmaceutical	213	Maltose	341.108	[M+H] ⁺	Food additive	256	Alantolactone	233.1535	[M+H] ⁺	Natural product	299	17beta-Trenbolone	271.1684	[M+H] ⁺	Pharmaceutical
171	dextrorphan	258.191	[M+H] ⁺	Pharmaceutical	214	Bufexamac	224.1264	[M+H] ⁺	Pharmaceutical	257	9,10-Phenanthredione	209.0581	[M+H] ⁺	Pesticide	300	5,7-Dimethoxycoumarin	207.0661	[M+H] ⁺	Pharmaceutical
172	Crotamiton	204.1382	[M+H] ⁺	Pharmaceutical	215	4-Guadinobutyric acid	146.0936	[M+H] ⁺	Natural product	258	Buphedrone	178.1219	[M+H] ⁺	Pharmaceutical	301	Norketamine	224.0866	[M+H] ⁺	Pharmaceutical
173	Isopregnanolone	319.2648	[M+H] ⁺	Pharmaceutical	216	Matrine	249.1971	[M+H] ⁺	Pharmaceutical	259	Fention sulfone	311.0237	[M+H] ⁺	Pesticide	302	2-Methylindole	132.0813	[M+H] ⁺	Natural product
174	Dibutyl phthalate	277.1433	[M+H] ⁺	Industrial chemical	217	Myosmine	147.0919	[M+H] ⁺	Natural product	260	Nalphenone	163.1115	[M+H] ⁺	Natural product	303	Nalmeferne	340.1974	[M+H] ⁺	Pharmaceutical
175	Mianserin N-oxide	279.1515	[M+H] ⁺	Pharmaceutical	218	Methacarbonyl	164.1086	[M+H] ⁺	Pharmaceutical	261	Olivetol	181.1245	[M+H] ⁺	Natural product	304	Rhein	285.0474	[M+H] ⁺	Natural product
176	Niclosamide	324.9763	[M+H] ⁺	Pesticide	219	Levosulpiride	342.1474	[M+H] ⁺	Pharmaceutical	262	N,N-Dimethyldecylamine oxide	202.2163	[M+H] ⁺	Industrial chemical	305	Mandrestrobin	314.1708	[M+H] ⁺	Pesticide
177	Tanshinone II	295.1354	[M+H] ⁺	Natural product	220	2,3,4,9-tetrahydro-1H-pyrido[3,4-b]indol-1-one	187.0846	[M+H] ⁺	Natural product	263	9-Fluorenone	181.0666	[M+H] ⁺	Industrial chemical	306	Endosulfan sulfate	418.8022	[M+H] ⁺	Pesticide
178	Epinastine	250.1346	[M+H] ⁺	Pharmaceutical	221	Decyldimethylamine	186.2236	[M+H] ⁺	Industrial chemical	264	Bisphenol A	229.1222	[M+H] ⁺	Industrial chemical	307	Formetate	222.1216	[M+H] ⁺	Pesticide
179	Meglutol	163.0618	[M+H] ⁺	Pharmaceutical	222	Gabapentin-lactam	154.1219	[M+H] ⁺	Pharmaceutical	265	Naphthalene-2-sulfonic acid	207.012	[M+H] ⁺	Industrial chemical	308	Acrylic acid	331.1896	[M+H] ⁺	Industrial chemical
180	Quinalphos	299.0675	[M+H] ⁺	Pesticide	223	Varenicline	212.1192	[M+H] ⁺	Pharmaceutical	266	N-Demethoxyluron	216.9938	[M+H] ⁺	Pesticide	309	Zamifenacin	416.2185	[M+H] ⁺	Pharmaceutical
181	4-METHOXYFLAVONE	253.0879	[M+H] ⁺	Natural product	224	Terephthalic acid	165.0183	[M+H] ⁺	Industrial chemical	267	3,4-Dichloroaniline	161.9898	[M+H] ⁺	Industrial chemical	310	Dihydrocapsaicin	308.2228	[M+H] ⁺	Pharmaceutical
182	Cholic acid	409.2935	[M+H] ⁺	Natural product	225	6-Phenyl-1,3,5-triazine-2,4-diamine	188.0934	[M+H] ⁺	Industrial chemical	268	Tryptantrine	249.0711	[M+H] ⁺	Natural product	311	Brompheniramine	319.082	[M+H] ⁺	Pharmaceutical
183	Elaidic Acid	283.2643	[M+H] ⁺	Natural product	226	3,4-Dimethoxysalicylic acid	199.0603	[M+H] ⁺	Pharmaceutical	269	Flutamide	277.0829	[M+H] ⁺	Pharmaceutical	312	N,N-Bis(2-hydroxyethyl)iodocanamide	288.2551	[M+H] ⁺	Personal care product
184	Nonanedioic acid	189.1133	[M+H] ⁺	Pesticide	227	Sulfathiazole	256.0193	[M+H] ⁺	Pharmaceutical	270	1-cyclohexyl-3-phenyl-urea	219.1494	[M+H] ⁺	Pesticide	313	2-(4-Nonylphenoxy)Acetic Acid	277.1808	[M+H] ⁺	Industrial chemical
185	Glycocholic acid	466.3205	[M+H] ⁺	Natural product	228	Senkirkine	366.1938	[M+H] ⁺	Natural product	271	Clomipramine	315.1616	[M+H] ⁺	Pharmaceutical	314	Benz[de]anthracen-7-one	231.0837	[M+H] ⁺	Industrial chemical
186	Imazaquin	310.1182	[M+H] ⁺	Pesticide	229	Dicyclohexylamine	182.1889	[M+H] ⁺	Industrial chemical	272	Diphenamid	240.1405	[M+H] ⁺	Pesticide	315	N-(2-hydroxyethyl)icosanamide	356.3513	[M+H] ⁺	Industrial chemical

Number	Name	M/Z	mode	Category	Number	Name	M/Z	mode	Category	Number	Name	M/Z	mode	Category
316	Novaluron	491.0022	[M-H] ⁻	Pesticide	375	Ellagic acid	303.0114	[M-H] ⁺	Pharmaceutical	434	Trichanolamine	150.1125	[M-H] ⁺	Industrial chemical
317	Triclocarban	312.97	[M-H] ⁻	Personal care product	376	Isoxafutole	360.0688	[M-H] ⁺	Pesticide	435	TriethyleneglycolDimethylEther	179.1278	[M-H] ⁺	Industrial chemical
318	Monomethyl phthalate	181.0501	[M-H] ⁻	Industrial chemical	377	Pyrazophos	374.0979	[M-H] ⁺	Pesticide	436	Triglycidylisocyanurate	298.1034	[M-H] ⁻	Industrial chemical
319	Vortioxetine	299.156	[M+H] ⁺	Natural product	378	Spingiosine	300.2895	[M-H] ⁺	Natural product	437	Triclosanchlorhexadecacts	286.9439	[M-H] ⁻	Personal care product
320	Norfloxacin	320.1391	[M+H] ⁺	Pharmaceutical	379	Haloxypol	360.0238	[M-H] ⁻	Pesticide	438	Tricyclanol	190.0433	[M-H] ⁻	Pesticide
321	3-Methylcatechol	125.0595	[M-H] ⁻	Natural product	380	Dehydroascrydiline	167.1812	[M-H] ⁺	Pharmaceutical	439	Hexamethylenediacrylate	227.1278	[M-H] ⁻	Industrial chemical
322	Benovamate	364.0865	[M-H] ⁻	Pesticide	381	Acetildenafil	467.2797	[M-H] ⁺	Pharmaceutical	440	Nitroglyram	271.0956	[M-H] ⁻	Pesticide
323	11-Keto-testosterone	303.1931	[M-H] ⁻	Natural product	382	1-Octylpyrrolidin-2-One	198.1866	[M-H] ⁺	Personal care product	441	N-Nitrosodimethylamine	75.0553	[M-H] ⁻	Industrial chemical
324	Genistein	269.0455	[M-H] ⁻	Natural product	383	N-Ethyl-4-menthane-3-carboxamide	212.2027	[M-H] ⁺	Food additive	442	N-Nitrosodiethylamine	103.0866	[M-H] ⁻	Industrial chemical
325	Retinoate	301.2155	[M-H] ⁻	Pharmaceutical	384	13a-Hydroxyspanin	265.1911	[M-H] ⁻	Natural product	443	N-Nitrosodipropylamine	131.1179	[M-H] ⁻	Industrial chemical
326	Paeonol	165.0419	[M-H] ⁻	Pharmaceutical	385	Vildagliptin	304.1986	[M-H] ⁺	Pharmaceutical	444	N-Nitrosodibutylamine	159.1492	[M-H] ⁻	Industrial chemical
327	2-(Thiocyanatomethylthio)benzotriazole	238.9752	[M-H] ⁻	Industrial chemical	386	Cycloheximide	282.1703	[M-H] ⁺	Pharmaceutical	445	N-Nitrosodiphenylamine	199.0866	[M-H] ⁻	Industrial chemical
328	Dimethyl isophthalate	195.0509	[M-H] ⁻	Industrial chemical	387	Dydrogesterone	313.2178	[M-H] ⁺	Pharmaceutical	446	N-Nitrosopyrrolidine	101.0709	[M-H] ⁻	Industrial chemical
329	Quinalofop-ethyl	373.1011	[M-H] ⁻	Pesticide	388	Scharol	399.2797	[M-H] ⁺	Natural product	447	Pyrazconil	315.1119	[M-H] ⁻	Pesticide
330	Glucoserin	420.052	[M-H] ⁻	Food additive	389	Flufenicol	358.0102	[M-H] ⁻	Pesticide	448	Pyrazoxone	439.0228	[M-H] ⁻	Pesticide
331	3,4-Dichlorophenylurea	202.9777	[M-H] ⁻	Pesticide	390	Tritosulfuron	446.0366	[M-H] ⁺	Pesticide	449	Pyridine	80.0495	[M-H] ⁺	Natural product
332	senegalensin	407.1836	[M-H] ⁻	Pharmaceutical	391	Linoleic acid	279.2336	[M-H] ⁻	Natural product	450	Ferizone	255.1604	[M-H] ⁻	Pesticide
333	Dinoterb	239.066	[M-H] ⁻	Pesticide	392	2,4,12-Octadecatrienamide	334.3134	[M-H] ⁺	Natural product	451	Butachlor/Pretilachlor*	312.173	[M-H] ⁻	Pesticide
334	Bupofezin	306.1644	[M+H] ⁺	Pesticide	393	HYOCHOLIC ACID	409.2935	[M-H] ⁺	Natural product	452	DimethylPhthalate	195.0652	[M-H] ⁺	Personal care product
335	Gamolenic acid	279.2326	[M-H] ⁻	Natural product	394	L-Thyroxine	777.6913	[M-H] ⁺	Pharmaceutical	453	DiethylPhthalate	247.0965	[M-H] ⁻	Industrial chemical
336	Pregnenolone acetate	359.254	[M+H] ⁺	Pharmaceutical	395	3-Methylsalicylic acid	153.0545	[M-H] ⁻	Natural product	454	DibutylPhthalate/DiisobutylPhthalate	279.1596	[M-H] ⁻	Industrial chemical
337	Coriolic acid	295.2242	[M-H] ⁻	Industrial chemical	396	Pantethine	555.254	[M-H] ⁺	Pharmaceutical	455	BenzyButylPhthalate	313.144	[M-H] ⁻	Industrial chemical
338	Salmeterol	416.2812	[M+H] ⁺	Pharmaceutical	397	Oleoyl-glycerol	357.3098	[M-H] ⁻	Personal care product	456	DicyclohexylPhthalate	331.1904	[M-H] ⁻	Industrial chemical
339	OPEO-8	559.3885	[M+H] ⁺	Industrial chemical	398	Gosypol	519.2037	[M-H] ⁺	Natural product	457	2-ButanoneOxime	88.0757	[M-H] ⁻	Industrial chemical
340	Triphenyl phosphate (TPHP)	327.0806	[M-H] ⁻	Industrial chemical	399	Diisononyl phthalate	419.3173	[M-H] ⁺	Industrial chemical	458	Flutolanil	324.1206	[M-H] ⁻	Pesticide
341	Zopiclone	389.1091	[M-H] ⁻	Pharmaceutical	400	UV Absorber 234	448.2388	[M-H] ⁻	Industrial chemical	459	Bromobutide	312.0957	[M-H] ⁻	Pesticide
342	OPEO-6	471.3353	[M-H] ⁻	Industrial chemical	401	Astaxanthin	565.4002	[M-H] ⁺	Natural product	460	Hexabromocyclododecane	634.6436	[M-H] ⁻	Industrial chemical
343	L-Aspartyl-L-Phenylalanine	281.1128	[M-H] ⁻	Food additive	402	Dipentyl phthalate	307.1891	[M-H] ⁺	Industrial chemical	461	Pentadecafluorooctanoic Acid	412.9664	[M-H] ⁻	Industrial chemical
344	N-(2-hydroxypropyl)ddscanamide	258.2437	[M-H] ⁻	Industrial chemical	403	Auraptene	297.1519	[M-H] ⁻	Natural product	462	Benobicyclon	447.0492	[M-H] ⁻	Pesticide
345	4-(2,5-Diethoxy-4-nitrophenyl)impropholine	297.1423	[M-H] ⁻	Natural product	404	Andrastin A	485.2564	[M-H] ⁻	Natural product	463	Benazon	239.0496	[M-H] ⁻	Pesticide
346	Estrone	271.1684	[M-H] ⁻	Pharmaceutical	405	Acrylamide	72.0444	[M-H] ⁺	Industrial chemical	464	Malathion	331.0433	[M-H] ⁻	Pesticide
347	Malaaxon	315.0708	[M-H] ⁻	Pesticide	406	Acetamidiprid	223.0745	[M-H] ⁺	Pesticide	465	GlycidylMethacrylate	143.0705	[M-H] ⁺	Industrial chemical
348	Oleic acid	283.2643	[M-H] ⁻	Personal care product	407	2-Aminopyridine	95.0604	[M-H] ⁺	Pharmaceutical	466	N-Methylidicylamine	312.3624	[M-H] ⁺	Pharmaceutical
349	Alumminicine	323.1774	[M-H] ⁻	Natural product	408	2-Ethylhexanoic acid	143.1078	[M-H] ⁻	Industrial chemical	467	1-Methyl-2-pyrrolidone	100.0757	[M-H] ⁺	Industrial chemical
350	Diosgenin	415.3216	[M-H] ⁻	Pharmaceutical	409	2-(2-Ethoxyethoxy)ethanol	135.1016	[M-H] ⁻	Personal care product	468	Metaminostrobin	284.1234	[M-H] ⁻	Pesticide
351	Diphenyl phosphate	251.035	[M-H] ⁻	Industrial chemical	410	Oryzastobin	392.1928	[M-H] ⁺	Pesticide	469	Melanine	127.0727	[M-H] ⁺	Industrial chemical
352	Casleran	207.175	[M+H] ⁺	Personal care product	411	Carbofuran	222.1125	[M-H] ⁻	Pesticide	470	Ethofumate	62.06	[M-H] ⁺	Personal care product
353	1-Naphthylamine	144.0827	[M-H] ⁻	Industrial chemical	412	Quinofop-ethyl	373.095	[M-H] ⁻	Pesticide	471	Molinate	188.1104	[M-H] ⁻	Pesticide
354	N,N-Dimethyl-N-p-tolylsulfamide	215.0855	[M-H] ⁻	Pesticide	413	2-Chloroaniline	128.0262	[M-H] ⁻	Industrial chemical	472	Tris(2-ethylhexyl)Phosphate	435.3598	[M-H] ⁻	Industrial chemical
355	8-Hydroxyquinoline-5-sulfonic acid	226.0172	[M-H] ⁻	Industrial chemical	414	3-Chloroaniline	128.0262	[M-H] ⁻	Industrial chemical	473	Tris(2-chloroethyl)Phosphate	284.9612	[M-H] ⁻	Industrial chemical
356	Isofos	314.0475	[M-H] ⁻	Pesticide	415	4-Chloroaniline	128.0262	[M-H] ⁻	Industrial chemical	474	TricresylPhosphate	369.125	[M-H] ⁻	Industrial chemical
357	Aflatoxin G1	329.0743	[M-H] ⁻	Natural product	416	Cyanazine	241.0963	[M-H] ⁻	Pesticide	475	TriphenylPhosphate	327.078	[M-H] ⁻	Industrial chemical
358	Acetazolamide	222.9945	[M-H] ⁻	Pharmaceutical	417	Disulfoton	275.0338	[M-H] ⁻	Pesticide	476	TributylPhosphate	267.1719	[M-H] ⁻	Industrial chemical
359	Fraxidin	223.0618	[M-H] ⁻	Pesticide	418	2,4-Dinitrophenol	183.0047	[M-H] ⁻	Industrial chemical	477	Dinotefuran-13CS	208.1301/206.1156	[M-H] ⁻	Pesticide
360	Tricosanoic acid	355.3594	[M-H] ⁻	Industrial chemical	419	Dinotefuran	201.0993	[M-H] ⁻	Pesticide	478	Duon-D-6	239.0620/2370.474	[M-H] ⁻	Industrial chemical
361	Benzoferap	431.0921	[M-H] ⁻	Pesticide	420	Diphenylamine	170.0965	[M-H] ⁺	Industrial chemical	479	loehol	820.88031	[M-H] ⁻	Industrial chemical
362	Flubromazolam	371.0294	[M-H] ⁻	Pharmaceutical	421	N,N-Dimethylacetamide	88.0757	[M-H] ⁺	Industrial chemical	480	DL-Arginine	174.11168	[M-H] ⁻	Industrial chemical
363	Hinokiflavone	539.097	[M-H] ⁻	Pharmaceutical	422	N,N-Dimethyldodecylamine	214.2529	[M-H] ⁺	Industrial chemical	481	Oleamide	281.27186	[M-H] ⁻	Industrial chemical
364	Tonalide	259.2079	[M-H] ⁻	Personal care product	423	Simetryn	214.1121	[M-H] ⁻	Pesticide	482	Ricinoleic acid	298.25079	[M-H] ⁻	Industrial chemical
365	Suxibuzone	439.1797	[M-H] ⁻	Pharmaceutical	424	Dymron	267.1503	[M-H] ⁻	Pesticide	483	Steraic acid	284.27153	[M-H] ⁻	Personal care product
366	Moectinostat	397.186	[M-H] ⁻	Pharmaceutical	425	Thiacloprid	253.0309	[M-H] ⁺	Pesticide	484	2,4,6-TBP	327.7734	[M-H] ⁻	Pesticide
367	Tetraethylene glycol monododecyl ether	363.3101	[M-H] ⁻	Industrial chemical	426	Thiadimil	266.016	[M-H] ⁻	Pesticide	485	4-Bromophenol (4-BP)	171.95238	[M-H] ⁻	Industrial chemical
368	Monomyristin	303.2501	[M-H] ⁻	Pesticide	427	Thioycalam	182.126	[M-H] ⁺	Pesticide	486	Cresyl diphenyl phosphate (CDP)	340.08645	[M-H] ⁻	Industrial chemical
369	GLYCOPYRRONIUM	319.2136	[M-H] ⁻	Pharmaceutical	428	Thiophanate-methyl	343.0529	[M-H] ⁻	Pesticide	487	Dimethyl phosphate (DMP)	126.0082	[M-H] ⁻	Pesticide
370	Hydroxyecdysone	481.1108	[M-H] ⁻	Natural product	429	2,4-Dichlorophenoxyacetic acid	218.9621	[M-H] ⁻	Pesticide	488	2-Ethylhexyl diphenyl phosphate (EHDP)	362.1647	[M-H] ⁻	Industrial chemical
371	1-Palmitoylethanolamine	452.2754	[M-H] ⁻	Pharmaceutical	430	Decanoic acid	171.1391	[M-H] ⁻	Industrial chemical	489	Tri(p-tert-butylphenyl) phosphate (TBPP)	494.2586	[M-H] ⁻	Industrial chemical
372	Thiophanate	371.1003	[M-H] ⁻	Pesticide	431	Tetrahydrodimethylphthalcanhydride	165.0557	[M-H] ⁻	Industrial chemical	490	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
373	Fenit	371.1003	[M-H] ⁻	Pharmaceutical	432	Tetraytrione	441.078	[M-H] ⁻	Pesticide	491	Trimethyl phosphate (TMP)	140.02385	[M-H] ⁻	Pesticide
374	Cefditoren	507.0565	[M-H] ⁻	Pharmaceutical	433	Terephthalic Acid	165.0193	[M-H] ⁻	Industrial chemical	492	Tri-n-butyl phosphate (TNBP)	266.1647	[M-H] ⁻	Industrial chemical
493	Tris(2-butoxyethyl) phosphate (TBEP)	398.24334	[M-H] ⁻	Industrial chemical	493	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	493	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
494	α-HBCD	641.64474	[M-H] ⁻	Industrial chemical	494	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	494	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
495	Nicotinamide	122.04801	[M-H] ⁻	Industrial chemical	495	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	495	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
496	2,2-methylbenzothiazole (MTBT)	149.02992	[M-H] ⁻	Food additive	496	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	496	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
497	Acetufurine	162.99393	[M-H] ⁻	Food additive	497	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	497	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
498	Saccharin	182.99901	[M-H] ⁻	Food additive	498	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	498	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
499	Sorbitol	182.07904	[M-H] ⁻	Food additive	499	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	499	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
500	Sucralose	396.01455	[M-H] ⁻	Food additive	500	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	500	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
501	Diemogest	311.18853	[M-H] ⁻	Pharmaceutical	501	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	501	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
502	Estriol (4 isomers)	288.17254	[M-H] ⁻	Pharmaceutical	502	Trichloroethylene	131.9723	[M-H] ⁻	Industrial chemical	502	Tris(2-chloro-2-propenyl) phosphate (TCPP)	326.00083	[M-H] ⁻	Industrial chemical
503	Etonogestrel													

