

Supporting Information

Chemical Isotope Labeling Exposome (CIL-EXPOSOME): One High-throughput Platform for Human Urinary Global Exposome Characterization

Platform for Human Urinary Global Exposome Characterization

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46 pages

8 tables

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Text S1. IsoMS Procedure ¹

IsoMS is a powerful platform to automate processing chemical isotope labeling LC-MS data by peak picking, peak pairing, peak-pair filtering, and peak-pair intensity ratio calculation. Briefly, convert the raw LC-MS data into a centroid peak list file; then use the IsoMS script to process all the files; finally, align the peak pairs and their ratios from the datasets generated to produce a final CSV file that can be exported for data and statistics analysis.

For more information please see the following website:

http://www.mycompoundid.org/mycompoundid_IsoMS/IsoMS.jsp

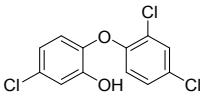
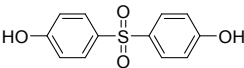
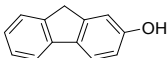
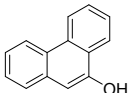
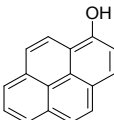
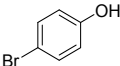
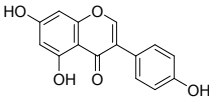
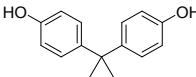
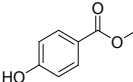
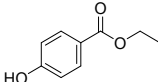
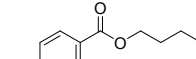
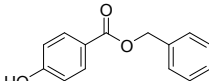
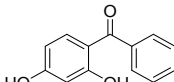
Text S2. Labelling Reaction Procedure

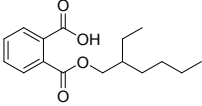
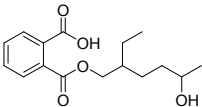
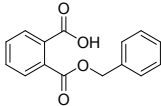
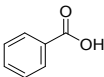
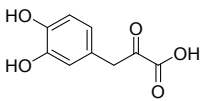
For dansylation reaction, 100 μ L of phenolic hydroxyl standard solutions or urine supernatants were mixed with an equal volume of sodium carbonate/sodium bicarbonate buffer (0.5 mol/L, pH 9.4). After vortex and spun down, mixed with 100 μ L of freshly prepared ^{12}C -dansyl chloride solution (18 mg/mL) (for light labeling) or $^{13}\text{C}_2$ -dansyl chloride (18 mg/mL) (for heavy labeling). The dansylation reaction was proceeded for 45 min at 40°C with shaking at 200 rpm in an incubator shaker. Then 20 μ L of 250 mM sodium hydroxide was added to quench the excess dansyl chloride. After an additional 10 min of 40°C incubation, 100 μ L of 20% formic acid was added to quench the excess sodium hydroxide. Samples were then centrifuged. For DmPA labeling reaction, about 100 μ L of carboxyl standard solutions or urine supernatants were mixed with an equal volume of triethylamine (20 mol/L). The solutions were vortexed, spun down, and mixed with 100 μ L freshly prepared ^{12}C -DmPA solution (18 mg/mL) (for light labeling) or $^{13}\text{C}_2$ -DmPA solution (18 mg/mL) (for heavy labeling). The reaction was allowed to proceed for 60 min at 90°C water bath. Then 200 μ L of 20% formic acid was added to quench the excess DmPA. After an additional 10 min of 90°C incubation, samples were centrifuged.

Text S3. LC-QTOF Analysis Procedure

A reversed-phase Atlantis T3 column (2.1 mm $\times$ 100 mm, 3 μ m particle size, 100 Å pore size, Waters Corporation, Milford, USA) was employed. Solvent A was 0.1% (v/v) LC/MS grade formic acid in LC/MS grade water, and solvent B was 0.1% (v/v) LC/MS grade formic acid in LC/MS grade ACN. The profile was as follows: t) 0 min, 5% B; t) 2 min, 5% B; t) 5 min, 70% B; t) 11 min, 95% B; t) 15 min, 5% B; t) 18 min, 5% B. The flow rate was 300 μ L/min, and the sample injection volume was 1 μ L or 10 μ L. All MS spectra were collected in positive ion mode at a spectral acquisition rate of 1 Hz. The MS² spectra of labelled standards were obtained under collision energy of 20 ~ 40 eV in a stepping mode. The width of mass window for precursor ion isolation in the MS/MS experiments was 6 Da.

Table S1. List of 20 tested environmental chemicals.

Name	CAS number	Chemical structure	Description	Exposure Source	Function Group
Triclosan	3380-34-5		Antibacterial	PPCP	
Bisphenol S	80-09-1		Plastic Additives	CP ^a	
1-Naphthol	90-15-3		Hydroxy-PAHs	Pollution	
2-Hydroxyfluorene	2443-58-5		Hydroxy-PAHs	Pollution	
9-Phenanthrol	484-17-3		Hydroxy-PAHs	Pollution	
1-Hydroxypyrene	5315-79-7		Hydroxy-PAHs	Pollution	
4-Bromophenol	106-41-2		Pesticide	Pesticide	Phenols
Genistein	446-72-0		Drug	PPCP	
Bisphenol A	80-05-7		Plastic Additives	CP	
Methylparaben	99-76-3		Preservatives	PPCP	
Ethylparaben	120-47-8		Preservatives	PPCP	
Butylparaben	94-26-8		Preservatives	PPCP	
Benzylparaben	94-18-8		Preservatives	PPCP	
Benzoresorcinol	611-99-4		Plastic Additives	CP	

Phthalic Acid Mono-2-Ethylhexyl Ester	4376-20-9		Plastic Additives	CP	
Mono-(2-Ethyl-5-Hydroxyhexyl) Phthalate	40321-99-1		Plastic Additives	CP	Carboxyl
Mono-Benzyl Phthalate	2528-16-7		Plastic Additives	CP	
Benzoic Acid	65-85-0		Antibiotic	PPCP	
3,5-DHPPA	4228-66-4		Food Additive	Diet	Phenols/ Carboxyl

a. CP short for consumer products

Table S2. Improved detection sensitivities of compounds by chemical labeling.

Name	LODs (ppb)		Improved folds	Median con. in Ref. (ppb)
	Unlabeled	Labeled		
Methylparaben	2.68	0.15	18	153 ²
Ethylparaben	2.01	0.09	23	2.8 ³
3,5-DHPPA (Dansylation)	38.96	0.63	62	16.4 ⁴
4-Bromophenol	5.17	0.12	44	NA
1-Naphthol	30.92	0.17	182	2.06 ⁵
Benzylparaben	5.31	0.25	22	< 0.18 ⁶
2-Hydroxyfluorene	153.84	0.13	1184	0.89 ⁵
Butylparaben	20.83	0.17	123	1.5 ³
Bisphenol S	1.11	0.43	3	0.26 ⁷
9-Phenanthrol	6.82	0.11	62	0.21 ⁵
Benzoresorcinol	0.97	0.18	6	4.91 ⁸
Triclosan	1.01	0.50	3	2.74 ⁹
1-Hydroxypyrene	3.95	0.52	8	3.37 ¹⁰
Bisphenol A	5.80	0.39	15	1.48 ¹¹
Genistein	2.75	1.06	3	50.1 ¹²
MEHP	4.72	0.19	25	5.49 ¹³
MEHHP	5.63	0.23	24	32.6 ⁹
Mono-Benzyl Phthalate	6.76	0.44	15	4.0 ¹⁴
Benzoic Acid	6.91	0.37	19	NA
3,5-DHPPA (DmPA)	39.96	1.45	27	16.4 ⁴

Table S3. Intra- and inter- performance of the method.

Name	RSD for intra-assay% (n=6)			RSD for inter-assay% (n=9)		
	100 ppt	10 ppb	1 ppm	100 ppt	10 ppb	1 ppm
Phenol (DNS)						
Methylparaben	13.81	11.79	10.46	7.71	0.52	2.46
Ethylparaben	10.67	12.57	14.00	17.38	0.75	2.50
3,5-DHPPA	2.80	14.50	14.80	8.35	2.70	2.48
4-Bromophenol	15.89	7.50	10.42	6.76	0.87	1.94
1-Naphthol	14.54	11.15	16.46	7.18	0.56	3.48
Benzylparaben	9.12	8.97	10.78	16.33	0.77	3.03
2-Hydroxyfluorene	16.95	4.03	11.51	5.86	0.83	3.07
Butylparaben	12.69	7.63	15.12	15.24	0.54	1.84
Bisphenol S	13.99	4.65	14.29	17.95	0.63	2.72
9-Phenanthrol	15.04	5.74	17.97	14.13	0.53	2.21
Benzoresorcinol	13.61	19.69	13.92	3.04	1.70	2.18
Triclosan	19.59	11.39	5.98	19.51	1.19	1.56
1-Hydroxypyrene	17.25	14.11	6.83	15.50	3.67	2.08
Bisphenol A	18.03	15.71	8.11	17.18	3.10	1.29
Genistein	16.80	18.29	13.60	12.23	0.69	3.49
Carboxylic acid (DmPA)	1 ppb	100 ppb	10 ppm	1 ppb	100 ppb	10 ppm
MEHP	18.45	12.87	4.83	14.33	17.24	6.79
MEHHP	17.62	15.49	3.01	16.74	10.32	8.32
Mono-Benzyl Phthalate	9.43	8.90	1.69	15.92	10.49	3.21
Benzoic Acid	19.22	12.55	2.51	18.37	11.76	5.46
Ampicillin	18.79	18.01	6.31	16.50	18.28	9.12
Ciprofloxacin	13.24	10.91	1.11	12.60	11.73	4.33
3,5-DHPPA	15.90	7.45	5.74	18.65	12.88	9.30

1 **Table S4.** Summary of stock stability of analytes (CV% responses).

Name	48 h at room temp., n=6	-20 °C for 30 d, n=6
Phenol (DNS)	1 ppm	1 ppm
Methylparaben	5.22	6.81
Ethylparaben	3.41	2.90
3,5-DHPPA	9.64	11.61
4-Bromophenol	5.11	6.52
1-Naphthol	3.58	3.20
Benzylparaben	16.82	15.71
2-Hydroxyfluorene	2.80	1.96
Butylparaben	3.79	3.59
Bisphenol S	18.22	16.59
9-Phenanthrol	6.13	9.39
Benzoresorcinol	3.24	2.62
Triclosan	8.23	7.52
1-Hydroxypyrene	12.76	10.85
Bisphenol A	6.17	9.51
Genistein	11.96	10.21
Carboxylic acid (DmPA)	10 ppm	10 ppm
MEHP	11.55	9.52
MEHHP	5.94	8.82
Mono-Benzyl Phthalate	7.09	5.58
Benzoic Acid	2.65	1.75
Ampicillin	7.17	6.42
Ciprofloxacin	3.36	2.82
3,5-DHPPA	8.67	12.52

3 **Table S5.** Derivatization efficiency, extraction efficiency and matrix effect from urine samples.

Name	Derivatization efficiency (n=5)			Extraction efficiency (n=5)			Matrix factor (n=5)		
	100 ppt	10 ppb	1 ppm	100 ppt	10 ppb	1 ppm	100 ppt	10 ppb	1 ppm
Methylparaben	92.5±4.4	95.4±8.6	91.2±4.3	82.4±5.6	88.8±7	92.7±6.7	66.4±3.6	65.6±7.6	72.7±6.3
Ethylparaben	91.6±1.8	92.7±5.4	92.6±9.4	84.0±7.4	82.3±5.4	90.9±4.5	64.0±4.9	62.3±5.1	70.5±4.2
3,5-DHPPA (DNS)	82.4±3.8	88.2±4.9	89.4±5.8	82.7±6.2	85.4±4.9	87.6±6.9	62.7±7.2	64.4±4.7	67.5±3.7
4-Bromophenol	85.6±6.9	84.2±9.3	88.7±6.7	79.2±4.4	82.7±5.2	96.1±7.2	61.2±7.4	66.7±4.6	71.2±7.6
1-Naphthol	92.8±4.2	95.6±3.8	107.4±8.4	77.4±9.2	92.9±6.8	93.8±6.4	62.4±4.2	64.3±6.7	75.7±6.4
Benzylparaben	94.9±12.5	92.6±6.2	99.2±6.1	82.4±6.3	90.2±7.2	92.5±8.3	65.4±7.1	70.2±7.6	62.5±4.3
2-Hydroxyfluorene	89.7±7.8	84.3±7.2	90.6±7.6	89.9±7.5	92.5±5.3	91.2±4.6	67.7±4.4	72.4±4.1	76.2±7.9
Butylparaben	96.6±5.1	95.8±8.6	97.1±6.4	80.6±11.2	90.3±4.1	94.1±6.2	60.3±6.8	70.3±4.5	74.6±6.2
Bisphenol S	87.3±7.2	89.2±6.7	102.8±10.8	84.2±8.1	112.6±7.5	96.5±4.9	65.5±4.6	62.5±7.6	67.1±4.7
9-Phenanthrol	92.4±6.2	92.7±5.2	105.2±6.7	79.2±6.7	82.3±5.2	92.6±11.6	76.6±15.3	63.2±4.2	71.2±5.5
Benzoresorcinol	87.2±13.6	86.9±3.7	87.6±5.8	82.8±9.0	95.6±4.1	90.5±7.2	61.2±4.9	72.6±4.6	70.6±7.0
Triclosan	81.5±5.9	91.2±12.5	90.8±6.2	77.2±12.3	90.4±6.3	91.2±3.3	70.5±4.6	70.4±6.0	75.4±4.2
1-Hydroxypyrene	91.3±4.1	90.3±3.6	102.8±7.1	80.6±16.1	92.1±10.2	96.4±2.9	60.6±4.6	67.2±2.1	63.4±6.7
Bisphenol A	82.5±10.9	85.6±5.2	106.4±9.8	84.2±8.7	101.6±9.9	98.6±7.2	64.1±6.6	65.3±7.7	73.6±7.6
Genistein	93.4±12.1	95.1±6.8	97.4±5.7	82.8±7.7	88.2±4.6	92.5±2.4	62.7±8.7	65.4±5.6	74.6±3.4
Carboxylic acid (DmPA)	5 ppb	500 ppb	50 ppm	5 ppb	500 ppb	50 ppm	5 ppb	500 ppb	50 ppm
MEHP	83.8±9.4	86.1±9.5	85.6±4.2	82.8±9.3	84.6±9.4	96.1±6.6	62.6±7.2	64.6±7.4	76.2±6.9
MEHHP	85.2±8.0	92.2±8.4	86.9±4.3	78.0±8.7	81.2±6.4	94.2±4.5	76.0±5.7	62.8±6.4	74.1±4.3
Mono-Benzyl Phthalate	89.4±7.1	83.6±6.9	88.4±5.7	79.8±9.1	86.4±4.6	93.6±6.8	77.8±7.0	61.4±4.6	75.6±6.1
Benzoic Acid	92.7±6.5	94.9±4.5	96.2±7.2	76.6±6.2	82.4±3.7	95.2±5.3	63.9±6.1	62.1±5.7	68.2±5.3
Ampicillin	87.2±7.4	81.2±8.0	89.5±6.2	74.7±12.4	88.6±7.2	93.3±7.4	74.7±8.4	69.6±4.1	76.3±5.8
Ciprofloxacin	86.3±9.2	92.6±7.2	94.1±6.5	79.2±5.7	85.3±5.6	91.5±4.3	77.2±6.7	68.0±8.6	73.6±4.9
3,5-DHPPA (DmPA)	91.9±8.9	90.4±4.7	93.7±4.1	88.7±6.1	84.6±4.8	99.4±8.2	66.7±6.0	64.3±5.9	77.4±6.2

5 **Table S6.** Database of 818 chemicals measured in human urine.

ID	HMDB_NO	Name	Accurate_Mass	MZ_light	Exposure_source	Component_group
1	HMDB00001	1-Methylhistidine	169.0851	403.1434	Endogenous	Histidine and derivatives
2	HMDB00002	1_3-Diaminopropane	74.0844	308.1427	Endogenous	Monoalkylamines
3	HMDB00002	1_3-Diaminopropane - multi-tags	74.0844	271.0583	Endogenous	Monoalkylamines
4	HMDB00020	p-Hydroxyphenylacetic acid	152.0473	386.1057	Food	Phenols
5	HMDB00021	Iodotyrosine	306.9705	387.5436	Endogenous	Carboxylic acids and derivatives
6	HMDB00022	3-Methoxytyramine	167.0946	317.6056	Endogenous	Phenols
7	HMDB00045	Adenosine monophosphate	347.0631	581.1214	Endogenous	Purine nucleotides
8	HMDB00050	Adenosine	267.0968	501.1551	Endogenous	Purine nucleotides
9	HMDB00051	Ammonia	17.0266	251.0849	Endogenous	Homogeneous other non metal
10	HMDB00056	Beta-Alanine	89.0477	323.1060	Endogenous	Carboxylic acids and derivatives
11	HMDB00064	Creatine	131.0695	365.1278	Endogenous	Carboxylic acids and derivatives
12	HMDB00070	D-Pipecolic acid	129.0790	363.1373	Endogenous	Carboxylic acids and derivatives
13	HMDB00085	Deoxyguanosine	267.0968	501.1551	Endogenous/Food	Purine nucleotides
14	HMDB00087	Dimethylamine	45.0578	279.1162	Endogenous/Food	Dialkylamines
15	HMDB00089	Cytidine	243.0855	477.1438	Endogenous/Food	Pyrimidine nucleosides
16	HMDB00089	Cytidine - H2O	243.0855	459.1333	Endogenous/Food	Pyrimidine nucleosides
17	HMDB00095	Cytidine monophosphate	323.0519	557.1102	Endogenous/Food	Pyrimidine nucleosides
18	HMDB00095	Cytidine monophosphate - Isomer	323.0519	557.1102	Endogenous/Food	Pyrimidine nucleosides
19	HMDB00099	L-Cystathionine	222.0674	345.0920	Endogenous/Food	Carboxylic acids and derivatives
20	HMDB00099	L-Cystathionine - Isomer	222.0674	345.0920	Endogenous/Food	Carboxylic acids and derivatives
21	HMDB00101	Deoxyadenosine	251.1018	485.1602	Endogenous	Purine nucleotides
22	HMDB00112	Gamma-Aminobutyric acid	103.0633	337.1216	Endogenous/Food	Carboxylic acids and derivatives
23	HMDB00112	Gamma-Aminobutyric acid - H2O	103.0633	319.1144	Endogenous/Food	Carboxylic acids and derivatives
24	HMDB00118	Homovanillic acid	182.0579	416.1162	Endogenous/Food	Methoxyphenols
25	HMDB00123	Glycine	75.0320	309.0903	Endogenous/Food	Carboxylic acids and derivatives

26	HMDB00128	Guanidoacetic acid	117.0538	351.1121	Endogenous	Carboxylic acids and derivatives
27	HMDB00130	Homogentisic acid	168.0423	318.0794	Endogenous/Food	Phenylacetic acids
28	HMDB00133	Guanosine	283.0917	517.1500	Endogenous/Food	Purine nucleotides
29	HMDB00148	L-Glutamic Acid	147.0532	381.1115	Endogenous/Food	Carboxylic acids and derivatives
30	HMDB00148	L-Glutamic Acid - H2O	147.0532	363.1009	Endogenous/Food	Carboxylic acids and derivatives
31	HMDB00149	Ethanolamine	61.0528	295.1111	Endogenous/Food	Amines
32	HMDB00152	Gentisic acid	154.0266	388.0849	Endogenous/Food	Hydroxybenzoic acid derivatives
33	HMDB00152	Gentisic acid - multi-tags	154.0266	311.0716	Endogenous/Food	Hydroxybenzoic acid derivatives
34	HMDB00153	Estriol	288.1725	522.2309	Endogenous/Food	Estrogens and derivatives
35	HMDB00157	Hypoxanthine + H2O	136.0385	388.1098	Endogenous/Food	Carboxylic acids and derivatives
36	HMDB00157	Hypoxanthine - multi-tags	136.0385	370.0968	Endogenous/Food	Carboxylic acids and derivatives
37	HMDB00157	Hypoxanthine - Isomer	136.0385	370.0968	Endogenous/Food	Carboxylic acids and derivatives
38	HMDB00158	L-Tyrosine	181.0739	324.5953	Endogenous/Food	Purines and purine derivatives
39	HMDB00159	L-Phenylalanine	165.0790	399.1373	Endogenous/Food	Amino Acids and Derivatives
40	HMDB00161	L-Alanine	89.0477	323.1060	Endogenous/Food	Carboxylic acids and derivatives
41	HMDB00162	L-Proline	115.0633	349.1216	Endogenous/Food	Carboxylic acids and derivatives
42	HMDB00164	Methylamine	31.0422	265.1005	Endogenous/Food	Monoalkylamines
43	HMDB00167	L-Threonine	119.0582	353.1166	Food	Amino Acids and Derivatives
44	HMDB00168	L-Asparagine	132.0535	366.1118	Endogenous/Food	Carboxylic acids and derivatives
45	HMDB00168	L-Asparagine - H2O	132.0535	348.1070	Endogenous/Food	Carboxylic acids and derivatives
46	HMDB00172	L-Isoleucine	131.0946	365.1529	Food	Amino Acids and Derivatives
47	HMDB00177	L-Histidine	155.0695	389.1278	Food	Amino Acids and Derivatives
48	HMDB00182	L-Lysine	146.1055	307.1111	Food	Amino Acids and Derivatives
49	HMDB00187	L-Serine	105.0426	339.1009	Endogenous/Food	Carboxylic acids and derivatives
50	HMDB00191	L-Aspartic Acid	133.0375	367.0958	Endogenous/Food	Carboxylic acids and derivatives
51	HMDB00192	L-Cystine	240.0238	354.0702	Endogenous/Food	Carboxylic acids and derivatives
52	HMDB00206	N6-Acetyl-L-Lysine	188.1161	422.1744	Endogenous/Food	Carboxylic acids and derivatives
53	HMDB00210	Pantothenic acid	219.1107	453.1690	Food	Amino acids

54	HMDB00214	Ornithine	132.0899	300.1033	Endogenous/Food	Carboxylic acids and derivatives
55	HMDB00224	O-Phosphoethanolamine	141.0191	375.0774	Endogenous	Organic phosphoric acids and derivatives
56	HMDB00228	Phenol	94.0419	327.0929	Pollutant	Phenols
57	HMDB00238	Sepiapterin	237.0862	471.1445	Endogenous	Pterins and derivatives
58	HMDB00239	Pyridoxine	169.0739	403.1322	Endogenous/Food	Pyridines and derivatives
59	HMDB00239	Pyridoxine - H2O	169.0739	385.1243	Endogenous/Food	Pyridines and derivatives
60	HMDB00251	Taurine	125.0147	359.0730	Food	Amino acids
61	HMDB00259	Serotonin	176.0950	322.1058	Endogenous/Food	Tryptamines and derivatives
62	HMDB00262	Thymine	126.0429	360.1012	Endogenous/Food	Hydroxypyrimidines
63	HMDB00265	Liothyronine	650.7900	884.8484	Endogenous	Carboxylic acids and derivatives
64	HMDB00271	Sarcosine	89.0477	323.1060	Endogenous	Carboxylic acids and derivatives
65	HMDB00279	Saccharopine	276.1321	510.1905	Endogenous/Food	Carboxylic acids and derivatives
66	HMDB00279	Saccharopine - H2O	276.1321	492.1799	Endogenous/Food	Carboxylic acids and derivatives
67	HMDB00291	Vanillylmandelic acid	198.0528	432.1111	Endogenous	Methoxyphenols
68	HMDB00291	Vanillylmandelic acid - H2O	198.0528	414.1005	Endogenous	Methoxyphenols
69	HMDB00292	Xanthine	152.0334	386.0917	Endogenous/Food	Purines and purine derivatives
70	HMDB00296	Uridine	244.0695	478.1279	Endogenous/Food	Pyrimidine nucleosides
71	HMDB00296	Uridine - H2O	244.0695	460.1173	Endogenous/Food	Pyrimidine nucleosides
72	HMDB00300	Uracil	112.0273	346.0856	Endogenous/Food	Pyrimidines and pyrimidine derivatives
73	HMDB00301	Urocanic acid	138.0429	372.1012	Endogenous/Food	Imidazolyl carboxylic acids and derivatives
74	HMDB00303	Tryptamine	160.1000	394.1584	Endogenous/Food	Tryptamines and derivatives
75	HMDB00306	Tyramine	137.0841	302.6004	Endogenous	Phenethylamines
76	HMDB00356	17-Epiestriol	288.1725	522.2309	Endogenous/Food	Estrogens and derivatives
77	HMDB00370	2-Amino-3-phosphonopropionic acid	169.0140	403.0723	Endogenous	Carboxylic acids and derivatives
78	HMDB00397	2-Pyrocatechuic acid	154.0266	388.0849	Endogenous/Food	Benzoic acids and derivatives
79	HMDB00440	3-Hydroxyphenylacetic acid	152.0473	386.1057	Food	Phenylacetic Acid Derivatives
80	HMDB00446	N-Alpha-acetylysine	188.1161	422.1744	Endogenous	Carboxylic acids and derivatives
81	HMDB00450	5-Hydroxylysine	162.1004	315.1085	Endogenous	Carboxylic acids and derivatives

82	HMDB00452	L-Alpha-aminobutyric acid	103.0633	337.1216	Endogenous/Food	Carboxylic acids and derivatives
83	HMDB00455	Allocystathionine	222.0674	345.0920	Endogenous	Carboxylic acids and derivatives
84	HMDB00455	Allocystathionine - Isomer	222.0674	345.0920	Endogenous	Carboxylic acids and derivatives
85	HMDB00468	Biopterin	237.0862	471.1445	Endogenous	Pterins and derivatives
86	HMDB00469	5-Hydroxymethyluracil	142.0378	376.0962	Endogenous	Pyrimidines and pyrimidine derivatives
87	HMDB00473	6-Dimethylaminopurine	163.0858	397.1441	Endogenous	Purines and purine derivatives
88	HMDB00479	3-methyl-histidine	169.0851	403.1434	Food	Amino acids
89	HMDB00484	Vanillic acid	168.0423	402.1006	Food	Polyphenols
90	HMDB00500	4-Hydroxybenzoic acid	138.0317	372.0900	Food	Benzoic Acid and Derivatives
91	HMDB00504	5-Hydroxy-L-tryptophan	220.0848	344.1007	Endogenous/Food	Tryptamines and derivatives
92	HMDB00510	Aminoadipic acid	161.0688	395.1271	Endogenous/Food	Carboxylic acids and derivatives
93	HMDB00517	L-Arginine	174.1117	408.1700	Food	Amino Acids and Derivatives
94	HMDB00557	L-Alloisoleucine	131.0946	365.1529	Endogenous/Food	Carboxylic acids and derivatives
95	HMDB00574	Cysteine	121.0197	355.0781	Endogenous	Carboxylic acids and derivatives
96	HMDB00592	Glucosamine 6-sulfate	259.0362	493.0945	Endogenous	Carbohydrates and carbohydrate conjugates
97	HMDB00615	Epinephrine	183.0895	417.1479	Endogenous	Phenols
98	HMDB00615	Epinephrine - Isomer	183.0895	417.1479	Endogenous	Phenols
99	HMDB00615	Epinephrine - Isomer	183.0895	417.1479	Endogenous	Phenols
100	HMDB00630	Cytosine	111.0433	345.1016	Endogenous	Pyrimidines and pyrimidine derivatives
101	HMDB00641	L-Glutamine	146.0691	380.1275	Endogenous/Food	Carboxylic acids and derivatives
102	HMDB00650	D-Alpha-aminobutyric acid	103.0633	337.1216	Endogenous/Food	Carboxylic acids and derivatives
103	HMDB00667	L-Thyroine	273.1001	370.6084	Endogenous	Carboxylic acids and derivatives
104	HMDB00669	Ortho-Hydroxyphenylacetic acid	152.0473	386.1057	Food	Phenylacetic Acid Derivatives
105	HMDB00670	Homo-L-arginine	188.1273	422.1856	Endogenous/Food	Carboxylic acids and derivatives
106	HMDB00676	L-Homocystine	268.0551	368.0859	Endogenous	Carboxylic acids and derivatives
107	HMDB00679	Homocitrulline	189.1113	423.1697	Endogenous	Carboxylic acids and derivatives
108	HMDB00684	L-Kynurenine	208.0848	442.1431	Endogenous	Alkyl-phenylketones
109	HMDB00684	L-Kynurenine - H2O	208.0848	424.1325	Endogenous	Alkyl-phenylketones