Number	Name	m/z	mode	Category	Number	Name	m/z	mode	Category	Number	Name	m/z	mode	Category	Number	Name	m/z	mode	Category
552	Fenpiclonil	235.9908	[M+H] ⁺	Pesticide	602	Perfluoro-2-propoxypropanoic acid (GenX)	329.975	[M-H] ⁻	Industrial chemical	652	Fcfofenadine	501.28791	[M+H] ⁺	Pharmaceutical	702	Sulfamethoxazole	253.05211	[M+H] ⁺	Pharmaceutical
553	Fenpropidin	273.24565	[M+H] ⁺	Pesticide	603	Perfluoro-2-propoxypropanoic acid (HPPO-DA)	329.975	[M-H] ⁻	Industrial chemical	653	Fluconazole	306.10407	[M+H] ⁺	Pharmaceutical	703	Sulindac	356.08824	[M+H] ⁺	Pharmaceutical
554	Fenpropimorph	303.25621	[M+H] ⁺	Pesticide	604	Perfluorobutane sulfonic acid (PFBS)	299.95027	[M-H] ⁻	Industrial chemical	654	Fluoxetine	309.13405	[M+H] ⁺	Pharmaceutical	704	Sulisobenzone	308.03546	[M+H] ⁺	Pharmaceutical
555	Fluazinam	463.95138	[M+H] ⁺	Pesticide	605	Perfluorobutanoic acid (PFBA)	213.98648	[M-H] ⁻	Industrial chemical	655	Glibenclamide	493.14382	[M+H] ⁺	Pharmaceutical	705	Tamoxifen	371.22491	[M+H] ⁺	Pharmaceutical
556	Fludoxonil	248.03973	[M+H] ⁺	Pesticide	606	Perfluorodecanoic acid (PFDA)	513.96732	[M-H] ⁻	Industrial chemical	656	Glimepiride	490.22499	[M+H] ⁺	Pharmaceutical	706	Terbutaline	225.13649	[M+H] ⁺	Pharmaceutical
557	Flufenacet	363.06646	[M+H] ⁺	Pesticide	607	Perfluorododecanoic acid (PFDDoDA)	613.96093	[M-H] ⁻	Industrial chemical	657	Haloperidol	375.14013	[M+H] ⁺	Pharmaceutical	707	Theobromine (Theophylline - isomere)	180.06473	[M+H] ⁺	Pharmaceutical
558	Flurtanone	333.09766	[M+H] ⁺	Pesticide	608	Perfluoroheptanoic acid (PFH7a)	363.9769	[M-H] ⁻	Industrial chemical	658	Hydrochlorothiazide (HCTZ)	296.96447	[M+H] ⁺	Pharmaceutical	708	Tiamulin	493.32258	[M+H] ⁺	Pharmaceutical
559	Flutrafal	301.10267	[M+H] ⁺	Pesticide	609	Perfluorohexadecanoic acid (PFH16DA)	813.94815	[M-H] ⁻	Industrial chemical	659	Ifosfamide	260.02482	[M+H] ⁺	Pharmaceutical	709	Tramadol	263.18853	[M+H] ⁺	Pharmaceutical
560	Foramsulfuron	452.11142	[M+H] ⁺	Pesticide	610	Perfluorohexane sulfonic acid (PFHS)	399.94388	[M-H] ⁻	Industrial chemical	660	Ivermectin B1a	874.50786	[M+H] ⁺	Pharmaceutical	710	Triclosan	287.95116	[M+H] ⁺	Pharmaceutical
561	Fuberidazole	184.06366	[M+H] ⁺	Pesticide	611	Perfluorohexanoic acid (PFH6a)	313.98009	[M-H] ⁻	Industrial chemical	661	Ketococonazole	530.14876	[M+H] ⁺	Pharmaceutical	711	Trimethoprim	290.13789	[M+H] ⁺	Pharmaceutical
562	Hexythiazox	352.10123	[M+H] ⁺	Pesticide	612	Perfluorononanoic acid (PFNA)	463.97051	[M-H] ⁻	Industrial chemical	662	Ketoprofen	254.09429	[M+H] ⁺	Pharmaceutical	712	Valproic acid	144.11503	[M+H] ⁺	Pharmaceutical
563	Isoproturon	206.14191	[M+H] ⁺	Pesticide	613	Perfluorooctane sulfonic acid (PFOS)	499.93749	[M-H] ⁻	Industrial chemical	663	Levamisole	204.07212	[M+H] ⁺	Pharmaceutical	713	Valsartan	435.22704	[M+H] ⁺	Pharmaceutical
564	Limaron	248.01193	[M+H] ⁺	Pesticide	614	Perfluorooctanoic acid (PFOA)	413.9737	[M-H] ⁻	Industrial chemical	664	Lidocaine	234.17321	[M+H] ⁺	Pharmaceutical	714	Venlafaxine	277.20418	[M+H] ⁺	Pharmaceutical
565	Mandipropamid	411.12374	[M+H] ⁺	Pesticide	615	Perfluoropentanoic acid (PFPeA)	263.98328	[M-H] ⁻	Industrial chemical	665	Loperamide	476.22306	[M+H] ⁺	Pharmaceutical	715	Verapamil	454.28316	[M+H] ⁺	Pharmaceutical
566	(4-Chloro-2-methylphenyl)acetic acid (MCPA)	200.02402	[M+H] ⁺	Pesticide	616	Perfluorotetradecanoic acid (PFTeDA)	713.95454	[M-H] ⁻	Industrial chemical	666	Loratadine	382.14481	[M+H] ⁺	Pharmaceutical	716	Benzyl butyl phthalate (BBP)	312.13616	[M+H] ⁺	Industrial chemical
567	Mecoprop	214.03967	[M+H] ⁺	Pesticide	617	Perfluoroundecanoic acid (PFUnDA)	563.96412	[M-H] ⁻	Industrial chemical	667	Losartan	422.16219	[M+H] ⁺	Pharmaceutical	717	Bis(2-ethylhexyl) phthalate (DEHP)	390.27701	[M+H] ⁺	Industrial chemical
568	Mesosulfuron-methyl	503.07807	[M+H] ⁺	Pesticide	618	10,11-Dihydro-10-hydroxycarbamazepine	254.10553	[M+H] ⁺	Pharmaceutical	668	Mebendazole	295.09569	[M+H] ⁺	Pharmaceutical	718	Dibutyl phthalate (DBP)	278.15181	[M+H] ⁺	Industrial chemical
569	Metazachlor	277.09819	[M+H] ⁺	Pesticide	619	10,11-Dihydrocarbamazepine	238.11061	[M+H] ⁺	Pharmaceutical	669	Meclofenamic acid	295.01668	[M+H] ⁺	Pharmaceutical	719	Monobenzyl Phthalate (MP)	256.07356	[M+H] ⁺	Industrial chemical
570	Methabenzthiazuron	221.06228	[M+H] ⁺	Pesticide	620	Aceclofenac	353.02216	[M+H] ⁺	Pharmaceutical	670	Mefenamic acid	241.11028	[M+H] ⁺	Pharmaceutical	720	Monobutyl Phthalate (MBP)	222.08921	[M+H] ⁺	Industrial chemical
571	Metrafenone	408.05724	[M+H] ⁺	Pesticide	621	Acetaminophen	151.06333	[M+H] ⁺	Pharmaceutical	671	Memantine	179.1674	[M+H] ⁺	Pharmaceutical	721	Dodecamethylpentaloxane	384.14599	[M+H] ⁺	Industrial chemical
572	Metribuzin	214.08883	[M+H] ⁺	Pesticide	622	Amitriptyline	277.18305	[M+H] ⁺	Pharmaceutical	672	Methadone	309.20926	[M+H] ⁺	Pharmaceutical	722	Hexamethylcyclotrisiloxane	222.05637	[M+H] ⁺	Industrial chemical
573	Metsulfuron methyl	381.0743	[M+H] ⁺	Pesticide	623	Amlodipine	408.1452	[M+H] ⁺	Pharmaceutical	673	Methotrexate	454.17132	[M+H] ⁺	Pharmaceutical	723	4-Dodecylbenzenesulfonic acid	326.19157	[M+H] ⁺	Industrial chemical
574	Onadiazon	344.06945	[M+H] ⁺	Pesticide	624	Amoxicillin	365.10454	[M+H] ⁺	Pharmaceutical	674	Metoprolol	267.18344	[M+H] ⁺	Pharmaceutical	724	Laureth-5	406.32944	[M+H] ⁺	Industrial chemical
575	Picloram	239.92601	[M+H] ⁺	Pesticide	625	Atenolol	266.16304	[M+H] ⁺	Pharmaceutical	675	Metronidazole	171.06439	[M+H] ⁺	Pharmaceutical	725	Laurilsulfate	266.15518	[M+H] ⁺	Industrial chemical
576	Picolinifen	376.08349	[M+H] ⁺	Pesticide	626	Atorvastatin	558.253	[M+H] ⁺	Pharmaceutical	676	Mirtazapine	265.1579	[M+H] ⁺	Pharmaceutical	726	Octaethylene glycol	370.22028	[M+H] ⁺	Industrial chemical
577	Pirimicarb	238.14298	[M+H] ⁺	Pesticide	627	Azithromycin	748.50853	[M+H] ⁺	Pharmaceutical	677	N,N-Dimethyltetradecylamine	241.27695	[M+H] ⁺	Industrial chemical	727	4-hydroximatoxifen	388.22711	[M+H] ⁺	Pharmaceutical
578	Propamocarb	188.15248	[M+H] ⁺	Pesticide	628	Bezafibrate	361.10809	[M+H] ⁺	Pharmaceutical	678	Natamycin	665.30474	[M+H] ⁺	Pharmaceutical	728	4-hydroxybenzothiazole/OBT	152.01646	[M+H] ⁺	Pharmaceutical
579	Propiconazole 1	341.06978	[M+H] ⁺	Pesticide	629	Bicalutamide	430.06104	[M+H] ⁺	Pharmaceutical	679	N-Desmethylcitalopram	310.14814	[M+H] ⁺	Pharmaceutical	729	Ambroxol	376.98586	[M+H] ⁺	Pharmaceutical
580	Propoxycarbazon	398.08962	[M+H] ⁺	Pesticide	630	Bisoprolol	325.22531	[M+H] ⁺	Pharmaceutical	680	Niflumic acid	282.06161	[M+H] ⁺	Pharmaceutical	730	Anastrozole	294.17132	[M+H] ⁺	Pharmaceutical
581	Propyzamide	255.02177	[M+H] ⁺	Pesticide	631	Budesonide	430.23554	[M+H] ⁺	Pharmaceutical	681	Norfloxacin	295.1184	[M+H] ⁺	Pharmaceutical	731	Azelastine	382.16807	[M+H] ⁺	Pharmaceutical
582	Proflumicarb	251.13439	[M+H] ⁺	Pesticide	632	Carazolol	296.16813	[M+H] ⁺	Pharmaceutical	682	Ofloxacine	361.14378	[M+H] ⁺	Pharmaceutical	732	Benzazone	239.04959	[M+H] ⁺	Pharmaceutical
583	Prothioconazole-desthio	311.05922	[M+H] ⁺	Pesticide	633	Carbamazepine	236.09496	[M+H] ⁺	Pharmaceutical	683	Omeprazole	345.11471	[M+H] ⁺	Pharmaceutical	733	Benzothiazium	412.32101	[M+H] ⁺	Pharmaceutical
584	Pyroxasulam	434.06202	[M+H] ⁺	Pesticide	634	Carbamazepine 10,11-epoxide	252.08988	[M+H] ⁺	Pharmaceutical	684	Oxazepam	286.05091	[M+H] ⁺	Pharmaceutical	734	Benzothiazole	136.02155	[M+H] ⁺	Pharmaceutical
585	Quimerac	221.02436	[M+H] ⁺	Pesticide	635	Cetirizine	388.15537	[M+H] ⁺	Pharmaceutical	685	Oxycodone	315.14706	[M+H] ⁺	Pharmaceutical	735	Bosentan	552.19113	[M+H] ⁺	Pharmaceutical
586	Quinoxifen	306.99967	[M+H] ⁺	Pesticide	636	Chloramphenicol	322.01233	[M+H] ⁺	Pharmaceutical	686	Parfenol	205.13141	[M+H] ⁺	Pharmaceutical	736	Bayoptol	240.11497	[M+H] ⁺	Pharmaceutical
587	Rimsulfuron	431.05694	[M+H] ⁺	Pesticide	637	Chloroquine	319.18153	[M+H] ⁺	Pharmaceutical	687	Paroxetine	329.14272	[M+H] ⁺	Pharmaceutical	737	Celecoxib	382.08316	[M+H] ⁺	Pharmaceutical
588	Silthiofam	267.11131	[M+H] ⁺	Pesticide	638	Ciprofloxacin	331.13322	[M+H] ⁺	Pharmaceutical	688	Phenazone	188.09496	[M+H] ⁺	Pharmaceutical	738	Cetirizine	389.16265	[M+H] ⁺	Pharmaceutical
589	Simazine	201.07812	[M+H] ⁺	Pesticide	639	Citalopram	324.16379	[M+H] ⁺	Pharmaceutical	689	Propranolol	259.15723	[M+H] ⁺	Pharmaceutical	739	Chloridazon	222.04287	[M+H] ⁺	Pharmaceutical
590	Spiroxamine I	297.26678	[M+H] ⁺	Pesticide	640	Clarithromycin	747.47689	[M+H] ⁺	Pharmaceutical	690	Pyridoxine	169.07389	[M+H] ⁺	Pharmaceutical	740	Chloroxuron	291.08948	[M+H] ⁺	Pharmaceutical
591	Sulfosulfuron	470.06784	[M+H] ⁺	Pesticide	641	Clindamycin	424.17987	[M+H] ⁺	Pharmaceutical	691	Pyrimethamine	248.08287	[M+H] ⁺	Pharmaceutical	741	Chlortoluron	213.07892	[M+H] ⁺	Pharmaceutical
592	Terbutylazine	229.10942	[M+H] ⁺	Pesticide	642	Clopidogrel	321.05903	[M+H] ⁺	Pharmaceutical	692	Ramipril	416.23112	[M+H] ⁺	Pharmaceutical	742	Clofibrac acid	213.0324	[M+H] ⁺	Pharmaceutical
593	Terbutryl	241.13612	[M+H] ⁺	Pesticide	643	Clozacin	326.12982	[M+H] ⁺	Pharmaceutical	693	Ranitidine	314.14126	[M+H] ⁺	Pharmaceutical	743	Clonidine	230.02463	[M+H] ⁺	Pharmaceutical
594	Thifensulfuron methyl	387.03072	[M+H] ⁺	Pesticide	644	Codine	299.15214	[M+H] ⁺	Pharmaceutical	694	Roxithromycin	836.52457	[M+H] ⁺	Pharmaceutical	744	Clopidrogel	322.0663	[M+H] ⁺	Pharmaceutical
595	Triadimefon	293.0931	[M+H] ⁺	Pesticide	645	Desvenlafaxine	263.18853	[M+H] ⁺	Pharmaceutical	695	Salbutamol	239.15214	[M+H] ⁺	Pharmaceutical	745	Cortisone	361.20095	[M+H] ⁺	Pharmaceutical
596	Trifloxystrobin	408.12969	[M+H] ⁺	Pesticide	646	Diclofenac	295.01668	[M+H] ⁺	Pharmaceutical	696	Sebacic acid	202.12051	[M+H] ⁺	Pharmaceutical	746	Cyclophosphamide	261.0321	[M+H] ⁺	Pharmaceutical
597	Trifluraluron-methyl	492.10389	[M+H] ⁺	Pesticide	647	Diltiazem	414.16133	[M+H] ⁺	Pharmaceutical	697	Setraline	305.0738	[M+H] ⁺	Pharmaceutical	747	Cyproterone	375.17215	[M+H] ⁺	Pharmaceutical
598	Trinexapac-ethyl	252.09977	[M+H] ⁺	Pesticide	648	Enalapril	376.19982	[M+H] ⁺	Pharmaceutical	698	Simvastatin	418.27192	[M+H] ⁺	Pharmaceutical	748	DEET	192.13829	[M+H] ⁺	Pesticide
599	Triticoazole	317.12949	[M+H] ⁺	Pesticide	649	Erythromycin	733.46124	[M+H] ⁺	Pharmaceutical	699	Sotalol	272.11946	[M+H] ⁺	Pharmaceutical	749	Desloratadine	311.13095	[M+H] ⁺	Pharmaceutical
600	N-Ethyl perfluorooctane sulfonamide (N-EtFOSA)	526.98478	[M+H] ⁺	Pesticide	650	Ferbendazole	299.07285	[M+H] ⁺	Pharmaceutical	700	Sparfloxacin	392.166	[M+H] ⁺	Pharmaceutical	750	Dexamethasone	393.20718	[M+H] ⁺	Pharmaceutical
601	N-Methyl perfluorooctane sulfonamide (N-MeFOSA)	512.96913	[M+H] ⁺	Industrial chemical	651	Fenofibrate	360.11284	[M+H] ⁺	Pharmaceutical	701	Sulfazoxime	284.01347	[M+H] ⁺	Pharmaceutical	751	Dichlorvos	220.95318	[M+H] ⁺	Pharmaceutical