110	HMDB00687	L-leucine	131.0946	365.1529	Food	Amino Acids and Derivatives
111	HMDB00696	L-Methionine	149.0510	383.1094	Food	Amino Acids and Derivatives
112	HMDB00704	Isoxanthopterin	179.0443	413.1026	Endogenous/Food	Pterins and derivatives
113	HMDB00704	Isoxanthopterin - Isomer	179.0443	413.1026	Endogenous/Food	Pterins and derivatives
114	HMDB00706	L-Aspartyl-L-phenylalanine	280.1059	514.1642	Food	Carboxylic acids and derivatives
115	HMDB00714	Hippuric acid	179.0582	340.1423	Food	Amino acids
116	HMDB00716	L-Pipecolic acid	129.0790	363.1373	Endogenous/Food	Carboxylic acids and derivatives
117	HMDB00719	L-Homoserine	119.0582	353.1166	Endogenous/Food	Carboxylic acids and derivatives
118	HMDB00719	L-Homoserine - H2O	119.0582	335.1060	Endogenous/Food	Carboxylic acids and derivatives
119	HMDB00721	Glycylproline	172.0848	406.1431	Endogenous	Carboxylic acids and derivatives
120	HMDB00725	Trans-4-Hydroxyl-L-Proline	131.0582	365.1166	Endogenous/Food	Carboxylic acids and derivatives
121	HMDB00734	Indoleacrylic acid	187.0633	421.1216	Endogenous/Food	Indoles
122	HMDB00750	3-Hydroxymandelic acid	168.0423	402.1006	Endogenous	Phenols
123	HMDB00750	3-Hydroxymandelic acid - COOH	168.0423	356.0951	Endogenous	Phenols
124	HMDB00755	Hydroxyphenyllactici acid	182.0579	416.1162	Endogenous	Phenylpropanoic acids
125	HMDB00759	Glycyl-L-Leucine	188.1161	422.1744	Endogenous	Carboxylic acids and derivatives
126	HMDB00763	5-Hydroxyindoleacetic acid	191.0582	425.1166	Endogenous	Indoles and derivatives
127	HMDB00819	Normetanephine	183.0895	325.6031	Endogenous	Methoxyphenols
128	HMDB00840	Salicyluric acid	195.0532	356.1372	Drug	Amino Acids and Derivatives
129	HMDB00881	Xanthurenic acid	205.0375	439.0958	Endogenous	Quinoline carboxylic acids
130	HMDB00881	Xanthurenic acid - multi-tags	205.0375	629.0732	Endogenous	Quinoline carboxylic acids
131	HMDB00883	L-Valine	117.0790	351.1373	Food	Amino Acids and Derivatives
132	HMDB00884	Ribothymidine	258.0852	492.1435	Endogenous	Pyrimidine nucleosides
133	HMDB00884	Ribothymidine - Isomer	258.0852	492.1435	Endogenous	Pyrimidine nucleosides
134	HMDB00884	Ribothymidine - H2O	258.0852	474.1329	Endogenous	Pyrimidine nucleosides
135	HMDB00897	7-Methylguanine	165.0651	399.1234	Endogenous	Purines and purine derivatives
136	HMDB00904	Citrulline	175.0957	409.1540	Endogenous/Food	Carboxylic acids and derivatives
137	HMDB00905	Deoxyadenosine monophosphate	331.0682	565.1265	Endogenous	Purine nucleotides

138	HMDB00929	L-Tryptophan	204.0899	438.1482	Food	Amino Acids and Derivatives
139	HMDB00939	S-Adenosylhomocysteine	384.1216	426.1191	Endogenous/Food	5'-deoxyribonucleosides
140	HMDB00954	trans-Ferulic acid	194.0579	428.1162	Food	Cinnamic Acid Derivatives
141	HMDB00955	Isoferulic acid	194.0579	427.1089	Food	Cinnamic Acid Derivatives
142	HMDB00957	pyrocatechol	110.0368	289.0767	Food	Phenols and Derivatives
143	HMDB00965	Hypotaurine	109.0197	343.0781	Endogenous	Sulfinic acids
144	HMDB00982	5-Methylcytidine	257.1012	491.1595	Endogenous	Pyrimidine nucleosides
145	HMDB00982	5-Methylcytidine - Isomer	257.1012	491.1595	Endogenous	Pyrimidine nucleosides
146	HMDB00991	2-aminooctanoic acid	159.1259	393.1842	Endogenous	Carboxylic acids and derivatives
147	HMDB01044	2'-Deoxyguanosine 5'-monophosphate	347.0631	581.1214	Endogenous	Purine nucleotides
148	HMDB01049	Gamma-Glutamylcysteine	250.0623	483.1211	Endogenous/Food	Carboxylic acids and derivatives
149	HMDB01065	2-Hydroxyphenethylamine	137.0841	371.1424	Endogenous	Aralkylamines
150	HMDB01065	2-Hydroxyphenethylamine - Isomer	137.0841	371.1424	Endogenous	Aralkylamines
151	HMDB01069	2-Phenylaminoadenosine	358.1390	592.1973	Endogenous	Purine nucleosides
152	HMDB01149	5-Aminolevulinic acid	131.0582	365.1166	Endogenous/Food	Carboxylic acids and derivatives
153	HMDB01169	4-Aminophenol	109.0528	343.1111	Endogenous	Benzene and substituted derivatives
154	HMDB01169	4-Aminophenol - multi-tags	109.0528	288.5847	Endogenous	Benzene and substituted derivatives
155	HMDB01173	5'-Methylthioadenosine	297.0896	531.1479	Endogenous/Food	5'-deoxyribonucleosides
156	HMDB01202	dCMP	307.0569	541.1153	Endogenous/Food	Pyrimidine nucleotides
157	HMDB01232	4-Nitrophenol	139.0269	373.0853	Endogenous	Phenols
158	HMDB01238	N-Acetylserotonin	218.1055	452.1638	Endogenous/Food	Indoles and derivatives
159	HMDB01254	Glucosamine 6-phosphate	259.0457	493.1040	Endogenous	Hexose phosphates
160	HMDB01257	Spermidine	145.1579	306.6373	Endogenous/Food	Dialkylamines
161	HMDB01336	3_4-Dihydroxybenzeneacetic acid	168.0423	318.0794	Endogenous/Food	Phenols
162	HMDB01341	ADP	427.0294	661.0877	Endogenous/Food	Purine nucleotides
163	HMDB01370	Diaminopimelic acid	190.0954	513.2707	Food	Carboxylic acids and derivatives
164	HMDB01370	Diaminopimelic acid - Isomer	190.0954	329.1060	Food	Carboxylic acids and derivatives
165	HMDB01392	p-Aminobenzoic acid	137.0477	371.1060	Drug	Benzoic Acid and Derivatives

166	HMDB01397	Guanosine monophosphate	363.0580	597.1163	Endogenous	Purine nucleotides
167	HMDB01398	Guaiacol	124.0524	358.1107	Endogenous/Food	Methoxyphenols
168	HMDB01413	Citicoline	488.1073	722.1657	Endogenous/Food	Pyrimidine nucleotides
169	HMDB01413	Citicoline - Isomer	488.1073	722.1657	Endogenous/Food	Pyrimidine nucleotides
170	HMDB01414	Putrescine	88.1000	278.1083	Endogenous/Food	Monoalkylamines
171	HMDB01431	Pyridoxamine	168.0899	318.1033	Endogenous/Food	Pyridines and derivatives
172	HMDB01432	Agmatine	130.1218	364.1802	Endogenous/Food	Guanidines
173	HMDB01432	Agmatine - multi-tags	130.1218	299.1192	Endogenous/Food	Guanidines
174	HMDB01476	3-Hydroxyanthranilic acid	153.0426	387.1009	Endogenous/Food	Hydroxybenzoic acid derivatives
175	HMDB01522	Methylguanidine	73.0640	307.1223	Endogenous/Food	Guanidines
176	HMDB01522	Methylguanidine - multi-tags	73.0640	270.5903	Endogenous/Food	Guanidines
177	HMDB01525	Imidazole	68.0374	302.0958	Food	Imidazoles
178	HMDB01545	Pyridoxal	167.0582	401.1166	Endogenous/Food	Pyridines and derivatives
179	HMDB01645	L-Norleucine	131.0946	365.1529	Endogenous	Carboxylic acids and derivatives
180	HMDB01713	m-Coumaric acid	164.0473	398.1057	Food	Polyphenols
181	HMDB01833	Aminopterin	440.1557	674.2140	Endogenous/Food	Hydroxycinnamic acids
182	HMDB01842	Guanidine	59.0483	293.1067	Endogenous/Food	Guanidines
183	HMDB01849	Propranolol	259.1572	493.2155	Drug	Naphthalenes
184	HMDB01855	5-Hydroxytryptophol	177.0790	411.1373	Endogenous/Food	Indoles and derivatives
185	HMDB01856	Protocatechuic acid	154.0266	311.0716	Food	Benzoic Acid and Derivatives
186	HMDB01858	p-Cresol	108.0575	342.1158	Endogenous/Food	Phenols
187	HMDB01859	Acetaminophen	151.0633	385.1216	Endogenous	Phenols
188	HMDB01861	3-Methylhistamine	125.0953	359.1536	Endogenous	Amines
189	HMDB01866	3_4-Dihydroxymandelic acid	184.0372	326.0769	Endogenous/Food	Phenols
190	HMDB01867	4-Aminohippuric acid	194.0691	428.1275	Endogenous	Benzoic acids and derivatives
191	HMDB01868	5-Methoxysalicylic acid	168.0423	402.1006	Food	Benzoic acids and derivatives
192	HMDB01885	3-Chlorotyrosine	215.0349	341.5758	Endogenous	Carboxylic acids and derivatives
193	HMDB01889	Theophylline	180.0647	414.1230	Endogenous/Food	Purines and purine derivatives

194	HMDB01891	m-Aminobenzoic acid	137.0477	371.1060	Drug	Benzoic acids and derivatives
195	HMDB01894	Aspartame	294.1216	528.1799	Food	Carboxylic acids and derivatives
196	HMDB01895	Salicylic acid	138.0317	403.0725	Food	Polyphenols
197	HMDB01901	Aminocaproic acid	131.0946	365.1529	Drug	Fatty Acids and Conjugates
198	HMDB01904	3-Nitrotyrosine	226.0590	335.1080	Endogenous	Carboxylic acids and derivatives
199	HMDB01904	3-Nitrotyrosine - H ₂ O	226.0590	347.0878	Endogenous	Carboxylic acids and derivatives
200	HMDB01906	2-Aminoisobutyric acid	103.0633	337.1216	Endogenous	Carboxylic acids and derivatives
201	HMDB01915	Alendronic acid	249.0167	483.0750	Endogenous	Bisphosphonates
202	HMDB01918	Thyroxine	776.6867	622.4017	Endogenous	Carboxylic acids and derivatives
203	HMDB01924	Atenolol	266.1630	500.2214	Drug	Ethers
204	HMDB01932	Metoprolol	267.1834	501.2418	Drug	Phenols
205	HMDB01937	Salbutamol	239.1521	473.2105	Drug	Benzyl alcohols
206	HMDB01937	Salbutamol - H ₂ O	239.1521	455.1999	Drug	Benzyl alcohols
207	HMDB01938	Lisinopril	405.2264	320.1460	Drug	Carboxylic acids and derivatives
208	HMDB01942	Phenylpropanolamine	151.0997	385.1580	Endogenous	Phenylpropanes
209	HMDB01943	Pseudoephedrine	165.1154	399.1737	Drug	Phenylpropanes
210	HMDB01964	Caffeic acid	180.0423	324.0800	Endogenous/Food	Hydroxycinnamic acids
211	HMDB01972	3-Aminosalicylic acid	153.0426	387.1009	Drug	Benzoic acids and derivatives
212	HMDB02005	Methionine Sulfoxide	165.0460	399.1043	Endogenous/Food	Carboxylic acids and derivatives
213	HMDB02005	Methionine Sulfoxide - Isomer	165.0460	399.1043	Endogenous/Food	Carboxylic acids and derivatives
214	HMDB02006	2_3-Diaminopropionic acid	104.0586	286.0876	Endogenous	Carboxylic acids and derivatives
215	HMDB02017	1-Phenylethylamine	121.0891	355.1475	Endogenous	Aralkylamines
216	HMDB02024	Imidazoleacetic acid	126.0429	360.1012	Endogenous/Food	Imidazolyl carboxylic acids and derivatives
217	HMDB02048	m-Cresol	108.0575	342.1158	Endogenous/Food	Phenols
218	HMDB02055	o-Cresol	108.0575	342.1158	Food	Phenols
219	HMDB02085	Syringic acid	198.0528	432.1111	Food	Benzoic acids and derivatives
220	HMDB02099	6-Methyladenine	149.0701	383.1285	Endogenous	Purines and purine derivatives
221	HMDB02099	6-Methyladenine - Isomer	149.0701	383.1285	Endogenous	Purines and purine derivatives

222	HMDB02108	Methylcysteine	135.0354	369.0937	Food	Amino Acids and Derivatives
223	HMDB02128	2_4-Diamino-6-hydroxypyrimidine	126.0542	360.1125	Drug	Pyrimidines and pyrimidine derivatives
224	HMDB02141	N-Methyl-a-aminoisobutyric acid	117.0790	351.1373	Endogenous	Carboxylic acids and derivatives
225	HMDB02182	Phenylephrine	167.0946	400.1456	Drug	Phenethylamines
226	HMDB02199	Desaminotyrosine	166.0630	400.1213	Endogenous/Food	Phenylpropanoic acids
227	HMDB02205	L-Homocysteic acid	183.0201	417.0785	Endogenous	Carboxylic acids and derivatives
228	HMDB02210	2-Phenylglycine	151.0633	385.1216	Endogenous	Carboxylic acids and derivatives
229	HMDB02322	Cadaverine	102.1157	285.1162	Endogenous/Food	Monoalkylamines
230	HMDB02339	5-Methoxytryptophan	234.1004	468.1588	Endogenous	Indoles and derivatives
231	HMDB02362	2_4-Diaminobutyric acid	118.0742	293.0954	Drug	Carboxylic acids and derivatives
232	HMDB02390	3-Cresotinic acid	152.0473	386.1057	Drug	Benzoic acids and derivatives
233	HMDB02393	N-methyl-D-aspartic acid	147.0532	381.1115	Endogenous	Carboxylic acids and derivatives
234	HMDB02658	6-Hydroxynicotinic acid	139.0269	373.0853	Endogenous	Pyridines and derivatives
235	HMDB02658	6-Hydroxynicotinic acid - Isomer	139.0269	373.0853	Endogenous	Pyridines and derivatives
236	HMDB02670	Naringenin	272.0685	370.0926	Food	Polyphenols
237	HMDB02706	Canavanine	176.0909	338.1822	Food	Carboxylic acids and derivatives
238	HMDB02706	Canavanine - Isomer	176.0909	338.1822	Food	Carboxylic acids and derivatives
239	HMDB02991	Cysteamine	77.0299	311.0882	Endogenous	Alkylthiols
240	HMDB03012	Aniline	93.0578	327.1162	Endogenous/Food	Benzene and substituted derivatives
241	HMDB03134	Biocytin	372.1831	606.2414	Endogenous	Carboxylic acids and derivatives
242	HMDB03157	Guanidinosuccinic acid	175.0593	409.1176	Endogenous	Carboxylic acids and derivatives
243	HMDB03164	Chlorogenic acid	354.0951	820.1971	Food	Polyphenols
244	HMDB03164	Chlorogenic acid - Isomer	354.0951	411.1059	Food	Polyphenols
245	HMDB03282	1-Methylguanine	165.0651	399.1234	Endogenous/Food	Purines and purine derivatives
246	HMDB03320	Indole-3-carboxylic acid	161.0477	395.1060	Food	Indoles and derivatives
247	HMDB03334	Symmetric dimethylarginine	202.1430	436.2013	Endogenous/Food	Carboxylic acids and derivatives
248	HMDB03337	Oxidized glutathione	612.1520	540.1343	Endogenous/Food	Carboxylic acids and derivatives
249	HMDB03338	Hydroxylamine	33.0215	267.0798	Endogenous/Food	Homogeneous other non metal

250	HMDB03355	5-Aminopentanoic acid	117.0790	351.1373	Endogenous	Homogeneous other non metal
251	HMDB03423	D-Glutamine	146.0691	380.1275	Endogenous	Homogeneous other non metal
252	HMDB03431	L-Histidinol	141.0902	375.1485	Endogenous/Food	Aralkylamines
253	HMDB03464	4-Guanidinobutanoic acid	145.0851	379.1434	Endogenous/Food	Carboxylic acids and derivatives
254	HMDB03464	4-Guanidinobutanoic acid - H2O	145.0851	361.1329	Endogenous/Food	Carboxylic acids and derivatives
255	HMDB03474	3_5-Diiodo-L-tyrosine	432.8672	666.9255	Endogenous	Carboxylic acids and derivatives
256	HMDB03474	3_5-Diiodo-L-tyrosine - multi-tags	432.8672	450.4919	Endogenous	Carboxylic acids and derivatives
257	HMDB03640	Beta-Leucine	131.0946	365.1529	Endogenous	Carboxylic acids and derivatives
258	HMDB03640	Beta-Leucine - H2O	131.0946	347.1424	Endogenous	Carboxylic acids and derivatives
259	HMDB03911	3-Aminoisobutanoic acid	103.0633	337.1216	Endogenous	Carboxylic acids and derivatives
260	HMDB03911	3-Aminoisobutanoic acid - H2O	103.0633	319.1110	Endogenous	Carboxylic acids and derivatives
261	HMDB04095	5-Methoxytryptamine	190.1106	424.1689	Endogenous	Indoles and derivatives
262	HMDB04122	Selenocystine	335.9128	402.0147	Endogenous	Carboxylic acids and derivatives
263	HMDB04437	Foodhanolamine	105.0790	339.1373	PPCP	Amines
264	HMDB04811	2_4-Dichlorophenol	161.9639	396.0222	Endogenous/sludge	Benzene and substituted derivatives
265	HMDB04815	4-Hydroxy-3-methylbenzoic acid	152.0473	386.1057	Endogenous	Hydroxybenzoic acid derivatives
266	HMDB04987	Alpha-Aspartyl-lysine	261.1325	364.6246	Food	Carboxylic acids and derivatives
267	HMDB04992	Benzocaine	165.0790	399.1373	PPCP	Benzoic acids and derivatives
268	HMDB06050	o-Tyrosine	181.0739	324.5953	Endogenous	Carboxylic acids and derivatives
269	HMDB11177	L-phenylalanyl-L-proline	262.1317	496.1901	Endogenous	Carboxylic acids and derivatives
270	HMDB11737	Gamma Glutamylglutamic acid	276.0958	510.1541	Endogenous	Carboxylic acids and derivatives
271	HMDB13243	Leucyl-phenylalanine	278.1630	512.2214	Endogenous	Carboxylic acids and derivatives
272	HMDB13302	Phenylalanylphenylalanine	312.1474	546.2057	Endogenous	Carboxylic acids and derivatives
273	HMDB28689	Alanyl-Histidine	226.1066	460.1649	Endogenous	Carboxylic acids and derivatives
274	HMDB28691	Alanyl-Leucine	202.1317	436.1901	Endogenous	Carboxylic acids and derivatives
275	HMDB28694	Alanyl-Phenylalanine	236.1161	470.1744	Endogenous	Carboxylic acids and derivatives
276	HMDB28698	Alanyl-Tryptophan	275.1270	509.1853	Endogenous	Carboxylic acids and derivatives
277	HMDB28699	Alanyl-Tyrosine	252.1110	360.1138	Endogenous	Carboxylic acids and derivatives

278	HMDB28716	Arginyl-Phenylalanine	321.1801	555.2384	Endogenous	Carboxylic acids and derivatives
279	HMDB28844	Glycyl-Isoleucine	188.1161	422.1744	Endogenous	Carboxylic acids and derivatives
280	HMDB28848	Glycyl-Phenylalanine	222.1004	456.1588	Endogenous	Carboxylic acids and derivatives
281	HMDB28852	Glycyl-Tryptophan	261.1113	495.1697	Endogenous	Carboxylic acids and derivatives
282	HMDB28853	Glycyl-Tyrosine	238.0954	353.1060	Endogenous	Carboxylic acids and derivatives
283	HMDB28854	Glycyl-Valine	174.1004	408.1588	Endogenous	Carboxylic acids and derivatives
284	HMDB28878	Histidiny-Alanine	226.1066	460.1649	Endogenous	Carboxylic acids and derivatives
285	HMDB28937	Leucyl-Proline	228.1474	462.2057	Endogenous	Carboxylic acids and derivatives
286	HMDB28940	Leucyl-Tryptophan	317.1739	551.2323	Endogenous	Carboxylic acids and derivatives
287	HMDB28941	Leucyl-Tyrosine	294.1580	381.1373	Endogenous	Carboxylic acids and derivatives
288	HMDB28988	Phenylalanyl-Alanine	236.1161	470.1744	Endogenous	Carboxylic acids and derivatives
289	HMDB28995	Phenylalanyl-Glycine	222.1004	456.1588	Endogenous	Carboxylic acids and derivatives
290	HMDB29001	Phenylalanyl-Methionine	296.1195	530.1778	Endogenous	Carboxylic acids and derivatives
291	HMDB29007	Phenylalanyl-Tyrosine	328.1423	398.1295	Endogenous	Carboxylic acids and derivatives
292	HMDB29008	Phenylalanyl-Valine	264.1474	498.2057	Endogenous	Carboxylic acids and derivatives
293	HMDB29043	Seriny-Leucine	218.1267	452.1850	Endogenous	Carboxylic acids and derivatives
294	HMDB29046	Seriny-Phenylalanine	252.1110	486.1693	Endogenous	Carboxylic acids and derivatives
295	HMDB29065	Threoniny-Leucine	232.1423	466.2006	Endogenous	Carboxylic acids and derivatives
296	HMDB29082	Tryptophyl-Glutamate	332.1246	566.1830	Endogenous	Carboxylic acids and derivatives
297	HMDB29087	Tryptophyl-Leucine	317.1739	551.2323	Endogenous	Carboxylic acids and derivatives
298	HMDB29090	Tryptophyl-Phenylalanine	351.1583	585.2166	Endogenous	Carboxylic acids and derivatives
299	HMDB29095	Tryptophyl-Tyrosine	367.1532	417.6349	Endogenous	Carboxylic acids and derivatives
300	HMDB29098	Tyrosyl-Alanine	252.1110	360.1138	Endogenous	Carboxylic acids and derivatives
301	HMDB29105	Tyrosyl-Glycine	238.0954	353.1060	Endogenous	Carboxylic acids and derivatives
302	HMDB29109	Tyrosyl-Leucine	294.1580	381.1373	Endogenous	Carboxylic acids and derivatives
303	HMDB29118	Tyrosyl-Valine	280.1423	374.1295	Endogenous	Carboxylic acids and derivatives
304	HMDB29306	4-Ethylphenol	122.0732	356.1315	Food	Phenols and Derivatives
305	HMDB59964	2_3_4-Trihydroxybenzoic acid	170.0215	319.0691	Endogenous	Benzoic Acid and Derivatives

306	HMDB59966	3_5-Dimethoxyphenol	154.0630	388.1213	Endogenous	Methoxyphenols
307	HMDB60003	Isovanillic acid	168.0423	402.1006	Endogenous	Benzoic Acid and Derivatives
308	HMDB29419	Gly-Gly-Gly-Gly	246.0964	480.1548	Endogenous	Carboxylic acids and derivatives
309	HMDB29083	Trp-Gly-Gly	318.1328	552.1911	Endogenous	Carboxylic acids and derivatives
310	HMDB94702	Gly-Norvaline	174.1005	408.1588	Endogenous	Carboxylic acids and derivatives
311	HMDB01645	Gly-Norleucine	188.1161	422.6993	Endogenous	Carboxylic acids and derivatives
312	HMDB94662	Phenyl-Leucine	278.1631	512.2214	Endogenous	Carboxylic acids and derivatives
313	HMDB12138	1-Naphthol	145.0647	378.1158	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
314	HMDB125533	3-(3,5-dihydroxyphenyl)propanoic acid	183.0651	344.1492	Food	Phenylpropanoic acids
315	HMDB61385	Triclosan	288.9584	522.0094	PPCP	Benzenoids
316		Bisphenol S	251.0372	717.1393	Plasticizer	Bisphenol
317		Tetrabromobisphenol A	540.7643	1006.8664	Flame retardant	Bromophenol
318	HMDB59801	9-Phenanthrol	195.0804	428.1314	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
319	HMDB62397	4-Bromophenol	171.9523	406.0107	Pesticides	Bromophenol
320	HMDB32133	Bisphenol A	229.1223	695.2244	Plasticizer	Bisphenol
321		Benzylparaben	229.0859	462.1369	PPCP	Phenol
322		2,4-Dihydroxybenzophenone	215.0702	681.1723	PPCP	Phenol
323	HMDB125533	3-(3,5-dihydroxyphenyl)propanoic acid	183.0651	649.1672	Food	Phenylpropanoic acids
324	HMDB13248	Phthalic acid mono-2-ethylhexyl ester	278.1518	440.2431	Plasticizer Phthalates	Phthalic acid
325	HMDB94679	mono-(2-Ethyl-5-hydroxyhexyl) phthalate	294.1467	456.2380	Plasticizer Phthalates	Phthalic acid
326	HMDB61744	Mono-Benzyl Phthalate	256.0735	418.1648	Plasticizer Phthalates	Phthalic acid
327	HMDB01870	Benzoic acid	122.0367	283.1208	Food	Benzoic Acid and Derivatives
328	HMDB14559	Ampicillin	349.1096	511.2009	Drug	Antibiotic
329	HMDB14677	Ciprofloxacin	331.1332	493.2245	Drug	Antibiotic
330	HMDB14653	Vancomycin	1447.4302	1609.5215	Drug	Antibiotic
331		10E-Octadecenoic acid (trans-18:1n-8)	282.2558	443.3399	Food	Fatty acids
332		11cis-Rumenic acid (9cis,11cis-18:2n-7)	280.2402	441.3242	Food	Fatty acids
333	HMDB34296	11-Eicosenoic acid (cis-20:1n-9)	310.2871	471.3712	Food	Fatty acids