Number	Name	m/z	mode	Category	Number	Name	m/z	mode	Category	Number	Name	m/z	mode	Category
752	Dimethachlor	256.10988	[M+H] ⁺	Pharmaceutical	810	Sulfapyridine	250.06447	[M+H] ⁺	Pharmaceutical	868	2,4-Dinitrophenol	184.11	[M-H] ⁻	Pesticide
753	Diphenhydramine	256.16959	[M+H] ⁺	Pharmaceutical	811	Terbinafine	292.20598	[M+H] ⁺	Pharmaceutical	869	Cyhalothop Butyl	357.38	[M-H] ⁻	Pesticide
754	Dodemorph	282.27914	[M+H] ⁺	Pharmaceutical	812	Triadimenol	296.11603	[M+H] ⁺	Pharmaceutical	870	Phenyl Ether	170.21	[M+H] ⁺	Personal care product
755	Domperidone	426.16913	[M+H] ⁺	Pharmaceutical	813	Triamcinolone	395.18644	[M+H] ⁺	Pharmaceutical	871	Dibutyltin dichloride	303.85	[M+H] ⁺	Industrial chemical
756	Drossiprenone	367.22677	[M+H] ⁺	Pharmaceutical	814	Triethylphosphate	183.07807	[M+H] ⁺	Pharmaceutical	872	Dibutyltin dilaurate	631.57	[M+H] ⁺	Industrial chemical
757	Dolasetine	298.12601	[M+H] ⁺	Pharmaceutical	815	Trimestopim	291.14517	[M+H] ⁺	Pharmaceutical	873	2,6-Di-tert-butyl-p-cresol	220.35	[M-H] ⁻	Food additive
758	EDDP	278.19033	[M+H] ⁺	Pharmaceutical	816	Methyl acrylate	86.09	[M+H] ⁺	Industrial chemical	874	Dibenzyl ether	198.26	[M-H] ⁻	Industrial chemical
759	Efavirenz	314.02011	[M-H] ⁻	Pharmaceutical	817	Ethyl acrylate	100.12	[M+H] ⁺	Industrial chemical	875	2,4-Di-tert-pentylphenol	234.38	[M-H] ⁻	Industrial chemical
760	Ethion	384.99489	[M+H] ⁺	Pharmaceutical	818	Butyl acrylate	128.17	[M+H] ⁺	Industrial chemical	876	N-[3-(dimethylamino)propyl] stearamide	368.64	[M+H] ⁺	Industrial chemical
761	Escmestane	297.18491	[M+H] ⁺	Pharmaceutical	819	2-Hydroxyethyl acrylate	116.12	[M+H] ⁺	Industrial chemical	877	Dimethyl Disulfide	94.2	[M+H] ⁺	Food additive
762	Fenoxycarb	302.13868	[M+H] ⁺	Pharmaceutical	820	Propenoic acid 2-(dimethylamino)ethyl ester	143.18	[M+H] ⁺	Industrial chemical	878	N,N-Dimethyldecylamine	213.4	[M+H] ⁺	Industrial chemical
763	Finasteride	373.28495	[M+H] ⁺	Pharmaceutical	821	2-Ethylhexyl acrylate	184.27	[M+H] ⁺	Industrial chemical	879	N,N-Dimethyldecylamine N-oxide	229.4	[M+H] ⁺	Personal care product
764	Flufenoxuron	487.02896	[M+H] ⁺	Pharmaceutical	822	Acetone	58.08	[M+H] ⁺	Industrial chemical	880	3-Dimethylamino-propylamine	102.18	[M+H] ⁺	Personal care product
765	Flumequine	262.0874	[M+H] ⁺	Pharmaceutical	823	Acetone Cyanohydrin	85.1	[M+H] ⁺	Industrial chemical	881	Dimethylformamide	73.1	[M+H] ⁺	Pesticide
766	Fluxoxamine	319.16279	[M+H] ⁺	Pharmaceutical	824	Acetaphate	183.17	[M+H] ⁺	Industrial chemical	882	Tetramethylammonium hydroxide	91.15	[M+H] ⁺	Industrial chemical
767	Genistin	433.11292	[M+H] ⁺	Pharmaceutical	825	2-Aminophenol	109.13	[M+H] ⁺	Industrial chemical	883	Thiourea	76.12	[M+H] ⁺	Pesticide
768	Hydroxychloroquine	336.18372	[M+H] ⁺	Pharmaceutical	826	3-Aminophenol	109.13	[M+H] ⁺	Industrial chemical	884	2,4-Dichlorophenoxyacetic acid	221.04	[M-H] ⁻	Pesticide
769	Imatinib	494.26629	[M+H] ⁺	Pharmaceutical	827	4-Aminophenol	109.13	[M+H] ⁺	Industrial chemical	885	Decanoic acid	172.26	[M-H] ⁻	Industrial chemical
770	Imazalil	297.0556	[M+H] ⁺	Pharmaceutical	828	Isobutyraldehyde	72.11	[M+H] ⁺	Industrial chemical	886	Decyl alcohol	158.28	[M-H] ⁻	Personal care product
771	Imipramine	281.20123	[M+H] ⁺	Pharmaceutical	829	2-Isobutoxyethanol	118.17	[M+H] ⁺	Industrial chemical	887	Tetraethylenepentamine	189.3	[M+H] ⁺	Industrial chemical
772	Lenacil	235.1441	[M+H] ⁺	Pharmaceutical	830	Isoprene	68.12	[M+H] ⁺	Industrial chemical	888	Tetrahydrodimethylphthalic anhydride	166.17	[M-H] ⁻	Industrial chemical
773	Lorazepam	321.01921	[M+H] ⁺	Pharmaceutical	831	Limone	136.23	[M+H] ⁺	Pharmaceutical	889	Phytol	296.53	[M-H] ⁻	Industrial chemical
774	Mebeverine	430.2588	[M+H] ⁺	Pharmaceutical	832	Ivermectin	875.11	[M+H] ⁺	Industrial chemical	890	Dimethyl Terephthalate	194.18	[M-H] ⁻	Industrial chemical
775	Medroxyprogesterone	345.24242	[M+H] ⁺	Pharmaceutical	833	Iminoctadine albesilate	1335.05	[M+H] ⁺	Industrial chemical	891	1-Dodecanol	186.33	[M-H] ⁻	Industrial chemical
776	Mefenamic acid	242.11756	[M+H] ⁺	Pharmaceutical	834	2-Ethyl hexanoic acid	144.21	[M-H] ⁻	Industrial chemical	892	Lauramidic Propylbetaine	342.52	[M-H] ⁻	Personal care product
777	Metamitron	203.09274	[M+H] ⁺	Pharmaceutical	835	Ethylene glycol	62.07	[M-H] ⁻	Industrial chemical	893	Methyl laurate	214.34	[M-H] ⁻	Industrial chemical
778	Metconazole	320.15242	[M+H] ⁺	Pharmaceutical	836	Ethylene glycol monoalkyl ether	90.12	[M-H] ⁻	Industrial chemical	894	Tert-dodecylthiol	202.4	[M-H] ⁻	Industrial chemical
779	Metroprolol	268.19072	[M+H] ⁺	Pharmaceutical	837	Ethylene glycol monoethyl ether acetate	160.21	[M+H] ⁺	Industrial chemical	895	Sodium dodecyl sulfate	288.38	[M-H] ⁻	Industrial chemical
780	Miconazole	414.9933	[M+H] ⁺	Pharmaceutical	838	Ethylendiamine	60.1	[M+H] ⁺	Industrial chemical	896	Triethylene Glycol Dimethyl Ether	178.23	[M+H] ⁺	Industrial chemical
781	Myclobetani	289.12145	[M+H] ⁺	Pharmaceutical	839	Ethylendiaminetetraacetic acid Alkylidimethylbenzylammonium chloride	292.24	[M+H] ⁺	Industrial chemical	897	Triglycidyl Isocyanurate	297.26	[M+H] ⁺	Industrial chemical
782	Mycophenolic acid	321.13326	[M+H] ⁺	Pharmaceutical	840	2-Chlorobenzyl Chloride	283.88	[M+H] ⁺	Pharmaceutical	898	Triclosan and chlorine adducts	289.55	[M-H] ⁻	Industrial chemical
783	Nitrofurantoin	237.02654	[M-H] ⁻	Pharmaceutical	841	Chloroethane	64.51	[M+H] ⁺	Industrial chemical	899	1,2,3-Trichloropropane	147.43	[M-H] ⁻	Industrial chemical
784	Norgestimate	370.23767	[M+H] ⁺	Pharmaceutical	842	1-Octanol	130.23	[M+H] ⁺	Industrial chemical	900	Trifluralin	335.28	[M+H] ⁺	Industrial chemical
785	Notriptyline	264.17468	[M+H] ⁺	Pharmaceutical	843	Captan	300.59	[M+H] ⁺	Pesticide	901	3,5,5-Trimethyl hexanol	144.25	[M+H] ⁺	Industrial chemical
786	Ondansetron	294.16009	[M+H] ⁺	Pharmaceutical	844	Glyphosate	169.07	[M+H] ⁺	Pesticide	902	Naphthalene	128.17	[M+H] ⁺	Industrial chemical
787	Oxizalin	347.10198	[M+H] ⁺	Pharmaceutical	845	Glufosinate	181.13	[M+H] ⁺	Pesticide	903	Hexamethylene diacrylate	226.27	[M+H] ⁺	Industrial chemical
788	Oxybutyrim	358.23767	[M+H] ⁺	Pharmaceutical	846	2-Cresol	108.14	[M+H] ⁺	Pesticide	904	Sodium nitroacetate	235.1	[M+H] ⁺	Industrial chemical
789	Pentoxifylline	279.14517	[M+H] ⁺	Pharmaceutical	847	3-Cresol	108.14	[M+H] ⁺	Pesticide	905	N-Nitrosodibutylamine	158.24	[M+H] ⁺	Industrial chemical
790	PFB5	298.94299	[M-H] ⁻	Industrial chemical	848	4-Cresol	108.14	[M+H] ⁺	Pesticide	906	2-Nitrotoluene	137.14	[M+H] ⁺	Industrial chemical
791	PFOA	412.96643	[M-H] ⁻	Industrial chemical	849	2-Chlorobenzyl Chloride	161.03	[M+H] ⁺	Pharmaceutical	907	3-Nitrotoluene	137.14	[M+H] ⁺	Industrial chemical
792	PFOS	498.93022	[M-H] ⁻	Industrial chemical	850	Chloroacetic Acid	94.5	[M+H] ⁺	Pesticide	908	4-Nitrotoluene	137.14	[M+H] ⁺	Industrial chemical
793	PFOSA	497.9462	[M+H] ⁺	Industrial chemical	851	Dichloroacetic Acid	128.94	[M+H] ⁺	Pharmaceutical	909	Nitrobenzene	123.11	[M+H] ⁺	Industrial chemical
794	Pindolol	249.15975	[M+H] ⁺	Pharmaceutical	852	Trichloroacetic Acid	163.39	[M+H] ⁺	Industrial chemical	910	Nitromethane	61.04	[M+H] ⁺	Industrial chemical
795	Pipamperone	376.23948	[M+H] ⁺	Pharmaceutical	853	2-Chloronitrobenzene	157.55	[M+H] ⁺	Industrial chemical	911	1-Nonanol	144.25	[M+H] ⁺	Industrial chemical
796	Pirimiphos-methyl	306.10358	[M+H] ⁺	Pesticide	854	3-Chloronitrobenzene	157.55	[M+H] ⁺	Industrial chemical	912	1-Hydroxyethane-1,1-diphosphonic Acid	206.03	[M+H] ⁺	Industrial chemical
797	Pravastatin	423.23883	[M-H] ⁻	Pharmaceutical	855	4-Chloronitrobenzene	157.55	[M+H] ⁺	Industrial chemical	913	Hydroquinone	110.11	[M-H] ⁻	Personal care product
798	Prednisone	359.1853	[M+H] ⁺	Pharmaceutical	856	Vinyl acetate	86.09	[M+H] ⁺	Industrial chemical	914	Biphenyl	154.21	[M-H] ⁻	Pesticide
799	Primidone	219.1128	[M+H] ⁺	Pharmaceutical	857	Propylene Oxide	58.08	[M+H] ⁺	Industrial chemical	915	Catechol	110.11	[M-H] ⁻	Industrial chemical
800	Propachlor	212.08367	[M+H] ⁺	Pharmaceutical	858	1,3-Dioxolane	74.08	[M+H] ⁺	Pharmaceutical	916	Fenrazamid	349.82	[M+H] ⁺	Pesticide
801	Propanil	218.0134	[M+H] ⁺	Pharmaceutical	859	Cyclohexanone	98.14	[M+H] ⁺	Pesticide	917	Phthalide	271.91	[M+H] ⁺	Pharmaceutical
802	Propylbenzazone	231.14919	[M+H] ⁺	Pharmaceutical	860	Cyclohexane	84.16	[M+H] ⁺	Pesticide	918	1,3-Butadiene	54.09	[M+H] ⁺	Industrial chemical
803	Pyramet	207.09505	[M+H] ⁺	Pharmaceutical	861	N-(cyclohexylthio) phthalimide	261.34	[M+H] ⁺	Industrial chemical	919	Diallyl Phthalate	246.26	[M+H] ⁺	Industrial chemical
804	Raloxifen	474.17336	[M+H] ⁺	Pharmaceutical	862	Dichlorobenzil	172.01	[M+H] ⁺	Pesticide	920	Diisobutyl Phthalate	278.34	[M+H] ⁺	Industrial chemical
805	Risperidone	411.21908	[M+H] ⁺	Pharmaceutical	863	2,4-Dichlorotoluene	161.03	[M+H] ⁺	Pesticide	921	Bis(2-methoxyethyl) phthalate	282.29	[M+H] ⁺	Industrial chemical
806	Ropinorel	261.19614	[M+H] ⁺	Pharmaceutical	864	1,3-Dichloro-2-propanol	128.99	[M+H] ⁺	Pesticide	922	2-Butanone Oxime	87.12	[M+H] ⁺	Industrial chemical
807	Spiroxamine	298.27406	[M+H] ⁺	Pharmaceutical	865	2-Dichlorobenzene	147	[M+H] ⁺	Pesticide	923	Tert-Butyl Hydroperoxide	90.12	[M+H] ⁺	Industrial chemical
808	Sulfadiazine	251.05972	[M+H] ⁺	Pharmaceutical	866	3-Dichlorobenzene	147	[M+H] ⁺	Pesticide	924	2-sec-Butylphenol	150.22	[M-H] ⁻	Industrial chemical
809	Sulfamethazine	272.09102	[M+H] ⁺	Pharmaceutical	867	4-Dichlorobenzene	147	[M+H] ⁺	Pesticide	925	4-tert-Butylphenol	150.22	[M-H] ⁻	Industrial chemical

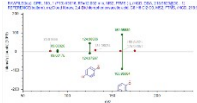
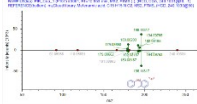
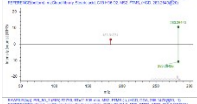
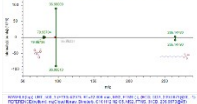
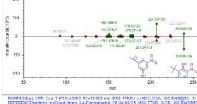
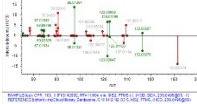
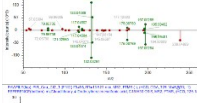
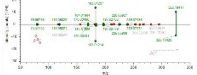
Table S5 List of compounds at confidence level 2 and their properties

Number	Precursor ion m/z	Mean RT (min)	Concentration by Quantem software (ng/L)				Neutral (Da)	Reference Ion	Mass error (ppm)	Chemical formula Chemspider	Mzcloud ion product matching	mzCloud matching scores	No. of proposed structures	B.P. (°C)	log Kow	CAS NO	Category
			CPR	PhR	PIR	UTR											
Penbutolol	292.2260	8.2	4.56	6.99	1.17	1.89	291.2198	[M+H] ⁺	-4.0	C18 H29 N O2		42.6	79	N/A	3.25	38363-40-5	Pharmaceutical
Lenacil	235.1430	7.4	26.9	11.5	5.76	38.9	234.1368	[M+H] ⁺	-4.8	C13 H18 N2 O2		44.3	403	N/A	1.9	2164-08-1	Pesticide
Acetamiprid	223.0734	8.7	13.1	6.96	1.95	2.17	222.0672	[M+H] ⁺	-4.8	C10 H11 Cl N4		47.4	20	N/A	0.8	135410-20-7	Pesticide
Terbuthylazine	230.1157	10.0	1.15	6.03	8.37	0.71	229.1094	[M+H] ⁺	-4.3	C9 H16 Cl N5		53.5	52	N/A	2.7	5915-41-3	Pesticide
Lidocaine	235.1794	7.9	0.58	1.62	0.39	0.77	234.1732	[M+H] ⁺	-4.8	C14 H22 N2 O		78.6	211	N/A	2.5	137-58-6	Pharmaceutical
Spiroxamine	298.2729	10.6	2.72	0.32	25.9	0.59	297.2668	[M+H] ⁺	-4.1	C18 H35 N O2		85.3	41	135	3.9	118134-30-8	Pharmaceutical
Benzyl butyl phthalate	313.1421	10.5	24.3	44.5	64.5	28.6	312.1362	[M+H] ⁺	-4.9	C19 H20 O4		89.9	199	370	4.9	85-68-7	Industrial chemical
Diuron	233.0232	9.7	48.5	78.8	223.2	43.3	232.0170	[M+H] ⁺	-4.6	C9 H10 Cl2 N2 O		94.6	54	N/A	2.9	330-54-1	Pesticide
Triazophos	314.0709	10.0	31.2	2.06	2.10	3.12	313.0650	[M+H] ⁺	-4.4	C12 H16 N3 O3 P S		99	41	N/A	3.7	24017-47-8	Pesticide
Propiconazole	342.0754	10.3	6435	254	330	0.00	341.0698	[M+H] ⁺	-4.7	C15 H17 Cl2 N3 O2		99.3	14	N/A	3.7	60207-90-1	Pesticide