334		12E-Octadecenoic acid (trans-18:1n-6)	282.2558	443.3399	Food	Fatty acids
335		13,16-Docosadienoic acid (cis-22:2n-6)	336.3028	499.4025	Food	Fatty acids
336	HMDB02068	13-Docosenoic acid (cis-22:1n-9)	338.3184	499.4025	Food	Fatty acids
337	HMDB35159	13-Eicosenoic acid (cis-20:1n-7)	310.2871	471.3712	Food	Fatty acids
338	HMDB02823	13Z,16Z,19Z-Docosatrienoic acid (cis-22:3n-3)	334.2871	495.3712	Food	Fatty acids
339	HMDB00001	1-Methylhistidine	169.0851	330.1691	Food	Amino acids
340	HMDB06511	2,3-Diketogulonic acid	192.0270	353.1110	Food	Carboxylic acids
341		3-(3,5-Dihydroxyphenyl)-1-propanoic acid	182.0579	648.1600	Food	Polyphenols
342	HMDB13677	3,5-Dihydroxybenzoic acid	154.0266	620.1287	Food	Polyphenols
343	HMDB13198	4-O-Methylgallic acid	184.0371	650.1392	Food	Polyphenols
344	HMDB00017	4-Pyridoxic acid	183.0531	344.1372	Food	Pyridines
345	HMDB31035	5-n-Heneicosylresorcinol (C21:0)	404.3654	870.4675	Food	Polyphenols
346	HMDB38530	5-n-Heptadecylresorcinol (C17:0)	348.3028	814.4049	Food	Polyphenols
347	HMDB30956	5-n-Nonadecylresorcinol (C19:0)	376.3341	842.4362	Food	Polyphenols
348	HMDB38485	5-n-Pentacosylresorcinol (C25:0)	460.4280	926.5301	Food	Polyphenols
349	HMDB38524	5-n-Tricosylresorcinol (C23:0)	432.3967	898.4988	Food	Polyphenols
350		7E-Hexadecenoic acid (trans-16:1n-9)	254.2245	415.3086	Food	Fatty acids
351	HMDB02186	7Z-Hexadecenoic acid (cis-16:1n-9)	254.2245	415.3086	Food	Fatty acids
352		8-Eicosenoic acid (cis-20:1n-12)	310.2871	471.3712	Food	Fatty acids
353		all-cis-7,10,13-Eicosatrienoic acid (cis-20:3n-7)	306.2558	467.3399	Food	Fatty acids
354	HMDB01388	alpha-Linolenic acid (ALA; cis-18:3n-3)	278.2245	439.3086	Food	Fatty acids
355	HMDB01893	alpha-Tocopherol	430.3810	663.4321	Food	Tocopherols
356	HMDB02124	Apigenin	270.0528	969.2059	Food	Polyphenols
357	HMDB02212	Arachidic acid (20:0)	312.3028	473.3868	Food	Fatty acids
358	HMDB01043	Arachidonic acid (AA; cis-20:4n-6)	304.2402	465.3242	Food	Fatty acids
359		Asclepic acid (cis-18:1n-7)	282.2558	443.3399	Food	Fatty acids
360	HMDB00944	Behenic acid (22:0)	340.3341	501.4181	Food	Fatty acids
361	HMDB06335	beta-Tocopherol	416.3654	649.4164	Food	Tocopherols

362	HMDB00030	Biotin	244.0881	405.1722	Food	Carboxylic acids
363	HMDB01964	Caffeic acid	180.0422	646.1443	Food	Polyphenols
364	HMDB00511	Capric acid (10:0)	172.1463	333.2303	Food	Fatty acids
365		cis-12-Linoelaidic acid (12cis-18:2n-6)	280.2402	441.3242	Food	Fatty acids
366		cis-9-Linoelaidic acid (9cis-18:2n-6)	280.2402	441.3242	Food	Fatty acids
367	HMDB02884	cis-Cetoleic acid (cis-22:1n-11)	338.3184	499.4025	Food	Fatty acids
368	HMDB41711	cis-Resveratrol 3-O-glucuronide	404.1107	870.2128	Food	Polyphenols
369	HMDB41713	cis-Resveratrol 4'-O-glucuronide	404.1107	870.2128	Food	Polyphenols
370	HMDB41714	cis-Resveratrol 4'-O-sulfate	308.0354	774.1375	Food	Polyphenols
371	HMDB02326	Coumestrol	268.0371	734.1392	Food	Polyphenols
372	HMDB03312	Daidzein	254.0579	720.1599	Food	Polyphenols
373	HMDB02902	delta-Tocopherol	402.3497	635.4008	Food	Tocopherols
374	HMDB02183	DHA (cis-22:6n-3)	328.2402	489.3242	Food	Fatty acids
375	HMDB02925	Dihomo-gamma-linolenic acid (DGLA; cis-20:3n-6)	306.2558	467.3399	Food	Fatty acids
376	HMDB05760	Dihydrodaidzein	256.0735	722.1756	Food	Polyphenols
377	HMDB05897	Dihydrogenistein	272.0684	971.2216	Food	Polyphenols
378		Docosatetraenoic acid (cis-22:4n-3)	332.2715	493.3555	Food	Fatty acids
379	HMDB02226	Docosatetraenoic acid (DTA; cis-22:4n-6)	332.2715	493.3555	Food	Fatty acids
380	HMDB06528	DPA (cis-22:5n-3)	330.2558	491.3399	Food	Fatty acids
381	HMDB05060	Eicosadienoic acid (cis-20:2n-6)	308.2715	469.3555	Food	Fatty acids
382	HMDB60039	Eicosatrienoic acid (ETE; cis-20:3n-3)	306.2558	467.3399	Food	Fatty acids
383	HMDB00573	Elaidic acid (trans-18:1n-9)	282.2558	443.3399	Food	Fatty acids
384	HMDB02899	Ellagic acid	302.0062	1234.2104	Food	Polyphenols
385	HMDB05056	Enterodiol	302.1518	941.2474	Food	Polyphenols
386	HMDB06101	Enterolactone	298.1205	764.2226	Food	Polyphenols
387	HMDB01999	EPA (cis-20:5n-3)	302.2245	463.3086	Food	Fatty acids
388	HMDB02209	Equol	242.0942	708.1962	Food	Polyphenols
389	HMDB05810	Eriodictyol	288.0633	1220.2675	Food	Polyphenols

390	HMDB10325	Ethyl glucuronide	222.0739	383.1580	Food	Carboxylic acids
391	HMDB00537	Ferulic acid	194.0579	427.1089	Food	Polyphenols
392	HMDB05807	Gallic acid	170.0215	869.1746	Food	Polyphenols
393	HMDB38365	Gallocatechin	306.0739	1471.3291	Food	Polyphenols
394	HMDB03073	gamma-Linolenic acid (GLA; cis-18:3n-6)	278.2245	439.3086	Food	Fatty acids
395	HMDB01492	gamma-Tocopherol	416.3654	649.4164	Food	Tocopherols
396	HMDB03217	Genistein	270.0528	970.2059	Food	Polyphenols
397	HMDB05781	Glycitein	284.0684	750.1704	Food	Polyphenols
398	HMDB02345	Heneicosanoic acid (21:0)	326.3184	487.4025	Food	Fatty acids
399	HMDB05782	Hesperetin	302.0790	1001.2321	Food	Polyphenols
400	HMDB00742	Homocysteine	135.0353	296.1194	Food	Amino acids
401	HMDB05784	Hydroxytyrosol	154.0629	620.1650	Food	Polyphenols
402	HMDB02655	Isorhamnetin	316.0583	1015.2114	Food	Polyphenols
403	HMDB05801	Kaempferol	286.0477	985.2008	Food	Polyphenols
404	HMDB00638	Lauric acid (12:0)	200.1776	361.2616	Food	Fatty acids
405	HMDB02003	Lignoceric acid (24:0)	368.3654	529.4494	Food	Fatty acids
406	HMDB06270	Linoelaidic acid (trans-18:2n-6)	280.2402	441.3242	Food	Fatty acids
407	HMDB00673	Linoleic acid (LA; cis-18:2n-6)	280.2402	441.3242	Food	Fatty acids
408	HMDB05800	Luteolin	286.0477	1218.2519	Food	Polyphenols
409	HMDB02259	Margaric acid (17:0)	270.2558	431.3399	Food	Fatty acids
410	HMDB35698	Matairesinol	358.1416	824.2437	Food	Polyphenols
411	HMDB10378	Mead acid (cis-20:3n-9)	306.2558	467.3399	Food	Fatty acids
412	HMDB00806	Myristic acid (14:0)	228.2089	389.2929	Food	Fatty acids
413	HMDB02000	Myristoleic acid (cis-14:1n-5)	226.1932	387.2773	Food	Fatty acids
414	HMDB02368	Nervonic acid (cis-24:1n-9)	366.3497	527.4338	Food	Fatty acids
415	HMDB01406	Nicotinamide	122.0480	355.0990	Food	Pyridines
416	HMDB04193	N-Methyl-2-pyridone-5-carboxamide	152.0585	385.1096	Food	Pyridines
417	HMDB04194	N-Methyl-4-pyridone-3-carboxamide	152.0585	385.1096	Food	Pyridines

418	HMDB03152	N-Methylnicotinamide	136.0636	369.1147	Food	Pyridines
419	HMDB04629	O-Desmethylangolensin	258.0892	957.2422	Food	Polyphenols
420	HMDB00207	Oleic acid (cis-18:1n-9)	282.2558	443.3399	Food	Fatty acids
421	HMDB02177	Omega-3 arachidonic acid (ETA; cis-20:4n-3)	304.2402	465.3242	Food	Fatty acids
422	HMDB01976	Osbond acid (cis-22:5n-6)	330.2558	491.3399	Food	Fatty acids
423	HMDB12328	Palmitelaidic acid (trans-16:1n-7)	254.2245	415.3086	Food	Fatty acids
424	HMDB00220	Palmitic acid (16:0)	256.2402	417.3242	Food	Fatty acids
425	HMDB03229	Palmitoleic acid (cis-16:1n-7)	254.2245	415.3086	Food	Fatty acids
426	HMDB02035	p-Coumaric acid	164.0473	397.0983	Food	Polyphenols
427	HMDB00826	Pentadecylic acid (15:0)	242.2245	403.3086	Food	Fatty acids
428		Petroselaidic acid (trans-18:1n-12)	282.2558	443.3399	Food	Fatty acids
429	HMDB03306	Phloretin	274.0841	1206.2883	Food	Polyphenols
430	HMDB00801	Phytanic acid	312.3028	473.3868	Food	Fatty acids
431	HMDB05794	Quercetin	302.0426	1234.2468	Food	Polyphenols
432	HMDB03797	Rumenic acid (9cis,11trans-18:2n-7)	280.2402	441.3242	Food	Fatty acids
433	HMDB13692	Secoisolariciresinol	362.1729	828.2750	Food	Polyphenols
434	HMDB00827	Stearic acid (18:0)	284.2715	445.3555	Food	Fatty acids
435	HMDB06547	Stearidonic acid (cis-18:4n-3)	276.2089	437.2929	Food	Fatty acids
436	HMDB02937	Tamarixetin	316.0583	1015.2114	Food	Polyphenols
437	HMDB00235	Thiamin	265.1123	466.1912	Food	Pyrimidines
438		trans-9-Tetradecenoic acid (trans-14:1n-5)	226.1932	387.2773	Food	Fatty acids
439	HMDB41782	trans-Resveratrol 3-O-glucuronide	404.1107	870.2128	Food	Polyphenols
440		trans-Resveratrol 3-O-sulfate	308.0354	774.1375	Food	Polyphenols
441	HMDB41784	trans-Resveratrol 4'-O-sulfate	308.0354	774.1375	Food	Polyphenols
442	HMDB01160	Tricosanoic acid (23:0)	354.3497	515.4338	Food	Fatty acids
443	HMDB00294	Urea	60.0323	526.1344	Food	Carboxamides
444	HMDB03231	Vaccenic acid (trans-18:1n-7)	282.2558	443.3399	Food	Fatty acids
445		4'-OH-PhIP	240.1011	706.2032	Food contaminants	Heterocyclic amines (HCA)

446		5-OH-PhIP	240.1011	706.2032	Food contaminants	Heterocyclic amines (HCA)
447		N-Acetyl-S-(3-amino-2-hydroxy-3-oxopropyl)cysteine	250.0623	379.1743	Food contaminants	Acrylamide
448		N-Acetyl-S-(3-amino-3-oxopropyl)cysteine	234.0674	363.1794	Food contaminants	Acrylamide
449	HMDB01926	17a-Ethynylestradiol	296.1776	529.2286	Drug	Steroids and Steroid Derivatives
450	HMDB01123	2-Aminobenzoic acid	137.0476	298.1317	Drug	Benzoic Acid and Derivatives
451	HMDB00405	2-Methoxyestradiol	302.1881	535.2392	Drug	Steroids and Steroid Derivatives
452	HMDB10316	Acetaminophen glucuronide	327.0954	488.1794	Drug	Sugar Acids and Derivatives
453	HMDB01879	Aspirin	180.0422	341.1263	Drug	Benzoic Acid and Derivatives
454	HMDB05006	Atorvastatin	558.2530	719.3370	Drug	Anilides
455	HMDB05014	Celecoxib	381.0758	614.1269	Drug	Phenylpyrazoles
456	HMDB05015	Gabapentin	171.1259	332.2099	Drug	Amino Acids and Derivatives
457	HMDB01514	Glucosamine	179.0793	412.1304	Drug	Monosaccharides
458	HMDB01925	Ibuprofen	206.1306	367.2147	Drug	Prenol Lipids
459	HMDB01929	Levofloxacin	361.1437	522.2278	Drug	Phenylpiperazines
460	HMDB01923	Naproxen	230.0942	391.1783	Drug	Acenes
461	HMDB02329	Oxalic acid	89.9953	412.1634	Drug	Carboxylic Acids and Derivatives
462	HMDB01878	Thymol	150.1044	383.1555	Drug	Prenol Lipids
463	HMDB01877	Valproic acid	144.1150	305.1990	Drug	Fatty Acids and Conjugates
464	HMDB32604	2-Methoxybenzoic acid	182.0579	343.1419	Food	Benzoic Acid and Derivatives
465	HMDB30254	3-(3,4,5-Trimethoxyphenyl)propanoic acid	240.0997	401.1838	Food	Phenols and Derivatives
466	HMDB34315	3-(3,4-Dimethoxyphenyl)-2-propenoic acid	208.0735	369.1576	Food	Cinnamic Acid Derivatives
467	HMDB00375	3-(3-Hydroxyphenyl)propanoic acid	166.0629	393.1385	Food	Phenols and Derivatives
468	HMDB01336	3,4-Dihydroxybenzeneacetic acid	168.0422	634.1443	Food	Phenols and Derivatives
469	HMDB00423	3,4-Dihydroxyhydrocinnamic acid	182.0579	648.1600	Food	Phenols and Derivatives
470	HMDB02466	3-Hydroxybenzoic acid	138.0316	403.0725	Food	Benzoic Acid and Derivatives
471	HMDB32606	3-Methoxybenzoic acid	152.0473	313.1314	Food	Benzoic Acid and Derivatives
472	HMDB41683	4-Hydroxyphenyl-2-propionic acid	166.0629	399.1140	Food	Phenols and Derivatives
473	HMDB02040	4-Methoxycinnamic acid	178.0629	339.1470	Food	Cinnamic Acid Derivatives

474	HMDB00448	Adipic acid	146.0579	468.2260	Food	Carboxylic Acids and Derivatives
475	HMDB01518	Alpha-CEHC	278.1518	511.2028	Food	Benzopyrans
476	HMDB06327	Alpha-Tocotrienol	424.3341	657.3851	Food	Prenol Lipids
477	HMDB00194	Anserine	240.1222	401.2063	Food	Peptidomimetics
478	HMDB00039	Butyric acid	88.0524	249.1364	Food	Fatty Acids and Conjugates
479	HMDB02780	Catechin	290.0790	1222.2832	Food	Flavonoids
480	HMDB00567	Cinnamic acid	148.0524	309.1364	Food	Cinnamic Acid Derivatives
481	HMDB02269	Curcumin	368.1259	834.2280	Food	Curcuminoids
482		Cyanidin	286.0477	1273.2470	Food	Flavonoids
483	HMDB00638	Dodecanoic acid	200.1776	361.2616	Food	Fatty Acids and Conjugates
484	HMDB02231	Eicosenoic acid	310.2871	471.3712	Food	Fatty Acids and Conjugates
485	HMDB01871	Epicatechin	290.0790	1222.2832	Food	Flavonoids
486	HMDB02068	Erucic acid	338.3184	499.4025	Food	Fatty Acids and Conjugates
487	HMDB05809	Eugenol	164.0837	397.1347	Food	Phenols and Derivatives
488	HMDB00121	Folic acid	441.1396	763.3078	Food	Pteridines and Derivatives
489	HMDB01931	Gamma-CEHC	264.1361	497.1872	Food	Benzopyrans
490	HMDB11628	Glycyrrhetic acid	470.3396	631.4236	Food	Prenol Lipids
491	HMDB00764	Hydrocinnamic acid	150.0680	311.1521	Food	Aromatic Homomonocyclic Compounds
492	HMDB00197	Indoleacetic acid	175.0633	336.1473	Food	Indoles
493	HMDB00718	Isovaleric acid	121.0891	354.1401	Food	Fatty Acids and Conjugates
494	HMDB00706	L-Aspartyl-L-phenylalanine	280.1059	602.2740	Food	Amino Acids and Derivatives
495	HMDB02755	Myricetin	318.0375	1483.2928	Food	Flavonoids
496	HMDB01488	Nicotinic acid	123.0320	284.1160	Food	Pyridines and Derivatives
497	HMDB12328	Palmitelaidic acid	254.2245	415.3086	Food	Fatty Acids and Conjugates
498	HMDB00020	p-Hydroxyphenylacetic acid	152.0473	385.0983	Food	Phenols and Derivatives
499	HMDB00070	Pipecolic acid	129.0789	290.1630	Food	Amino Acids and Derivatives
500	HMDB00237	Propionic acid	74.0367	235.1208	Food	Carboxylic Acids and Derivatives
501	HMDB01852	Retinoic acid	300.2089	461.2929	Food	Prenol Lipids

502	HMDB03141	Retinoyl b-glucuronide	476.2410	637.3250	Food	Prenol Lipids
503	HMDB10340	Retinyl beta-glucuronide	462.2617	623.3458	Food	Prenol Lipids
504	HMDB03572	Rosmarinic acid	360.0845	1292.2887	Food	Cinnamic Acid Derivatives
505	HMDB03070	Shikimic acid	174.0528	335.1368	Food	Cyclic Alcohols and Derivatives
506	HMDB00848	Stearoylcarnitine	427.3661	588.4502	Food	Fatty Acid Esters
507	HMDB13078	Stearoylethanolamide	327.3137	560.3647	Food	Fatty Amides
508	HMDB05789	Tetrahydrocurcumin	372.1572	838.2593	Food	Phenols and Derivatives
509	HMDB01846	Tetrahydrofolic acid	445.1709	767.3391	Food	Pteridines and Derivatives
510	HMDB00892	Valeric acid	102.0680	263.1521	Food	Fatty Acids and Conjugates
511	HMDB12308	Vanillin	152.0473	385.0983	Food	Phenols and Derivatives
512		2,3,4,6-Tetrachlorophenol (2,3,4,6-TeCP)	229.8859	462.9370	Pesticides	Organohalogenes
513		2,3,4-Trichlorophenol (2,3,4-TCP)	195.9249	428.9759	Pesticides	Organohalogenes
514		2,4,5-Trichlorophenol (2,4,5-TCP)	195.9249	428.9759	Pesticides	Organohalogenes
515		2,4,6-Trichlorophenol (2,4,6-TCP)	195.9249	428.9759	Pesticides	Organohalogenes
516	HMDB04811	2,4-Dichlorophenol (2,4-DCP)	161.9639	395.0149	Pesticides	Organohalogenes
517	HMDB41800	2,5-Dichlorophenol (2,5-DCP)	161.9639	395.0149	Pesticides	Organohalogenes
518		2,6-Dichlorophenol (2,6-DCP)	161.9639	395.0149	Pesticides	Organohalogenes
519	HMDB32582	2-Phenylphenol (2-PP)	170.0731	403.1242	Pesticides	Phenols
520	HMDB41807	3-Phenoxybenzoic acid (PBA)	214.0629	375.1470	Pesticides	Benzoic acids
521		4-Monochlorophenol (4-MCP)	128.0028	361.0539	Pesticides	Organohalogenes
522		4-Phenylphenol (4-PP)	170.0731	403.1242	Pesticides	Phenols
523	HMDB41974	Pentachlorophenol (PCP)	263.8470	496.8980	Pesticides	Organohalogenes
524		2-(N-Ethyl-perfluorooctane sulfonamido) acetic acid	584.9902	746.0743	Pollutant	Perfluorinated Compounds
525		2-(N-Methyl-perfluorooctane sulfonamido) acetic acid	570.9746	732.0586	Pollutant	Perfluorinated Compounds
526		4-Ethylbenzoic acid	150.0680	311.1521	Pollutant	Benzoic Acid and Derivatives
527		Alpha-Hydroxyisobutyric acid	104.0473	265.1314	Pollutant	Hydroxy Acids and Derivatives
528		Perfluorodecanoic acid	513.9673	675.0513	Pollutant	Perfluorinated Compounds
529		Perfluorononanoic acid	463.9705	625.0545	Pollutant	Perfluorinated Compounds

530		Perfluorooctanoic acid	413.9737	575.0577	Pollutant	Perfluorinated Compounds
531		1-Hydroxybenzo[a]anthracene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
532		1-Hydroxybenzo[c]phenanthrene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
533		1-Hydroxychrysene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
534		1-Hydroxyfluorene	182.0731	415.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
535	HMDB12138	1-Hydroxynaphthalene	144.0575	377.1085	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
536	HMDB59797	1-Hydroxyphenanthrene	194.0731	427.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
537	HMDB13139	1-Hydroxypyrene	218.0731	451.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
538	HMDB59759	1-Hydroxypyrene glucuronide	394.1052	555.1893	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
539		2,4,5-Tribromophenol	327.7734	560.8244	Pollutant	Organohalogens
540	HMDB29642	2,4,6-Tribromophenol	327.7734	560.8244	Pollutant	Organohalogens
541	HMDB32079	2,4-Dibromophenol	249.8628	482.9139	Pollutant	Organohalogens
542		2,9-Hydroxyphenanthrene	210.0680	676.1701	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
543		2-Hydroxybenzo[c]phenanthrene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
544		2-Hydroxychrysene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
545	HMDB13163	2-Hydroxyfluorene	182.0731	416.1314	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
546	HMDB12322	2-Hydroxynaphthalene	144.0575	377.1085	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
547	HMDB59798	2-Hydroxyphenanthrene	194.0731	427.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
548		3-Hydroxybenzo[a]anthracene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
549		3-Hydroxybenzo[a]pyrene	268.0888	501.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
550		3-Hydroxybenzo[c]phenanthrene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
551		3-Hydroxychrysene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
552		3-Hydroxyfluoranthene	218.0731	451.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
553	HMDB59802	3-Hydroxyfluorene	182.0731	415.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
554	HMDB59799	3-Hydroxyphenanthrene	194.0731	427.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
555		3-OH-BDE-100	575.6206	808.6716	Pollutant	Polybrominated diphenyl ethers (PBDE)
556		3-OH-BDE-7	341.8891	574.9401	Pollutant	Polybrominated diphenyl ethers (PBDE)
557		3-OH-PCB-118	339.8783	572.9293	Pollutant	Polychlorinated biphenyls (PCB)

558		3'-OH-PCB-138	373.8393	606.8903	Pollutant	Polychlorinated biphenyls (PCB)
559		3-OH-PCB-153	373.8393	606.8903	Pollutant	Polychlorinated biphenyls (PCB)
560		3'-OH-PCB-180	407.8003	640.8514	Pollutant	Polychlorinated biphenyls (PCB)
561		3'-OH-PCB-187	407.8003	640.8514	Pollutant	Polychlorinated biphenyls (PCB)
562		4-Hydroxychrysene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
563	HMDB59800	4-Hydroxyphenanthrene	194.0731	427.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
564		4'-OH-BDE-49	497.7101	730.7611	Pollutant	Polybrominated diphenyl ethers (PBDE)
565		4-OH-PCB-107	339.8783	572.9293	Pollutant	Polychlorinated biphenyls (PCB)
566		4-OH-PCB-109	339.8783	572.9293	Pollutant	Polychlorinated biphenyls (PCB)
567		4'-OH-PCB-120	339.8783	572.9293	Pollutant	Polychlorinated biphenyls (PCB)
568		4'-OH-PCB-127	339.8783	572.9293	Pollutant	Polychlorinated biphenyls (PCB)
569		4'-OH-PCB-130	373.8393	606.8903	Pollutant	Polychlorinated biphenyls (PCB)
570		4-OH-PCB-146	373.8393	606.8903	Pollutant	Polychlorinated biphenyls (PCB)
571		4-OH-PCB-163	373.8393	606.8903	Pollutant	Polychlorinated biphenyls (PCB)
572		4'-OH-PCB-172	407.8003	640.8514	Pollutant	Polychlorinated biphenyls (PCB)
573		4-OH-PCB-187	407.8003	640.8514	Pollutant	Polychlorinated biphenyls (PCB)
574		4-OH-PCB-193	407.8003	640.8514	Pollutant	Polychlorinated biphenyls (PCB)
575		5-OH-BDE-47	497.7101	730.7611	Pollutant	Polybrominated diphenyl ethers (PBDE)
576		5'-OH-BDE-99	575.6206	808.6716	Pollutant	Polybrominated diphenyl ethers (PBDE)
577		6-Hydroxychrysene	244.0888	477.1398	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
578		6-OH-BDE-47	497.7101	730.7611	Pollutant	Polybrominated diphenyl ethers (PBDE)
579		6-OH-BDE-85	575.6206	808.6716	Pollutant	Polybrominated diphenyl ethers (PBDE)
580	HMDB59803	9-Hydroxyfluorene	182.0731	415.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
581	HMDB59801	9-Hydroxyphenanthrene	194.0731	427.1242	Pollutant	Polycyclic aromatic hydrocarbons (PAH)
582	HMDB33141	AalphaC	183.0796	416.1306	Pollutant	Heterocyclic amines (HCA)
583	HMDB15497	Benzophenone-3 (BP-3)	228.0786	461.1296	Pollutant	Phenols
584	HMDB32133	Bisphenol A (BPA)	228.1150	694.2171	Pollutant	Phenols
585	HMDB32575	Butylparaben (BP)	194.0942	421.1698	PPCP	Phenols

586		Dichloroacetic acid	127.9431	289.0272	Pollutant	Organohalogens
587	HMDB32573	Ethylparaben	166.0629	393.1385	PPCP	Phenols
588	HMDB32572	Methylparaben	153.0546	386.1056	PPCP	Phenols
589		Mono(2-carboxymethylhexyl) phthalate (MCMHP)	308.1259	630.2941	Pollutant	Phthalates
590		Mono(2-ethyl-5-carboxypentyl) phthalate (MECPP)	308.1259	630.2941	Pollutant	Phthalates
591		Mono(2-ethyl-5-hydroxyhexyl) phthalate (MEHHP)	294.1467	455.2307	Pollutant	Phthalates
592		Mono(2-ethyl-5-oxohexyl) phthalate (MEOHP)	292.1310	614.2992	Pollutant	Phthalates
593	HMDB13248	Mono(2-ethylhexyl) phthalate (MEHP)	278.1518	439.2358	Pollutant	Phthalates
594		Mono(3-carboxypropyl) phthalate (MCP)	252.0633	574.2315	Pollutant	Phthalates
595		Mono(4-hydroxypentyl) phthalate (MHPP)	252.0997	413.1838	Pollutant	Phthalates
596		Mono(carboxy-isooctyl) phthalate (MCOP)	322.1416	644.3097	Pollutant	Phthalates
597		Monobenzyl phthalate (MBzP)	256.0735	417.1576	Pollutant	Phthalates
598		Mono-carboxy-isodecyl phthalate (cx-MiDP)	336.1572	658.3254	Pollutant	Phthalates
599		Mono-carboxy-isononyl phthalate (cx-MiNP)	322.1416	644.3097	Pollutant	Phthalates
600	HMDB31331	Monochloroacetic acid	93.9821	255.0662	Pollutant	Organohalogens
601		Mono-cyclohexyl phthalate (MCHP)	248.1048	409.1889	Pollutant	Phthalates
602	HMDB02120	Monoethyl phthalate (MEP)	194.0579	355.1419	Pollutant	Phthalates
603		Mono-hydroxy-iso-butyl phthalate (OH-MiBP)	238.0841	399.1681	Pollutant	Phthalates
604		Mono-hydroxy-isodecyl phthalate (OH-MiDP)	322.1780	483.2620	Pollutant	Phthalates
605		Mono-hydroxy-isononyl phthalate (OH-MiNP)	308.1623	469.2464	Pollutant	Phthalates
606		Mono-hydroxy-n-butyl phthalate (OH-MnBP)	238.0841	399.1681	Pollutant	Phthalates
607	HMDB02056	Mono-isobutyl phthalate (MiBP)	222.0892	383.1732	Pollutant	Phthalates
608		Mono-isononyl phthalate (MiNP)	292.1674	453.2515	Pollutant	Phthalates
609		Mono-isopentyl phthalate (MiPP)	236.1048	397.1889	Pollutant	Phthalates
610	HMDB02130	Monomethyl phthalate (MMP)	180.0422	341.1263	Pollutant	Phthalates
611	HMDB13247	Mono-n-butyl phthalate (MnBP)	222.0892	383.1732	Pollutant	Phthalates
612		Mono-n-octyl phthalate (MnOP)	278.1518	439.2358	Pollutant	Phthalates
613		Mono-n-pentyl phthalate (MnPP)	236.1048	397.1889	Pollutant	Phthalates