Tramadol	264.1949	8.2	8.28	6.52	19.2	3.77	263.1885	[M+H] ⁺ 1	-3.4	C ₁₆ H ₂₅ N O ₂		99.9	260	N/A	1.35	27203-73-2	Pharmaceutical
Clomazone	240.0774	9.8	146	3.00	2.63	2.45	239.0713	[M+H] ⁺ 1	-4.8	C ₁₂ H ₁₄ Cl N O ₂		99	154	275	2.45	81777-89-1	Pesticide
Venlafaxine	278.2105	8.3	1.86	3.73	5.67	35.4	277.2042	[M+H] ⁺ 1	-3.6	C ₁₇ H ₂₇ N O ₂		31.1	126	N/A	2.1	93413-62-8	Pharmaceutical
17beta-Estradiol	273.1840	9.8	9.10	30.4	15.3	25.5	272.1776	[M+H] ⁺ 1	-3.5	C ₁₈ H ₂₄ O ₂		34	151	N/A	3.7	50-28-2	Pharmaceutical
Primidone	219.1118	7.9	18.3	18.2	50.0	31.7	218.1055	[M+H] ⁺ 1	-4.9	C ₁₂ H ₁₄ N ₂ O ₂		37.3	540	N/A	0.25	125-33-7	Pharmaceutical
Normeperidine	234.1479	7.6	6.46	4.70	4.30	12.7	233.1416	[M+H] ⁺ 1	-4.2	C ₁₄ H ₁₉ N O ₂		52.8	587	N/A	1.6	77-17-8	Pharmaceutical
Ciprofloxacin	332.1390	8.1	0.69	32.0	5.37	8.14	331.1332	[M+H] ⁺ 1	-4.7	C ₁₇ H ₁₈ F N ₃ O ₃		67.2	75	N/A	-0.45	85721-33-1	Pharmaceutical
Hexazinone	253.1649	9.4	4.03	49.3	0.69	0.65	252.1586	[M+H] ⁺ 1	-4.2	C ₁₂ H ₂₀ N ₄ O ₂		67.1	39	N/A	1.2	51235-04-2	Pesticide
Galaxolidone	273.1839	10.5	933	2046	7120	6131	272.1776	[M+H] ⁺ 1	-3.9	C ₁₈ H ₂₄ O ₂		69.3	151	142.5	5.6	1222-05-5	Personal care product
Phenolphthalein	319.0951	9.3	10.1	60.9	42.8	37.1	318.0892	[M+H] ⁺ 1	-4.4	C ₂₀ H ₁₄ O ₄		86	86	N/A	2.45	77-09-8	Industrial chemical
Metolachlor morpholinone	234.1478	7.7	29.3	29.2	5.21	10.5	233.1416	[M+H] ⁺ 1	-4.5	C ₁₄ H ₁₉ N O ₂		51.9	587	N/A	N/A	120375-14-6	Pesticide

Triphenylphosphine oxide	279.0923	9.9	61.5	53.5	45.2	83.9	278.0861	[M+H] ⁺	-3.8	C18 H15 O P		90.1	6	360	3.65	791-28-6	Industrial chemical
Climbazole	293.1041	9.6	3.24	1.89	105	2.03	292.0979	[M+H] ⁺	-3.7	C15 H17 Cl N2 O2		61	73	N/A	3.3	38083-17-9	Personal care product
Pendimethalin	282.1439	10.8	0.00	43322	0.00	0.00	281.1376	[M+H] ⁺	-3.5	C13 H19 N3 O4		57.2	2	200	5.1	40487-42-1	Pesticide
Metalaxyl	280.1533	9.6	85.4	27.5	246	65.0	279.1471	[M+H] ⁺	-3.8	C15 H21 N O4		96.4	305	N/A	1.7	57837-19-1	Pesticide
Buprofezin	306.1621	10.6	4.90	3.57	7.09	12.3	305.1562	[M+H] ⁺	-4.4	C16 H23 N3 O S		96.5	20	N/A	4.1	69327-76-0	Pesticide
Pretilachlor	312.1711	10.5	52.5	3.30	306	1.42	311.1652	[M+H] ⁺	-4.7	C17 H26 Cl N O2		83.7	66	N/A	3.9	51218-49-6	Pesticide
Tebuconazole	308.1511	10.2	19.0	0.76	0.89	0.80	307.1451	[M+H] ⁺	-4.4	C16 H22 Cl N3 O		97.3	11	N/A	3.7	107534-96-3	Pesticide
Atrazine	216.1000	9.8	1157	0	18112	0	215.0938	[M+H] ⁺	-4.9	C8 H14 Cl N5		70.8	48	N/A	2.6	1912-24-9	Pesticide
Erucamide	338.3401	12.1	12398	28985	0	24226	337.3345	[M+H] ⁺	-5.0	C22 H43 N O		97.3	25	202.5	7.35	112-84-5	Industrial chemical
Oleamide	282.2781	11.1	0.00	17509	0	20379	281.2719	[M+H] ⁺	-4.0	C18 H35 N O		98	54	202.5	6.35	301-02-0	Industrial chemical
17beta-Trenbolone	271.1682	10.2	678	1899	908	3311	270.1620	[M+H] ⁺	-3.8	C18 H22 O2		74.9	164	N/A	3.9	10161-22-9	Pharmaceutical

Sulfadiazine	251.0588	7.5	3.04	31.1	217.2	6.85	250.0525	[M+H] ⁺	-3.8	C10 H10 N4 O2 S	
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2,4-Dichlorophenoxyacetic acid	218.9622	12.0	7.38	278	311	290	219.9694	[M-H]-1	0.1	C ₈ H ₆ Cl ₂ O ₃		91.4	41	N/A	2.8	94-75-7	Pesticide
Mefenamic acid	240.1031	13.0	3.48	1.94	63.0	230	241.1103	[M-H]-1	0.4	C ₁₅ H ₁₅ N O ₂		93	474	N/A	5	61-68-7	Pharmaceutical
Stearic acid	283.2642	11.9	0.90	3.41	267	138	284.2715	[M-H]-1	-0.1	C ₁₈ H ₃₆ O ₂		50	148	376	8.23	57-11-4	Personal care product
Lauryl sulfate	265.1478	11.5	10.4	6.57	435	212	266.1552	[M-H]-1	-0.5	C ₁₂ H ₂₆ O ₄ S		99.2	6	N/A	Not applicable	151-21-3	Industrial chemical
Dinoterb	239.0674	12.8	10.3	11.4	16.9	118	240.0746	[M-H]-1	0.2	C ₁₀ H ₁₂ N ₂ O ₅		64.2	70	N/A	4.5	1420-07-1	Pesticide
2,4-Dinitrophenol	183.0047	13.7	96.6	1.47	1.51	96.0	184.0120	[M-H]-1	-0.3	C ₆ H ₄ N ₂ O ₅		35.5	24	290	1.65	51-28-5	Pesticide
Bentazone	239.0498	11.7	148	4.94	2.99	167	240.0569	[M-H]-1	0.8	C ₁₀ H ₁₂ N ₂ O ₃ S		88.6	72	N/A	0.77	25057-89-0	Pharmaceutical
4-Dodecylbenzenesulfonic acid	325.1839	13.5	0	18699	9623	25836 2	326.1916	[M-H]-1	-1.3	C ₁₈ H ₃₀ O ₃ S		99.4	19	N/A	6.25	27176-87-0	Industrial chemical

B.P. (°C) and log Kow collected from PubChem database; ChemSpider database; EPA, 2011; Li Xie et al., 2021

Table S6 List of compounds at confidence level 3 and their properties

Number	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral mass (Da)	Reference Ion	Mass error (ppm)	Chemical formula Chemspider	Product ion (m/z) matching	No. of proposed structures	B.P.(°C)	log Kow	CAS NO	Category
			CPR	PhR	PIR	UTR										
Hexa(methoxymethyl)melamine	391.2281	15.1	180.8	0.0	116.0	72.1	390.2227	[M+H] ⁺ 1	-4.8	C15 H30 N6 O6	177.0877, 253.1387	28	N/A	2	3089-11-0	Industrial chemical
Lopinavir	651.3518	9.5	13.9	41.0	13.4	15.5	628.3625	[M+Na] ⁺ 1	0.2	C37 H48 N4 O5	447.2640, 183.1130	10	N/A	5.1	192725-17-0	Pharmaceutical
Estradiol benzoate	377.2123	9.2	57.6	20.6	15.1	1045.8	376.2038	[M+H] ⁺ 1	3.1	C25 H28 O3	255.1746, 271.1694	45	N/A	5.7	50-50-0	Pharmaceutical
Methylprednisolone	375.2173	13.6	0.0	67.0	174.9	0.0	374.2093	[M+H] ⁺ 1	1.9	C22 H30 O5	357.206, 339.195	62	N/A	1.55	83-43-2	Pharmaceutical
Spirotetramat	374.1975	10.0	46.2	63.3	43.4	440.1	373.1889	[M+H] ⁺ 1	3.3	C21 H27 N O5	304.1905, 79.0211	48	N/A	3.6	203313-25-1	Pesticide
Quisalofop-ethyl	373.0955	2.9	0.0	2910.4	3210.0	1642.0	372.0877	[M+H] ⁺ 1	1.6	C19 H17 Cl N2 O4	299.06064, 91.05712	48	N/A	4.5	76578-14-8	Pesticide
Pyridaben	365.1466	10.6	0.0	10.6	10.7	0.0	364.1376	[M+H] ⁺ 1	4.6	C19 H25 Cl N2 O S	307.2709, 240.23117	39	N/A	6.3	96489-71-3	Pesticide
Nalmefene	340.1925	10.0	2137.6	21.1	82.7	20.2	339.1834	[M+H] ⁺ 1	5.0	C21 H25 N O3	340.20828, 204.13713	125	N/A	2.4	55096-26-9	Pharmaceutical
Mandestrobin	314.1737	10.4	14.3	16.4	16.8	455.5	313.1678	[M+H] ⁺ 1	-4.3	C19 H23 N O3	200.06921, 242.11644	4	N/A	3.4	173662-97-0	Pesticide
N-Methylidodecylamine	312.3611	14.6	84.1	30.3	0.0	78.6	311.3552	[M+H] ⁺ 1	-4.5	C21 H45 N	312.36124, 60.08089	6	210	6.5	20630-75-5	Pharmaceutical
Dipentyl phthalate	307.1890	9.8	10703.1	13493.5	4305.4	8222.9	306.1831	[M+H] ⁺ 1	-4.7	C18 H26 O4	145.10030, 119.08504	137	338	5.75	131-18-0	Industrial chemical
Tetra(methoxymethyl)melamine (TMMM)	303.1763	8.8	456.1	54.8	128.0	1243.3	302.1703	[M+H] ⁺ 1	-4.1	C11 H22 N6 O4	165.08725, 147.07936	15	N/A	1	4124-78-1	Industrial chemical
Vortioxetine	299.1581	7.8	31.1	95.0	44.9	52.9	298.1504	[M+H] ⁺ 1	1.4	C18 H22 N2 S	283.02939, 268.99603	27	N/A	3.25	508233-74-7	Natural product
Isoprothiolane	291.0708	10.0	2025.2	28.0	186.2	13.5	290.0647	[M+H] ⁺ 1	-4.3	C12 H18 O4 S2	188.96626, 144.97681	8	N/A	2.5	31088-93-4	Pesticide
N,N-Bis(2-hydroxyethyl)dodecanamide	288.2522	9.8	32589.9	16.8	21358.6	33.7	287.2460	[M+H] ⁺ 1	-4.1	C16 H33 N O3	227.19928, 106.08596	21	N/A	N/A	120-40-1	Personal care product
Vulgarin	265.1425	17.3	10.9	33.1	10.7	27.9	264.1362	[M+H] ⁺ 1	-3.7	C15 H20 O4	194.94771, 176.93719	405	N/A	N/A	1773016	Pharmaceutical
Galaxolide	259.2048	11.0	161.3	109.8	445.1	233.2	258.1984	[M+H] ⁺ 1	-3.2	C18 H26 O	185.02849, 175.11078	109	143	5.6	1222-05-5	Personal care product
1-Tetradecanamine	258.2784	9.9	51.3	16.8	0.0	0.0	257.2719	[M+H] ⁺ 1	-3.1	C16 H35 N O	85.10096, 57.07006	18	268	6.2	112-72-1	Industrial chemical
N-(2-hydroxypropyl)dodecanamide dimethachlor	258.2420	10.6	75.5	20.1	18.4	19.6	257.2355	[M+H] ⁺ 1	-3.1	C15 H31 N O2	198.22054, 57.07006	50	N/A	N/A	4292-10-8	Industrial chemical
	256.1088	10.1	66.0	20.0	337.1	22.0	255.1026	[M+H] ⁺ 1	-4.3	C13 H18 Cl N O2	148.11111, 133.08786	128	N/A	2.55	50563-36-5	Pharmaceutical
Lamotrigine	256.0142	0.7	83.5	92.0	72.2	79.9	255.0079	[M+H] ⁺ 1	-3.5	C9 H7 Cl2 N5	218.98257, 190.98746	25	N/A	0.85	84057-84-1	Pharmaceutical
Alibendol	252.1220	9.5	88.4	19.1	36.2	849.1	251.1158	[M+H] ⁺ 1	-4.0	C13 H17 N O4	206.11656, 192.10063	393	N/A	N/A	73504-20-8	Pharmaceutical
Matrine	249.1968	9.6	16.6	20.1	14.9	17.8	248.1889	[M+H] ⁺ 1	2.7	C15 H24 N2 O	231.18623, 161.10789	162	N/A	0	519-02-8	Pharmaceutical
Reynosin	249.1475	19.8	96.8	205.7	87.1	181.0	248.1412	[M+H] ⁺ 1	-4.1	C15 H20 O3	207.05280, 163.02669	512	N/A	N/A	56834-45-8	Natural product