614		Mono-oxo-isodecyl phthalate (oxo-MiDP)	320.1623	481.2464	Pollutant	Phthalates
615		Mono-oxo-isononyl phthalate (oxo-MiNP)	306.1467	467.2307	Pollutant	Phthalates
616	HMDB00228	Phenol	94.0418	327.0929	Pollutant	Phenol
617	HMDB02107	Phthalic acid (PA)	166.0266	488.1947	Pollutant	Phthalates
618	HMDB32574	Propylparaben (PP)	180.0786	407.1541	Pollutant	Phenols
619		TBBPA	539.7570	1005.8591	Pollutant	Organohalogens
620	HMDB02349	trans,trans-Muconic acid	142.0266	464.1947	Pollutant	Carboxylic acids
621	HMDB42048	Trichloroacetic acid	161.9042	322.9882	Pollutant	Organohalogens
622		Mecoprop	214.0397	376.1310	Pesticides	Acidic pesticides
623		Dichlorophenoxybutyric acid	248.0007	410.0920	Pesticides	Acidic pesticides
624	HMDB14910	Malathion	330.0361	478.1118	Pesticides	Acidic pesticides
625	HMDB29628	Chlorthal	301.8707	624.0388	Pesticides	Acidic pesticides
626		MCPB	228.0553	390.1467	Pesticides	Acidic pesticides
627		Ethirimol	209.1528	443.2111	Pesticides	Acidic pesticides
628		1-Naphthoxyacetic acid	202.0630	364.1543	Pesticides	Acidic pesticides
629		Bromofenofos	577.6765	811.7348	Pesticides	Acidic pesticides
630		Imazapyr	261.1113	423.2027	Pesticides	Acidic pesticides
631	HMDB37112	Acifluorfen	360.9965	523.0878	Pesticides	Acidic pesticides
632		Fenoxaprop-p	333.0404	495.1317	Pesticides	Acidic pesticides
633		Fluoroglycofen	419.0020	581.0933	Pesticides	Acidic pesticides
634	HMDB11625	Cacodylic acid	137.9662	300.0575	Pesticides	Acidic pesticides
635		Dalapon	141.9588	304.0502	Pesticides	Acidic pesticides
636		Glyphosate	169.0140	331.1053	Pesticides	Acidic pesticides
637		Glufosinate	181.0504	343.1417	Pesticides	Acidic pesticides
638		Picloram	239.9260	402.0174	Pesticides	Acidic pesticides
639		Clopyralid	190.9541	353.0454	Pesticides	Acidic pesticides
640	HMDB29581	Sorbic acid	112.0524	274.1438	Pesticides	Acidic pesticides
641		Trichlorobenzoic acid	223.9199	386.0112	Pesticides	Acidic pesticides

642		Triclopyr	254.9257	417.0170	Pesticides	Acidic pesticides
643		Fluroxypyr	253.9661	416.0575	Pesticides	Acidic pesticides
644		Chloramben	204.9697	367.0611	Pesticides	Acidic pesticides
645		Endothall	186.0528	348.1442	Pesticides	Acidic pesticides
646		2,4,5-trichlorophenoxyacetic acid	253.9304	416.0217	Pesticides	Acidic pesticides
647		Dicamba	219.9694	382.0607	Pesticides	Acidic pesticides
648	HMDB41797	Dichlorophenoxyacetic acid	219.9694	382.0607	Pesticides	Acidic pesticides
649		4-Chlorophenoxyacetic acid	186.0084	348.0997	Pesticides	Acidic pesticides
650		Chlorophenoxyacetic acid	186.0084	348.0997	Pesticides	Acidic pesticides
651	HMDB31609	Phenoxyacetic acid	152.0473	314.1387	Pesticides	Acidic pesticides
652		Fenoprop	267.9461	430.0374	Pesticides	Acidic pesticides
653		Dichlorprop	233.9850	396.0764	Pesticides	Acidic pesticides
654		Benzadox	195.0532	357.1445	Pesticides	Acidic pesticides
655		MCPA	200.0240	362.1154	Pesticides	Acidic pesticides
656	HMDB32559	Dinoseb	240.0746	474.1329	Pesticides	Phenolic pesticides
657		Dinoterb	240.0746	474.1329	Pesticides	Phenolic pesticides
658		Subutex	467.3036	701.3619	Pesticides	Phenolic pesticides
659		Hymecromone	176.0473	410.1056	Pesticides	Phenolic pesticides
660	HMDB32582	2-Phenylphenol	170.0732	404.1315	Pesticides	Phenolic pesticides
661		Dinitrocyclohexylphenol	266.0903	500.1486	Pesticides	Phenolic pesticides
662		Phenylchlorophenol	204.0342	438.0925	Pesticides	Phenolic pesticides
663		Dibutyl dimethylbenzylphenol	324.2453	558.3036	Pesticides	Phenolic pesticides
664		Tetrachlorophenol	229.8860	463.9443	Pesticides	Phenolic pesticides
665		Ioxynil	370.8304	604.8887	Pesticides	Phenolic pesticides
666		Bromoxynil	274.8581	508.9165	Pesticides	Phenolic pesticides
667		DNOC (2,4-Dinitro-o-kresol)	198.0277	432.0860	Pesticides	Phenolic pesticides
668		2-tert-Butylphenol	150.1045	384.1628	Antioxidants	Phenols
669		2-sec-Butylphenol	150.1045	384.1628	Antioxidants	Phenols

670		4-Butylphenol	150.1045	384.1628	Antioxidants	Phenols
671		4-sec-Butylphenol	150.1045	384.1628	Antioxidants	Phenols
672	HMDB32063	4-tert-Butylphenol	150.1045	384.1628	Antioxidants	Phenols
673		4-Butoxyphenol	166.0994	400.1577	Antioxidants	Phenols
674		4-Cyclopentylphenol	162.1045	396.1628	PPCP	Phenols
675	HMDB32575	Butyl paraben	194.0943	428.1526	PPCP	Phenols
676		2-sec-Pentylphenol	164.1201	398.1784	Pollutant	Phenols
677		4-Isopentylphenol	164.1201	398.1784	Pollutant	Phenols
678		4-Pentylphenol	164.1201	398.1784	Pollutant	Phenols
679		4-sec-Pentylphenol	164.1201	398.1784	Pollutant	Phenols
680		4-tert-Pentylphenol	164.1201	398.1784	Pollutant	Phenols
681	HMDB59925	Butylated hydroxyanisole	180.1150	414.1734	Pollutant	Phenols
682		4-(Phenylazo)phenol	198.0793	432.1376	Pollutant	Phenols
683		3-Phenylphenol	170.0732	404.1315	Pollutant	Phenols
684		4-Phenylphenol	170.0732	404.1315	Pollutant	Phenols
685		4-Phenoxyphenol	186.0681	420.1264	Pollutant	Phenols
686		4,4'-Biphenol	186.0681	420.1264	Pollutant	Phenols
687		4,4'-Thiodiphenol	186.0681	420.1264	Pollutant	Phenols
688		2-Bromo-4-cyclohexylphenol	254.0306	488.0890	Pollutant	Phenols
689		2-Chloro-4-cyclohexylphenol	210.0811	444.1395	Pollutant	Phenols
690		2-Cyclohexylphenol	176.1201	410.1784	Pollutant	Phenols
691		4-Cyclohexylphenol	176.1201	410.1784	Pollutant	Phenols
692		4-Hexylphenol	178.1358	412.1941	Pollutant	Phenols
693		4-Hexyloxyphenol	194.1307	428.1890	Pollutant	Phenols
694		Bis(ethylthio)methyl-2-methoxyphenol	258.0748	492.1331	Pollutant	Phenols
695		2-Bromo-4-(2,4,6-tribromo-phenoxy)phenol	497.7101	731.7685	Pollutant	Phenols
696		4-(2,4,6-Tribromo-phenoxy)phenol	419.7996	653.8579	Pollutant	Phenols
697		2-(2H-Benzotriazol-2-yl)-4-methylphenol	225.0902	459.1485	Pollutant	Phenols

698		4-Benzylphenol	184.0888	418.1471	Pollutant	Phenols
699	HMDB41808	4,4'-Methylenebis(phenol)	200.0837	434.1421	Pollutant	Phenols
700		Bisphenol F	200.0837	434.1421	Pollutant	Phenols
701		4-(Benzylamino)phenol	199.0997	433.1580	Pollutant	Phenols
702		4-Heptyloxyphenol	208.1463	442.2047	Pollutant	Phenols
703		1-Hydroxyphenanthrene	194.0732	428.1315	Pollutant	Phenols
704		2-Hydroxyphenanthrene	194.0731	428.1314	Pollutant	Phenols
705		3-Hydroxyphenanthrene	228.0786	462.1369	Pollutant	Phenols
706	HMDB15497	2-Hydroxy-4-methoxybenzophenone	228.0786	462.1369	Pollutant	Phenols
707		4-((4-(Allyloxy)phenyl)sulfonyl)phenol	290.0612	524.1196	Pollutant	Phenols
708		4-Phenethylphenol	198.1044	432.1627	Pollutant	Phenols
709		4,4'-Ethylene diphenol	214.0993	681.2087	Pollutant	Phenols
710	HMDB13816	2,4-Di-tert-butylphenol	206.1670	440.2253	Pollutant	Phenols
711		2,6-Di-tert-butylphenol	206.1670	440.2253	Pollutant	Phenols
712		4-Octylphenol	206.1670	440.2253	Pollutant	Phenols
713	HMDB13825	4-tert-Octylphenol	206.1670	440.2253	Pollutant	Phenols
714	HMDB14999	Diflunisal	250.0441	645.1865	Pollutant	Phenols
715		Bisphenol AF	336.0584	803.1678	Pollutant	Phenols
716		Tetrachlorobisphenol A	363.9591	831.0685	Pollutant	Phenols
717		3,3',5-Tribromobisphenol A	461.8465	928.9559	Pollutant	Phenols
718		3,3'-Dibromobisphenol A	383.9360	851.0454	Pollutant	Phenols
719		3-Monobromobisphenol A	306.0255	773.1349	Pollutant	Phenols
720		4-Cumylphenol	212.1201	446.1784	Pollutant	Phenols
721		3,5-Di-tert-Butylsalicylic acid	250.1568	645.2992	Pollutant	Phenols
722	HMDB38982	4-Nonylphenol	220.1827	454.2410	Pollutant	Phenols
723		4-tert-Nonylphenol	220.1827	454.2410	Pollutant	Phenols
724		Bisphenol B	242.1306	476.1890	Pollutant	Phenols
725		4-(1-Adamantyl)phenol	228.1514	462.2097	Pollutant	Phenols

726		2,4-bis(1,1-Dimethylpropyl)phenol	234.1983	468.2566	Pollutant	Phenols
727		Octylphenol monoethoxylate	250.1932	484.2516	Pollutant	Phenols
728	HMDB30105	Diphenolic acid	286.1205	914.3139	Pollutant	Phenols
729		Bisphenol C	256.1463	257.1536	Pollutant	Phenols
730		1,7-bis(4-Hydroxyphenylthio)-3,5-dioxaheptane	352.0803	819.1896	Pollutant	Phenols
731		Nonylphenol monoethoxylate	264.2089	498.2672	Pollutant	Phenols
732	HMDB37521	Citrus Red No. 2	308.1160	542.1744	Pollutant	Phenols
733		4,4'-Cyclohexylidenebisphenol	268.1463	735.2557	Pollutant	Phenols
734		Bisphenol Z	268.1463	735.2557	Pollutant	Phenols
735	HMDB00145	Estrone	270.1619	504.2203	Pollutant	Phenols
736		2,4,6-tris(1,1-Dimethylethyl)phenol	262.2296	496.2879	Pollutant	Phenols
737		2,6-bis(1,1-Dimethylethyl)-4-(1-methylpropyl)phenol	262.2296	496.2879	Pollutant	Phenols
738		4-Dodecylphenol	262.2296	496.2879	Pollutant	Phenols
739		4-Isododecylphenol	262.2296	496.2879	Pollutant	Phenols
740		Octylphenol	206.1670	440.2253	Pollutant	Phenols
741		Nonylphenol	220.1827	454.2410	Pollutant	Phenols
742		Bisphenol AP	290.1306	757.2400	Pollutant	Phenols
743		2-(2H-Benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol	323.1997	557.2580	Pollutant	Phenols
744		Bisphenol TMC	310.1932	777.3026	Pollutant	Phenols
745		Bisphenol G	312.2089	779.3183	Pollutant	Phenols
746		4,4'-(Octahydro-4,7-methano-5H-inden-5-ylidene)bisphenol	320.1776	787.2870	Pollutant	Phenols
747		2-(2H-Benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)phenol	351.2310	585.2893	Pollutant	Phenols
748		4,4'-Thiobis[2-(1,1-dimethylethyl)-5-methylphenol]	359.2039	825.3060	Pollutant	Phenols
749		2,4-bis(1-Methyl-1-phenylethyl)phenol	330.1983	564.2566	Pollutant	Phenols
750		Bisphenol M	346.1932	813.3026	Pollutant	Phenols
751		Bisphenol P	346.1932	813.3026	Pollutant	Phenols
752		Bisphenol BP	352.1463	819.2557	Pollutant	Phenols