Number	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral mass (Da)	Reference Ion	Mass error (ppm)	Chemical formula Chemspider	Product ion (m/z) matching	No. of proposed structures	B.P.(°C)	log Kow	CAS NO	Category
			CPR	PhR	PIR	UTR										
Diallyl Phthalate	247.0956	9.5	1198.3	1406.4	503.2	2409.6	246.0892	[M+H] ⁺ 1	-3.8	C14 H14 O4	131.0848, 105.06961	269	290	2.5	131-17-9	Industrial chemical
Allylescaline	238.1427	0.8	57.2	112.1	69.6	962.2	237.1365	[M+H] ⁺ 1	-4.8	C13 H19 N O3	163.08549, 91.05713	321	N/A	N/A	16840-08-7	Pharmaceutical
Buturon	237.0781	12.3	3878.3	8182.4	0.0	4537.4	236.0716	[M+H] ⁺ 1	-3.4	C12 H13 Cl N2 O	223.06244, 91.05708	97	N/A	2.6	3766-06-1	Pesticide
Pterodin G	235.1319	9.3	11329.9	17140.3	4239.4	16015.6	234.1256	[M+H] ⁺ 1	-4.3	C14 H18 O3	119.08506, 105.06960	518	N/A	N/A	31835-23-1	Natural product
N,N-Dimethyldodecylamine-N-oxide	230.2468	9.7	356.6	198.2	148.3	0.0	229.2406	[M+H] ⁺ 1	-4.4	C14 H31 N O	83.08527, 57.07006	23	N/A	2.5	1643-20-5	Industrial chemical
Formetanate	222.1229	16.2	220.5	382.4	210.9	110.8	221.1164	[M+H] ⁺ 1	-3.6	C11 H15 N3 O2	194.09196, 180.07628	239	N/A	1.6	22259-30-9	Pesticide
2,3,4,9-Tetrahydro-6-methoxy-1H-pyrido(3,4-b)indol-1-one	217.0972	9.7	245.1	107.2	2292.9	16.6	216.0899	[M+H] ⁺ 1	0.0	C12 H12 N2 O2	158.05904, 130.06444	594	N/A	N/A	105051-22-3	Pharmaceutical
Ethyl butylacetylaminopropionate	216.1584	9.4	527.1	1274.1	171.7	1132.0	215.1521	[M+H] ⁺ 1	-4.8	C11 H21 N O3	188.10579, 160.07483	174	N/A	N/A	52304-43-5	Personal care product
3,4-Dimethoxycinnamic acid	209.0798	9.0	1380.3	583.9	578.7	2079.1	208.0736	[M+H] ⁺ 1	-4.8	C11 H12 O4	127.12236, 91.05399	2	N/A	2	2316-09-8	Food additive
Aspirin	181.0488	15.9	0.0	0.0	0.0	518.5	180.0423	[M+H] ⁺ 1	-4.0	C9 H8 O4	102.96997, 84.95947	175	140	1.3	50-78-2	Pharmaceutical
Hydroxycinnamic acid	165.0538	7.6	33.5	49.1	26.2	47.2	164.0473	[M+H] ⁺ 1	-4.7	C9 H8 O3	137.02853, 105.00304	207	N/A	2	14755-02-3	Pharmaceutical
Nicotine	163.1237	9.3	15.4	19.4	13.1	16.9	162.1157	[M+H] ⁺ 1	4.7	C10 H14 N2	105.03323, 95.04897	4	247	1.17	54-11-5	Pharmaceutical
Meglutol	163.0595	8.9	0.0	0.0	0.0	102.1	162.0528	[M+H] ⁺ 1	-4.0	C6 H10 O5	115.05383, 91.05405	120	N/A	N/A	322-79-2	Pharmaceutical
3,4-Dihydrocoumarin	149.0596	17.0	81.7	188.0	0.0	0.0	148.0524	[M+H] ⁺ 1	-0.6	C9 H8 O2	84.95952, 70.98031	168	261	1.55	119-84-6	Food additive
Glycidyl methacrylate	143.0695	7.9	612.1	0.0	0.0	163.7	142.0630	[M+H] ⁺ 1	-4.7	C7 H10 O3	69.03339, 55.05424	381	189	0.8	106-91-2	Industrial chemical
N-Nitrosodipropylamine	131.1172	7.9	21.7	192.8	25.9	220.4	130.1106	[M+H] ⁺ 1	-4.9	C6 H14 N2 O	98.98386, 72.04423	167	206	1.4	621-64-7	Industrial chemical
Melamine	127.0721	0.8	186.1	133.6	108.7	314.0	126.0654	[M+H] ⁺ 1	-4.7	C3 H6 N6	85.0510, 68.0244	6	350	-0.75	108-78-1	Industrial chemical
3-Methylcatechol	125.0591	8.3	1412.9	817.3	3236.7	1723.2	124.0524	[M+H] ⁺ 1	-4.8	C7 H8 O2	108.0210, 123.0440	157	243	1.65	503-86-6	Natural product
Indoline	120.0803	2.8	14.9	64.0	15.8	137.0	119.0735	[M+H] ⁺ 1	-4.1	C8 H9 N	103.0595, 91.5399	65	221	2	496-15-1	Pharmaceutical
N-Nitrosodiethylamine	103.0863	13.9	69.5	39.5	67.4	143.0	102.0793	[M+H] ⁺ 1	-3.0	C4 H10 N2 O	75.091, 103.0862	61	177	0.5	55-18-5	Industrial chemical
N-Nitrosopyrrolidine	101.0707	0.8	35.0	14.0	60.0	11.1	100.0637	[M+H] ⁺ 1	-2.5	C4 H8 N2 O	70.0651, 55.0542	77	214	0.25	930-55-2	Industrial chemical
1-Methyl-2-pyrrolidone	100.0754	9.4	0.0	0.0	0.0	4570.0	99.0684	[M+H] ⁺ 1	-3.3	C5 H9 N O	69.03291, 58.02891	132	202	-0.6	872-50-4	Industrial chemical
Cyclohexanone	99.0802	5.1	0.0	0.0	10847.9	10739.8	98.0732	[M+H] ⁺ 1	-2.8	C6 H10 O	70.0651, 55.0542	242	156	0.9	108-94-1	Pesticide
N,N-Dimethylacetamide	88.0754	6.8	20322.4	10461.5	12509.7	11012.2	87.0684	[M+H] ⁺ 1	-2.9	C4 H9 N O	58.0281, 43.0184	90	166	-0.7	127-19-5	Industrial chemical
Pyridine	80.0493	15.6	60.3	113.2	81.5	56.1	79.0422	[M+H] ⁺ 1	-2.8	C5 H5 N	53.0416, 52.0338	11	115	0.65	110-86-1	Natural product
N-Nitrosodimethylamine	75.0551	1.9	847.9	919.0	1262.6	1089.2	74.0480	[M+H] ⁺ 1	-2.2	C2 H6 N2 O	58.0281, 75.0551	14	153	-0.35	62-75-9	Industrial chemical

Number	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral mass (Da)	Reference Ion	Mass error (ppm)	Chemical formula Chemspider	Product ion (m/z) matching	No. of proposed structures	B.P.(°C)	log Kow	CAS NO	Category
			CPR	PhR	PIR	UTR										
Dimethylformamide	74.0599	4.1	9487.7	11353.1	0.0	0.0	73.0528	[M+H] ⁺ 1	-2.6	C3 H7 N O	59.0604, 74.05985	29	153	-0.9	68-12-2	Pesticide
Isobutyraldehyde	73.0646	5.8	0.0	10955.9	10828.5	13560.2	72.0575	[M+H] ⁺ 1	-2.4	C4 H8 O	57.0332, 73.06462	36	64	0.7	78-84-2	Industrial chemical
Acrylamide	72.0442	7.8	0.0	169.4	0.0	791.7	71.0371	[M+H] ⁺ 1	-2.2	C3 H5 N O	55.0297, 72.04424	29	125	-0.7	79-06-1	Industrial chemical
Acetone	59.0493	2.1	21049.2	24746.7	28751.0	43086.1	58.0419	[M+H] ⁺ 1	2.3	C3 H6 O	59.04927*	19	56	-0.24	67-64-1	Industrial chemical
4-(2,5-Diethoxy-4-nitrophenyl)morpholine	297.1434	0.9	9.4	45.8	18.3	36.6	296.1372	[M+H] ⁺ 1	-3.5	C14 H20 N2 O5	283.02933, 268.99814	63	N/A	N/A	5220-41-7	Natural product
Diethanolamine	106.0860	5.4	38.1	50.7	50.7	84.6	105.0790	[M+H] ⁺ 1	-2.3	C4 H11 N O2	72.99792, 56.04966	34	270	-1.45	111-42-2	Personal care product
Tert-Butyl Hydroperoxide	91.0751	1.8	676.8	543.1	511.2	512.8	90.0681	[M+H] ⁺ 1	-2.2	C4 H10 O2	73.0650, 53.00252	34	111	0.6	75-91-2	Industrial chemical
Paconol	165.0558	10.7	333.7	295.5	153.1	107.1	166.0630	[M-H] ⁻ 1	1.0	C9 H10 O3	149.0603, 121.0666	421	N/A	1.65	103-93-5	Pharmaceutical
(4-Chloro-2-methylphenoxy)acetic acid (MCPA)	199.0168	11.3	0.5	3.5	2.3	12.0	200.0240	[M-H] ⁻ 1	0.5	C9 H9 Cl O3	155.0268, 141.0113	144	N/A	2.65	94-74-6	Pesticide
Saccharin	181.9919	2.7	8.5	1.1	17.9	2825.0	182.9990	[M-H] ⁻ 1	0.7	C7 H5 N O3 S	139.0241, 121.0135	14	229	-0.85	81-07-2	Food additive
Sebacic acid	201.1134	13.6	311.9	0.0	0.0	0.0	202.1205	[M-H] ⁻ 1	0.7	C10 H18 O4	157.1330, 139.1224	269	343	1.6	111-20-6	Pharmaceutical
Benzothiazole-2-sulfonic acid	213.9640	10.3	1479.3	239.6	232.6	2636.1	214.9711	[M-H] ⁻ 1	0.8	C7 H5 N O3 S2	134.00700, 57.97505	6	N/A	N/A	87-03-6	Industrial chemical
Dibutyl phthalate	277.1445	13.0	2301.0	2595.1	2749.1	2085.8	278.1518	[M-H] ⁻ 1	-0.1	C16 H22 O4	149.0234, 121.0285	248	340	4.6	84-74-2	Industrial chemical
2-(4-Nonylphenoxy)Acetic Acid	277.1809	13.2	599.1	16.0	237.0	906.0	278.1882	[M-H] ⁻ 1	0.0	C17 H26 O3	219.1749, 112.9889	158	N/A	5.5	3115-49-9	Industrial chemical
Linoleic acid	279.2329	13.7	10.4	155.5	96.9	23.9	280.2402	[M-H] ⁻ 1	-0.2	C18 H32 O2	261.2218, 245.2269	192	230	6.25	60-33-3	Natural product
Triclosan	286.9440	13.0	6.3	51.5	276.8	36.1	287.9512	[M-H] ⁻ 1	0.2	C12 H7 Cl3 O2	183.17546, 80.91653	14	N/A	4.85	3380-34-5	Pharmaceutical
Coriolic acid	295.2278	13.1	20.1	443.8	191.5	92.6	296.2351	[M-H] ⁻ 1	-0.1	C18 H32 O3	295.13675, 57.03394	122	N/A	N/A	17290-79-8	Industrial chemical
Imazaquin	310.1201	11.8	5.7	20.4	15.0	342.8	311.1270	[M-H] ⁻ 1	1.1	C17 H17 N3 O3	217.01302, 183.01196	2	N/A	0.1	81335-37-7	Pesticide
Sucralose	395.0075	8.4	0.9	0.0	435.5	0.0	396.0146	[M-H] ⁻ 1	0.8	C12 H19 Cl3 O8	383.19266, 361.0385	3	N/A	-0.5	56038-13-2	Food additive
Benzoic acid	121.0296	12.7	881.3	271.9	309.7	0.0	122.0368	[M-H] ⁻ 1	0.5	C7 H6 O2	108.02184, 95.0183	45	249.2	1.87	65-85-0	Food additive
Monobutyl Phthalate (MBP)	221.0819	14.2	422.4	0.0	0.0	17.5	222.0892	[M-H] ⁻ 1	0.1	C12 H14 O4	149.0971, 121.0290	635	N/A	2	131-70-4	Industrial chemical

B.P. (°C), log Kow and Product ion (m/z) matching collected from PubChem database; ChemSpider database; EPA, 2011; Li Xie et al., 2021; Pandey et al. 2024

Table S7 List of compounds at confidence level 4-5 and their properties

Name	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral (Da)	Reference Ion	Mass error (ppm)	B.P.(°C)	log Kow	CAS NO	Chemical formula	Category
			CPR	PhR	PIR	UTR								
Pantethine	555.2530	9.6	16.6	20.3	33.4	14.5	554.2444	[M+H] ⁺ 1	2.3	987.2	-0.06	303-05-9	C22 H42 N4 O8 S2	Pharmaceutical
Telmisartan	515.2436	9.1	9.3	15.5	7.9	9.9	514.2369	[M+H] ⁺ 1	-1.14	771.9	8.42	144701-48-4	C33 H30 N4 O2	Pharmaceutical
Acetildenafil	467.2759	10.1	65.0	93.6	41.7	75.2	466.2692	[M+H] ⁺ 1	-1.31	760	N/A	831217-01-7	C25 H34 N6 O3	Pharmaceutical
UV Absorber 234	448.2379	9.8	2202.1	1251.2	701.2	531.5	447.2311	[M+H] ⁺ 1	-0.9	589.3	6.78	70321-86-7	C30 H29 N3 O	Industrial chemical
Irbesartan	429.2377	12.0	0.0	0.0	0.0	350.2	428.2325	[M+H] ⁺ 1	-4.87	648.6	5.31	138402-11-6	C25 H28 N6 O	Pharmaceutical
Cholic acid	409.2941	10.8	0.0	0.0	18.2	77.2	408.2876	[M+H] ⁺ 1	-1.89	583.9	2.02	81-25-4	C24 H40 O5	Natural product
Azoxystrobin	404.1258	7.3	0.0	63.0	0.0	0.0	403.1168	[M+H] ⁺ 1	4.11	581.3	2.5	131860-33-8	C22 H17 N3 O5	Pesticide
Dexamethasone	393.2070	9.3	17.7	963.8	20.7	94.0	392.1999	[M+H] ⁺ 1	-0.42	568.2	1.83	50-02-2	C22 H29 F O5	Pharmaceutical
Bis-(2-ethylhexyl) phthalate	391.2829	10.2	82.9	94.5	157.8	208.9	390.2770	[M+H] ⁺ 1	-3.62	385	7.5	117-81-7	C24 H38 O4	Industrial chemical
Pregnenolone acetate	359.2571	10.4	354.8	84.8	15.9	114.7	358.2508	[M+H] ⁺ 1	-2.82	457.3	4.3	1778-02-5	C23 H34 O3	Pharmaceutical
BISPHENOL A (2 3-DIHYDROXYPROPYL) GLYCID	359.1836	18.8	6.2	90.5	5.7	6.3	358.1780	[M+H] ⁺ 1	-4.82	460	3.4	76002-91-0	C21 H26 O5	Industrial chemical
Dicyclohexyl phthalate	331.1888	18.8	17.7	219.4	6.1	6.8	330.1831	[M+H] ⁺ 1	-4.83	451.8	4.82	84-61-7	C20 H26 O4	Industrial chemical
Flutolanil	324.1193	9.9	10.5	12.4	10.7	10.1	323.1133	[M+H] ⁺ 1	-3.95	420	3.5	66332-96-5	C17 H16 F3 N O2	Pesticide
Chlorpromazine	319.1044	0.9	0.0	10.4	94.1	9.6	318.0958	[M+H] ⁺ 1	3.98	400	5.3	50-53-3	C17 H19 Cl N2 S	Pharmaceutical
Brompheniramine	319.0798	8.8	12.6	45.7	12.1	28.3	318.0732	[M+H] ⁺ 1	-2.12	380	3.5	86-22-6	C16 H19 Br N2	Pharmaceutical
Traversianal	317.2100	9.6	191.6	243.4	129.4	260.7	316.2038	[M+H] ⁺ 1	-3.53	458.9	N/A	108605-66-9	C20 H28 O3	Pesticide
Progesterone	315.2309	10.2	48.5	69.1	22.9	90.1	314.2246	[M+H] ⁺ 1	-3.11	537.7	3.87	57-83-0	C21 H30 O2	Pharmaceutical
L-Glutamic acid	313.0694	9.7	11.4	35.3	13.1	23.7	312.0634	[M+H] ⁺ 1	-4.22	215	-3.22	56-86-0	C17 H12 O6	Food additive
Sclareol	309.2776	10.4	13.6	46.2	13.4	22.7	308.2715	[M+H] ⁺ 1	-4.06	218–220 (at 19 mmHg)	N/A	515-03-7	C20 H36 O2	Natural product
Betaxolol	308.2207	9.1	31.2	51.4	51.8	28.2	307.2147	[M+H] ⁺ 1	-4.17	448 (at 760 mmHg)	2.78	63659-18-7	C18 H29 N O3	Pharmaceutical
Tolnaftate	308.1112	8.3	35.6	166.1	18.1	31.0	307.1031	[M+H] ⁺ 1	2.63	437.6	5.3	2398-96-1	C19 H17 N O S	Pesticide

Name	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral (Da)	Reference Ion	Mass error (ppm)	B.P.(°C)	log Kow	CAS NO	Chemical formula	Category
			CPR	PhR	PIR	UTR								
cis-3-(2,5-Dimethylphenyl)-4-hydroxy-8-methoxy-1-azaspiro[4.5]decan-2-one	304.1894	9.2	37.8	21.3	15.3	31.2	303.1834	[M+H] ⁺ 1	-4.28	521.4 (at 760 mmHg)	3.31	203312-38-3	C18 H25 N O3	Pesticide
11-Keto-testosterone	303.1941	9.3	212.6	309.6	109.6	225.7	302.1882	[M+H] ⁺ 1	-4.5	476.8	3.61	564-35-2	C19 H26 O3	Natural product
Phenmedipham	301.1185	9.6	16.2	21.4	14.8	18.2	300.1110	[M+H] ⁺ 1	0.69	81.6	N/A	13684-63-4	C16 H16 N2 O4	Pesticide
Quinalphos	299.0611	8.7	12.0	42.6	30.0	13.6	298.0541	[M+H] ⁺ 1	-0.88	142	4.4	13593-03-8	C12 H15 N2 O3 P S	Pesticide
Cryptotanshinone	297.1471	9.7	288.4	62.5	26.1	133.5	296.1412	[M+H] ⁺ 1	-4.8	459 ± 45 (at 760 mmHg)	4.4	35825-57-1	C19 H20 O3	Natural product
Tanshinone II	295.1316	9.5	10.7	14.9	10.3	44.6	294.1256	[M+H] ⁺ 1	-4.22	480.7 (at 760 mmHg)	4.4	568-72-9	C19 H18 O3	Natural product
Tutin	295.1164	18.8	9.4	77.3	0.0	9.4	294.1103	[M+H] ⁺ 1	-3.97	356.07	-0.36	2571-22-4	C15 H18 O6	Natural product
Paclitaxel	294.1353	9.9	46.1	14.6	12.8	12.2	293.1295	[M+H] ⁺ 1	-4.98	460.9 ± 55.0	3.2	76738-62-0	C15 H20 Cl N3 O	Pesticide
BENZYL-DIPHENYLPHOSPHINE OXIDE	293.1100	7.7	16.3	118.5	18.2	34.1	292.1017	[M+H] ⁺ 1	3.48	399	N/A	2959-74-2	C19 H17 O P	Industrial chemical
2-(2-Ethoxyethoxy)ethanol	291.1790	0.5	11.4	16.9	21.4	45.6	134.0943	[2M+Na] ⁺ 1	0.7	196–202	-0.54	111-90-0	C6 H14 O3	Personal care product
Androstenedione	287.1995	9.3	35.3	52.5	20.2	54.8	286.1933	[M+H] ⁺ 1	-3.67	431.4	2.75	63-05-8	C19 H26 O2	Pharmaceutical
Metominostrobin	285.1241	10.0	14.7	18.2	14.1	14.4	284.1161	[M+H] ⁺ 1	2.57	N/A	N/A	133408-50-1	C16 H16 N2 O3	Pesticide
Bis(2-methoxyethyl) phthalate	283.1165	8.7	3432.6	1823.5	932.7	3582.5	282.1103	[M+H] ⁺ 1	-3.74	340	2.9	117-82-8	C14 H18 O6	Industrial chemical
Cycloheximide	282.1691	0.8	14.4	63.1	256.5	779.6	281.1627	[M+H] ⁺ 1	-3.37	N/A	N/A	66-81-9	C15 H23 N O4	Pharmaceutical
L-Aspartyl-L-Phenylalanine	281.1120	8.0	106.4	253.4	34.3	68.9	280.1059	[M+H] ⁺ 1	-4.21	528.4 ± 60.0	1.79	13433-09-5	C13 H16 N2 O5	Food additive
Metolachlor OA	280.1532	7.6	63.8	68.5	15.1	63.9	279.1471	[M+H] ⁺ 1	-3.98	100	N/A	152019-73-3	C15 H21 N O4	Pesticide
Shogaol	277.1787	18.6	0.0	134.8	0.0	0.0	276.1725	[M+H] ⁺ 1	-4.01	427.5	N/A	23513-13-5	C17 H24 O3	Natural product
Dihydromethysticin	277.1061	9.2	82.8	88.2	62.9	95.2	276.0998	[M+H] ⁺ 1	-3.5	476.1	N/A	19902-91-1	C15 H16 O5	Pharmaceutical
Nandrolone	275.1996	9.6	120.7	205.0	148.2	163.3	274.1933	[M+H] ⁺ 1	-3.35	~357.4 (estimated)	~3.00	434-22-0	C18 H26 O2	Pharmaceutical
Nitenpyram	271.0952	9.4	98.5	26.1	32.1	89.1	270.0884	[M+H] ⁺ 1	-1.5	N/A	N/A	150824-47-8	C11 H15 Cl N4 O2	Pesticide
Metoprolol	268.1896	9.8	114.2	201.2	0.0	103.2	267.1834	[M+H] ⁺ 1	-3.78	398.6 (at 760 mmHg)	1.79	37350-58-6	C15 H25 N O3	Pharmaceutical
Tributyl phosphate	267.1733	10.5	0.0	12.6	18.9	26.7	266.1647	[M+H] ⁺ 1	4.93	289	N/A	126-73-8	C12 H27 O4 P	Industrial chemical
Albendazole	266.0950	9.8	12.4	15.2	36.9	12.9	265.0885	[M+H] ⁺ 1	-3.01	N/A	N/A	54965-21-8	C12 H15 N3 O2 S	Pharmaceutical

Name	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral (Da)	Reference Ion	Mass error (ppm)	B.P.(°C)	log Kow	CAS NO	Chemical formula	Category
			CPR	PhR	PIR	UTR								
Phebalosin	259.0956	9.9	81.3	22.9	116.5	45.2	258.0892	[M+H] ⁺ 1	-3.33	418.8	N/A	6545-99-9	C15 H14 O4	Pharmaceutical
dextrophan	258.1846	8.3	14.8	151.9	149.0	37.0	257.1780	[M+H] ⁺ 1	-2.44	229–232	2.9	125-71-3	C17 H23 N O	Pharmaceutical
1-(2,4-Dichlorophenyl)-2-(1,2,4-triazol-1-yl)ethanol	258.0187	9.4	386.5	20.3	13.4	16.1	257.0123	[M+H] ⁺ 1	-3.18	N/A	2.1	79017-06-0	C10 H9 Cl2 N3 O	Pesticide
Pterostilbene	257.1164	9.4	98.8	84.4	26.8	364.2	256.1099	[M+H] ⁺ 1	-3.3	~420	3.6	537-42-8	C16 H16 O3	Natural product
Diphenyl phosphate	251.0476	8.8	13.4	45.5	11.3	48.7	250.0395	[M+H] ⁺ 1	3.24	280	4.1	115-86-6	C12 H11 O4 P	Industrial chemical
3-(4-hydroxy-5-oxo-3-phenyl-2H-furan-2-yl)propanoic acid	249.0749	8.4	128.8	202.4	100.1	128.9	248.0685	[M+H] ⁺ 1	-3.6	N/A	N/A	105364-56-5	C13 H12 O5	Pharmaceutical
Suberosin	245.1163	9.6	987.1	1000.1	506.8	1227.9	244.1099	[M+H] ⁺ 1	-3.76	393.3	N/A	18942-62-0	C15 H16 O3	Natural product
Eleutherol	245.0799	9.5	28.6	18.1	42.5	60.0	244.0736	[M+H] ⁺ 1	-3.99	N/A	N/A	574-84-5	C14 H12 O4	Pesticide
Cyanazine	241.0967	9.8	19.4	26.5	18.5	25.9	240.0890	[M+H] ⁺ 1	1.68	N/A	2.3	21725-46-2	C9 H13 Cl N6	Pesticide
Costunolide	233.1526	18.6	73.0	116.5	55.1	118.0	232.1463	[M+H] ⁺ 1	-4.53	N/A	2.6	553-21-9	C15 H20 O2	Pharmaceutical
osthenol	231.1007	9.2	1052.2	1002.6	430.7	1035.0	230.0943	[M+H] ⁺ 1	-3.88	N/A	N/A	481-46-9	C14 H14 O3	Natural product
Pteleine	230.0802	9.1	107.8	145.6	110.1	135.8	229.0739	[M+H] ⁺ 1	-4.35	N/A	N/A	477-90-7	C13 H11 N O3	Natural product
Bisphenol A	229.1214	9.7	598.7	1036.7	238.1	1383.7	228.1150	[M+H] ⁺ 1	-4.12	220–250	3.3	80-05-7	C15 H16 O2	Industrial chemical
cis-Resveratrol	229.0851	9.2	160.9	90.5	19.4	183.3	228.0786	[M+H] ⁺ 1	-3.75	N/A	3.1	501-36-0	C14 H12 O3	Natural product
Dicyclohexylurea	225.1950	19.0	5.2	24.0	24.5	22.8	224.1889	[M+H] ⁺ 1	-4.91	N/A	4.2	101-83-7	C13 H24 N2 O	Industrial chemical
Bufexamac	224.1270	3.7	20.3	37.3	0.0	6.1	223.1208	[M+H] ⁺ 1	-4.98	N/A	3.1	2438-72-4	C12 H17 N O3	Pharmaceutical
Mexacarbate	223.1430	7.6	259.9	57.6	29.0	159.3	222.1368	[M+H] ⁺ 1	-4.82	N/A	2.7	315-18-4	C12 H18 N2 O2	Pesticide
Carbofuran	222.1114	18.7	7.4	232.9	127.6	145.1	221.1052	[M+H] ⁺ 1	-4.85	170–172	2.3	1563-66-2	C12 H15 N O3	Pesticide
Pterosin B	219.1369	7.9	10.8	6131.8	18.6	288.9	218.1307	[M+H] ⁺ 1	-4.94	N/A	N/A	10440-05-4	C14 H18 O2	Natural product
Pyracarbolid	218.1165	9.0	231.6	105.3	126.6	299.8	217.1103	[M+H] ⁺ 1	-4.75	N/A	N/A	34622-58-7	C13 H15 N O2	Pesticide
Imidacloprid urea	212.0588	7.3	84.4	46.6	10.7	15.3	211.0512	[M+H] ⁺ 1	1.22	N/A	N/A	155584-75-7	C9 H10 Cl N3 O	Pesticide
Desnitro-imidacloprid	211.0741	9.6	79.3	122.0	30.5	83.3	210.0672	[M+H] ⁺ 1	-1.71	N/A	N/A	135410-20-7	C9 H11 Cl N4	Pesticide
Dexibuprofen	207.1370	9.9	435.6	700.0	271.7	657.2	206.1307	[M+H] ⁺ 1	-4.56	157–158	3.5	51146-56-6	C13 H18 O2	Pharmaceutical

Name	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral (Da)	Reference Ion	Mass error (ppm)	B.P.(°C)	log Kow	CAS NO	Chemical formula	Category
			CPR	PhR	PIR	UTR								
5,7-Dimethoxycoumarin	207.0642	0.5	0.0	6.4	4.6	3.9	206.0579	[M+H] ⁺ 1	-4.73	N/A	N/A	531-59-9	C11 H10 O4	Pharmaceutical
Monuron	199.0635	7.0	4.8	9.3	5.1	12.4	198.0560	[M+H] ⁺ 1	1.13	180-182	2.1	150-68-5	C9 H11 Cl N2 O	Pesticide
7-Methoxy-4-methylcoumarin	191.0693	8.4	146.4	168.5	17.3	50.3	190.0630	[M+H] ⁺ 1	-4.94	N/A	N/A	121-33-5	C11 H10 O3	Natural product
Benzo[g]quinoline	180.0799	6.7	22.3	565.1	225.4	417.0	179.0735	[M+H] ⁺ 1	-4.76	N/A	N/A	85-02-9	C13 H9 N	Industrial chemical
5-Phenylvaleric acid	179.1059	11.9	0.0	146.7	0.0	0.0	178.0994	[M+H] ⁺ 1	-4.21	N/A	N/A	45508	C11 H14 O2	Natural product
Deisopropylatrazine	174.0538	8.1	23.3	126.1	18.9	120.3	173.0468	[M+H] ⁺ 1	-1.51	N/A	N/A	6190-65-4	C5 H8 Cl N5	Pesticide
Propenoic acid 2-(dimethylamino)ethyl ester	144.1010	8.9	18.6	53.5	17.8	34.3	143.0946	[M+H] ⁺ 1	-4.42	N/A	N/A	105-63-5	C7 H13 N O2	Industrial chemical
Butyl acrylate	129.0904	14.2	0.0	170.9	0.0	0.0	128.0837	[M+H] ⁺ 1	-4.82	145	2.3	141-32-2	C7 H12 O2	Industrial chemical
Naphthalene	129.0693	9.5	35.9	56.6	22.0	87.8	128.0626	[M+H] ⁺ 1	-4.84	218	3.3	91-20-3	C10 H8	Industrial chemical
Nitrobenzene	124.0388	5.6	0.0	0.0	1192.3	0.0	123.0320	[M+H] ⁺ 1	-4.49	210.9	1.85	98-95-3	C6 H5 N O2	Industrial chemical
2-Isobutoxyethanol	119.1062	3.7	13.3	8.6	0.0	0.0	118.0994	[M+H] ⁺ 1	-2.5	N/A	N/A	14634-35-6	C6 H14 O2	Industrial chemical
2-Hydroxyethyl acrylate	117.0542	7.7	0.0	197.3	0.0	97.2	116.0473	[M+H] ⁺ 1	-3.76	213	0.47	818-61-1	C5 H8 O3	Industrial chemical
2-Aminophenol	110.0598	8.5	1456.6	0.0	791.4	1081.6	109.0528	[M+H] ⁺ 1	-2.67	174	0.62	95-55-6	C6 H7 N O	Industrial chemical
Ethyl acrylate	101.0595	5.6	0.0	2849.6	2095.1	3468.2	100.0524	[M+H] ⁺ 1	-2.55	99.4	1.2	140-88-5	C5 H8 O2	Industrial chemical
Methyl acrylate	87.0438	8.0	0.0	696.2	3659.1	732.8	86.0368	[M+H] ⁺ 1	-2.52	80	0.73	96-33-3	C4 H6 O2	Industrial chemical
Acetone Cyanohydrin	86.0598	2.1	110.7	130.1	0.0	151.6	85.0528	[M+H] ⁺ 1	-2.94	120	-0.2	75-86-5	C4 H7 N O	Industrial chemical
Cyclohexane	85.1010	20.1	12.8	5.5	34.4	18.0	84.0939	[M+H] ⁺ 1	0.05	80.7	3.4	110-82-7	C6 H12	Pesticide
1,3-Dioxolane	75.0439	8.6	0.0	70.1	0.0	39.4	74.0368	[M+H] ⁺ 1	-2.14	74	-0.37	646-06-0	C3 H6 O2	Pharmaceutical
Acrylic acid	73.0282	3.8	0.0	617.2	0.0	466.9	72.0211	[M+H] ⁺ 1	-2.46	141	0.35	79-10-7	C3 H4 O2	Industrial chemical
Isoprene	69.0698	20.1	270.8	439.8	968.5	397.3	68.0626	[M+H] ⁺ 1	-1.16	34	2.42	78-79-5	C5 H8	Industrial chemical
Ethanolamine	62.0601	1.3	12.7	0.0	0.0	0.0	61.0528	[M+H] ⁺ 1	1.13	170	-1.31	141-43-5	C2 H7 N O	Personal care product
1,3-Butadiene	55.0545	16.2	83.9	0.0	81.5	0.0	54.0470	[M+H] ⁺ 1	3.5	-4.4	1.99	106-99-0	C4 H6	Industrial chemical
Acesulfame	161.9867	2.1	1.1	49.8	45.6	98.0	162.9939	[M-H] ⁻ 1	0.45	N/A	-1.3	33665-90-6	C4 H5 N O4 S	Food additive

Name	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral (Da)	Reference Ion	Mass error (ppm)	B.P.(°C)	log Kow	CAS NO	Chemical formula	Category
			CPR	PhR	PIR	UTR								
Decanoic acid	171.1390	12.8	2.3	1.3	1.3	15.4	172.1463	[M-H]-1	-0.07	268	4.09	334-48-5	C10 H20 O2	Industrial chemical
Benzotrichloride	192.9384	12.5	2.9	16.4	2.8	28.1	193.9457	[M-H]-1	0.14	213	3.3	98-07-7	C7 H5 Cl3	Pesticide
dinotefuran	201.0995	9.4	2.5	2.4	50.9	2.8	202.1066	[M-H]-1	1.12	136	-0.55	165252-70-0	C7 H14 N4 O3	Pesticide
3,4-Dichlorophenylurea	202.9786	11.9	1.1	3.7	8.1	14.3	203.9857	[M-H]-1	0.53	N/A	N/A	101-20-2	C7 H6 Cl2 N2 O	Pesticide
Mecoprop	213.0326	9.8	1.1	0.6	1.5	1.8	214.0397	[M-H]-1	0.78	200	2.8	93-65-2	C10 H11 Cl O3	Pesticide
Clofibric acid	213.0327	9.4	1.7	1.7	154.9	2.0	214.0397	[M-H]-1	1.51	242	2.4	882-09-7	C10 H11 Cl O3	Pharmaceutical
N-Demethoxylinuron	216.9940	12.1	638.2	7.4	75.9	18.8	218.0014	[M-H]-1	-0.26	N/A	N/A	330-55-2	C8 H8 Cl2 N2 O	Pesticide
Genistein	269.0457	12.4	2.6	4.2	10.5	28.1	270.0528	[M-H]-1	0.43	482	2.9	446-72-0	C15 H10 O5	Natural product
Mianserin N-oxide	279.1506	13.0	14.5	3.9	5.1	29.4	280.1576	[M-H]-1	0.96	N/A	N/A	24219-97-4	C18 H20 N2 O	Pharmaceutical
Benomyl	289.1296	10.0	60.9	212.1	73.9	108.9	290.1379	[M-H]-1	-3.36	325	1.5	17804-35-2	C14 H18 N4 O3	Pesticide
Tetradecyl sulfate	293.1779	12.9	6.9	41.9	36.9	43.4	294.1865	[M-H]-1	-4.33	N/A	N/A	1191-50-0	C14 H30 O4 S	Industrial chemical
Ricinoleic acid	297.2435	11.2	3.8	28.3	495.0	178.1	298.2508	[M-H]-1	0.06	313	4	141-22-0	C18 H34 O3	Industrial chemical
Perfluorobutane sulfonic acid (PFBS)	298.9431	13.5	16.3	4.4	4.8	35.7	299.9503	[M-H]-1	0.41	N/A	N/A	375-73-5	C4 H F9 O3 S	Industrial chemical
sulisobenzene	307.0284	11.3	1.5	11.3	82.3	45.2	308.0355	[M-H]-1	0.59	360	2.3	4065-45-6	C14 H12 O6 S	Pharmaceutical
Triclocarban	312.9709	12.9	4.8	2.5	2.2	27.3	313.9781	[M-H]-1	0.26	250	4.9	101-20-2	C13 H9 Cl3 N2 O	Personal care product
Maltose	341.1076	9.8	2.3	0.7	3.0	6.4	342.1162	[M-H]-1	-3.83	N/A	-3.7	69-79-4	C12 H22 O11	Food additive
Fipronil-desulfinyl	386.9649	12.4	2.2	3.1	11.7	24.4	387.9717	[M-H]-1	1.26	N/A	N/A	205650-65-3	C12 H4 Cl2 F6 N4	Pesticide
Fipronil sulfide	418.9369	14.4	6.1	1.6	2.2	9.0	419.9438	[M-H]-1	0.96	N/A	N/A	120068-37-3	C12 H4 Cl2 F6 N4 S	Pesticide
Fipronil	434.9316	12.5	3.6	3.9	27.1	36.2	435.9387	[M-H]-1	0.43	200	4	120068-37-3	C12 H4 Cl2 F6 N4 O S	Pesticide
1-Palmitoylcephalin	452.2784	13.3	8.6	19.0	17.2	25.5	453.2855	[M-H]-1	0.38	N/A	N/A	65172-31-2	C21 H44 N O7 P	Pharmaceutical
Andrastin A	485.2543	14.5	766.5	43.5	39.9	140.5	486.2618	[M-H]-1	-0.36	N/A	N/A	1000385-21-2	C28 H38 O7	Natural product
Novaluron	491.0041	13.1	5.4	2.1	2.1	22.0	492.0123	[M-H]-1	-1.85	500	5.3	116714-46-6	C17 H9 Cl F8 N2 O4	Pesticide

Name	Precursor ion m/z	Mean RT (min)	Average peak intensity (10 ⁵)				Neutral (Da)	Reference Ion	Mass error (ppm)	B.P.(°C)	log Kow	CAS NO	Chemical formula	Category
			CPR	PhR	PIR	UTR								
Heptadecafluorooctanesulfonic Acid	498.9304	12.8	6.3	15.0	12.6	50.4	499.9375	[M-H]-1	0.41	N/A	4.49	1763-23-1	C ₈ H ₉ F ₁₇ O ₃ S	Industrial chemical
Methyl 2,4-Dihydroxy-3,6-Dimethylbenzoate	197.0799	8.8	235.8	52.9	229.3	378.8	196.0736	[M+H] ⁺ 1	-4.7	360.7	2.6	4707-47-5	C ₁₀ H ₁₂ O ₄	Personal care product
Monobenzyl Phthalate (MP)	255.0663	12.5	5.6	5.3	24.4	50.1	256.0736	[M-H]-1	0.1	359.5	1.06	2528-16-7	C ₁₅ H ₁₂ O ₄	Industrial chemical

B.P. (°C) and log Kow collected from PubChem database; ChemSpider database; EPA, 2011; Li Xie et al., 2021

Table S8 PNEC concentrations in each compound

No.	Category	Name	Category	Formula	PNEC concentration (µg/L)	Reference
1	Pharmaceutical	Bentazone	Pharmaceutical	C10 H12 N2 O3 S	270	7
2		Lidocaine	Pharmaceutical	C14 H22 N2 O	8.20	8
3		Primidone	Pharmaceutical	C12 H14 N2 O2	9.30	ECOTOX
4		Sulfadiazine	Pharmaceutical	C10 H10 N4 O2 S	1.35	9
5		Trimethoprim	Pharmaceutical	C14 H18 N4 O3	1.00	10
6		Mefenamic acid	Pharmaceutical	C15 H15 N O2	0.428	11
7		Ciprofloxacin	Pharmaceutical	C17 H18 F N3 O3	0.100	9
8		Venlafaxine	Pharmaceutical	C17 H27 N O2	0.092	9
9		17beta-Trenbolone	Pharmaceutical	C18 H22 O2	0.078	12
10		Spiroxamine	Pharmaceutical	C18 H35 N O2	0.020	7
11		Tramadol	Pharmaceutical	C16 H25 N O2	0.007	13
12		17beta-Estradiol	Pharmaceutical	C18 H24 O2	0.002	14
13	Pesticide	Metalaxyl	Pesticide	C15 H21 N O4	120	7
14		Pretilachlor	Pesticide	C17 H26 Cl N O2	32.0	6
15		Dinoterb	Pesticide	C10 H12 N2 O5	18.60	15
16		2,4-Dinitrophenol	Pesticide	C6 H4 N2 O5	4.00	ECOTOX
17		2,4-Dichlorophenoxyacetic acid	Pesticide	C8 H6 Cl2 O3	1.30	16
18		Tebuconazole	Pesticide	C16 H22 Cl N3 O	0.578	7
19		Acetamiprid	Pesticide	C10 H11 Cl N4	0.500	6
20		Diuron	Pesticide	C9 H10 Cl2 N2 O	0.320	ECOTOX
21		Terbuthylazine	Pesticide	C9 H16 Cl N5	0.224	17
22		Lenacil	Pesticide	C13 H18 N2 O2	0.170	17

23		Clomazone	Pesticide	C12 H14 Cl N O2	0.167	ECOTOX
24		Thiamethoxam	Pesticide	C8 H10 Cl N5 O3 S	0.140	7
25		Ametryn	Pesticide	C9 H17 N5 S	0.100	7
26		Hexazinone	Pesticide	C12 H20 N4 O2	0.048	7
27		Imidacloprid	Pesticide	C9 H10 Cl N5 O2	0.008	7
28		Buprofezin	Pesticide	C16 H23 N3 O S	0.003	ECOTOX
29		Triazophos	Pesticide	C12 H16 N3 O3 P S	0.003	18
30	Personal care product	Butylparaben	Personal care product	C11 H14 O3	20.1	19
31		Galaxolidone	Personal care product	C18 H24 O2	18.4	20
32		Stearic acid	Personal care product	C18 H36 O2	1.50	21
33		Propylparaben	Personal care product	C10 H12 O3	1.00	22
34	Industrial chemical	Lauryl sulfate	Industrial chemical	C12 H26 O4 S	137	ECOTOX
35		Terephthalic acid	Industrial chemical	C8 H6 O4	380	ECOTOX
36		Perfluorooctanoic acid (PFOA)	Industrial chemical	C8 H F15 O2	18.7	23
37		Benzyl butyl phthalate	Industrial chemical	C19 H20 O4	3.30	24
38		Phenolphthalein	Industrial chemical	C20 H14 O4	0.219	ECOTOX
39		Triphenylphosphine oxide	Industrial chemical	C18 H15 O P	0.012	25

ECOTOX is a website <https://cfpub.epa.gov/ecotox/> comprehensive ecotoxicology database maintained by the U.S. Environmental Protection Agency (EPA).

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