753		4,4'-Isopropylidenebis(2-phenylphenol)	380.1776	847.2870	Pollutant	Phenols
754		Bisphenol PH	380.1776	847.2870	Pollutant	Phenols
755		2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol	447.2310	681.2893	Pollutant	Phenols
756		2,2'-methylenebis(4-methyl-6-nonylphenol)	480.3967	947.5061	Pollutant	Phenols
757		2,3-Dibromo-1-propanol	215.8785	449.9368	Pollutant	Phenols
758		2,3,5,6-Tetrachlorophenol	229.8859	463.9443	Pollutant	Phenols
759		2,3,6-Trichlorophenol	195.9249	429.9832	Pollutant	Phenols
760		2,4,6-Trichlorophenol	195.9249	429.9832	Pollutant	Phenols
761		2,3-Dichlorophenol	161.9639	396.0222	Pollutant	Phenols
762	HMDB04811	2,4-Dichlorophenol	161.9639	396.0222	Pollutant	Phenols
763	HMDB41800	2,5-Dichlorophenol	161.9639	396.0222	Pollutant	Phenols
764		3,4-Dichlorophenol	161.9639	396.0222	Pollutant	Phenols
765		2,4-Dinitrophenol	184.0120	418.0703	Pollutant	Phenols
766		2-Chlorophenol	128.0028	362.0612	Pollutant	Phenols
767		3-Chlorophenol	128.0028	362.0612	Pollutant	Phenols
768		4-Chlorophenol	128.0028	362.0612	Pollutant	Phenols
769		Pentabromophenol	483.5944	717.6527	Pollutant	Phenols
770	HMDB41974	Pentachlorophenol	263.8470	497.9053	Pollutant	Phenols
771		4-Amino-2-nitrophenol	154.0378	388.0961	Pollutant	Phenols
772		3-Trifluoromethyl-4-nitrophenol	207.0143	441.0726	Pollutant	Phenols
773		2-Chloro-4-methylphenol	142.0185	376.0768	Pollutant	Phenols
774		4-Chloro-2-methylphenol	142.0185	376.0768	Pollutant	Phenols
775		4-Chloro-3-methylphenol	142.0185	376.0768	Pollutant	Phenols
776	HMDB02055	2-Methylphenol	108.0575	342.1158	Pollutant	Phenols
777	HMDB01858	4-Methylphenol	108.0575	342.1158	Pollutant	Phenols
778		2-Ethylphenol	122.0731	356.1314	Pollutant	Phenols
779	HMDB59873	3-Ethylphenol	122.0731	356.1314	Pollutant	Phenols
780		3'-Hydroxyacetophenone	136.0524	370.1107	Pollutant	Phenols

781		4-Hydroxyacetophenone	136.0524	370.1107	Pollutant	Phenols
782		4-Chloro-3,5-dimethylphenol	156.0341	390.0925	Pollutant	Phenols
783		Ethyl-p-hydroxybenzoate (Ethyl paraben)	166.0629	400.1213	Pollutant	Phenols
784	HMDB29667	2,3,6-Trimethylphenol	136.0888	370.1471	Pollutant	Phenols
785	HMDB32625	4-Propylphenol	136.0888	370.1471	Pollutant	Phenols
786	HMDB41804	2-Isopropoxyphenol	152.0837	386.1420	Pollutant	Phenols
787		4-Propoxyphenol	152.0837	386.1420	Pollutant	Phenols
788		4-Pentyloxyphenol	180.1150	414.1733	Pollutant	Phenols
789		4-Hydroxycoumarin	162.0316	396.0900	Pollutant	Phenols
790		4-(Imidazol-1-yl)phenol	161.0709	394.1219	Pollutant	Phenols
791		Monoallyl phthalate	207.0651	368.1492	Pollutant	Phthalate metabolites
792		Monopropyl phthalate	209.0808	370.1648	Pollutant	Phthalate metabolites
793	HMDB61748	Mono 3-carboxypropyl phthalate	253.0706	575.2387	Pollutant	Phthalate metabolites
794	HMDB13247	Monobutyl phthalate	223.0964	384.1805	Pollutant	Phthalate metabolites
795		Monopentyl phthalate	237.1121	398.1961	Pollutant	Phthalate metabolites
796		Monocyclohexyl phthalate	249.1121	410.1961	Pollutant	Phthalate metabolites
797		Monoheptyl phthalate	251.1277	412.2118	Pollutant	Phthalate metabolites
798		1,2-Benzenedicarboxylic acid	251.1277	489.2020	Pollutant	Phthalate metabolites
799	HMDB61744	Monobenzyl phthalate	257.0808	418.1648	Pollutant	Phthalate metabolites
800		Monoheptyl phthalate	265.1434	426.2274	Pollutant	Phthalate metabolites
801	HMDB94645	Mono (2-ethyl-5-oxohexyl) phthalate	293.1383	454.2224	Pollutant	Phthalate metabolites
802		Mono (2-carboxymethylhexyl) phthalate	309.1332	631.3013	Pollutant	Phthalate metabolites
803	HMDB94647	Mono (2-ethyl-5-carboxypentyl) phthalate	309.1332	631.3013	Pollutant	Phthalate metabolites
804		Monocarboxyheptyl phthalate	323.1489	645.3170	Pollutant	Phthalate metabolites
805	HMDB13248	Mono (2-ethylhexyl) phthalate	279.1590	440.2431	Pollutant	Phthalate metabolites
806		Monooctyl phthalate	279.1590	440.2431	Pollutant	Phthalate metabolites
807		Mono (2-ethylhydroxyhexyl) phthalate	295.1540	456.2380	Pollutant	Phthalate metabolites
808		Mono (4-methyl-7-oxo-octyl)phthalate	307.1540	468.2380	Pollutant	Phthalate metabolites

809		Monoisononyl phthalate	293.1747	454.2587	Pollutant	Phthalate metabolites
810		Monohydroxyisononyl phthalate	309.1696	470.2537	Pollutant	Phthalate metabolites
811		Monodecyl phthalate	307.1903	468.2744	Pollutant	Phthalate metabolites
812		Monoisodecyl phthalate	306.1831	468.2744	Pollutant	Phthalate metabolites
813		Monoisoundecyl phthalate	306.1831	468.2744	Pollutant	Phthalate metabolites
814		Monoundecyl phthalate	306.1831	468.2744	Pollutant	Phthalate metabolites
815		Monododecyl phthalate	335.2216	496.3057	Pollutant	Phthalate metabolites
816	HMDB02130	Monomethyl phthalate	181.0495	342.1335	Pollutant	Phthalate metabolites
817		3-Bromo-6-phenoxybenzene-1,2-diol	279.9735	747.0828	Pollutant	OH-BDEs
818		4-(4-Bromophenoxy)benzene-1,2-diol	264.9858	731.0879	Pollutant	OH-BDEs

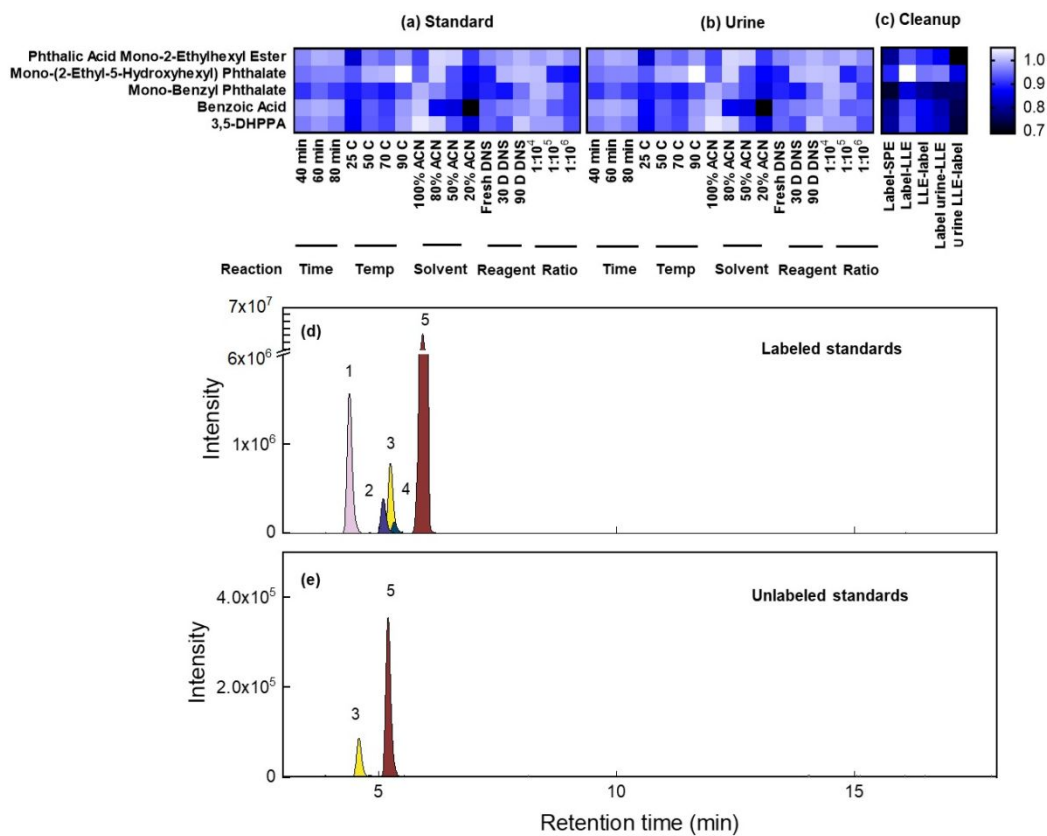
7 **Table S7.** Final results from IsoMS processing of the LC-qTOF runs of ten $^{12}\text{C}_2$ -/ $^{13}\text{C}_2$ -danylated standards.

Sample	rt	mz_light	mz_heavy	distance	int_light	int_heavy	ratio_light to heavy	nCharge	nTag	pairLev	isSaturated
1-Naphthol	349	378.1839	380.1905	2.0066	676696.2	658765.5	1.02	1	1	1	0
Methylparaben	335	386.1315	388.1385	2.0067	115759.3	110386.5	1.04	1	1	1	0
Ethylparaben	343	400.1199	402.1268	2.0068	862217.2	936830.5	0.92	1	1	1	0
4-Bromophenol	348	406.1432	408.1498	2.0065	610783.3	518722.4	1.17	1	1	1	0
2-Hydroxyfluorene	358	416.1175	418.1242	2.0067	9500841	10343000	0.91	1	1	1	0
9-Phenanthrol	365	428.1283	430.137	2.0064	360809.7	303016.3	1.19	1	1	1	0
Butylparaben	360	428.1506	430.1582	2.0067	787148.2	903222.8	0.87	1	1	1	0
1-Hydroxypyrene	381	452.1305	454.1371	2.0066	594840.9	643760.6	0.92	1	1	1	0
Benzylparaben	354	462.1359	464.1425	2.0066	277583.6	316245.8	0.87	1	1	1	0
Triclosan	377	522.0883	524.0946	2.0062	1157763	1154707	1.00	1	1	1	0

Table S8. List of suspect features that were detected in greater than 80% of urine samples (N=35).

Formula	Names	Isomers	MZ_light	Exposure Source
C ₁₄ H ₂₂ O	2,4-Di-tert-butylphenol	4	440.2253	Plastic Additives
	2,6-Di-tert-butylphenol			
	4-Octylphenol			
	4-tert-Octylphenol			
C ₇ H ₈ O	2-Methylphenol	2	342.1158	Preservatives
	4-Methylphenol			
C ₉ H ₁₂ O ₂	2-Isopropoxyphenol	2	314.1750	Plastic Additives
	4-Propoxyphenol			
C ₁₆ H ₂₂ O ₄	Monooctyl phthalate	3	440.2431	Plastic Additives
	Monoisooctyl phthalate			
	Mono-2-ethylhexylphthalate			

Figure S1. Comparison of DmPA derivatization efficiencies for 5 carboxylic acids (a) standards in MiliQ water and (b) spiked urine under different labeling reaction conditions. From left to right: reaction time, reaction temperature, incubation solvent, DmPA prepared time, and effect of compound/DmPA mole ratio. (c) Comparison of cleanup method optimization for phenol standards under different cleanup procedures. All data in (a) (b) (c) are presented as the mean from three independent experiments (n = 3) of three level QC working solution (5, 50, and 500 ppb). Base peak ion chromatograms of labelled standard mixture (d) after derivatization and (e) before derivatization (50 ppb each). The compounds are shown as follows: 1, 3,5-DHPPA Phthalic Acid; 2, Benzoic Acid; 3, Mono-(2-Ethyl-5-Hydroxyhexyl) Phthalate; 4, Mono-Benzyl Phthalate; 5, Mono-2-Ethylhexyl Ester.



25 **Figure S2.** Base peak ion chromatograms of labelled standard mixture in urine (a) after
 26 derivatization and (b) before derivatization. The compounds are shown as follows: 1,
 27 Methylparaben; 2, Benzoic Acid; 3, Mono-(2-Ethyl-5-Hydroxyhexyl) Phthalate; 4, Mono-
 28 Benzyl Phthalate; 5, Mono-2-Ethylhexyl Ester; 6, Ethylparaben; 7, 4-Bromophenol; 8, 1-
 29 Naphthol; 9, Benzylparaben; 10, 2-Hydroxyfluorene; 11, Butylparaben; 12, 9-Phenanthrol;
 30 13, Bisphenol S; 14, Benzoorsorcinol; 15, 1-Hydroxypyrene; 16, Triclosan; 17, Bisphenol
 31 A; 18, Genistein; 19, 3,5-DHPPA.

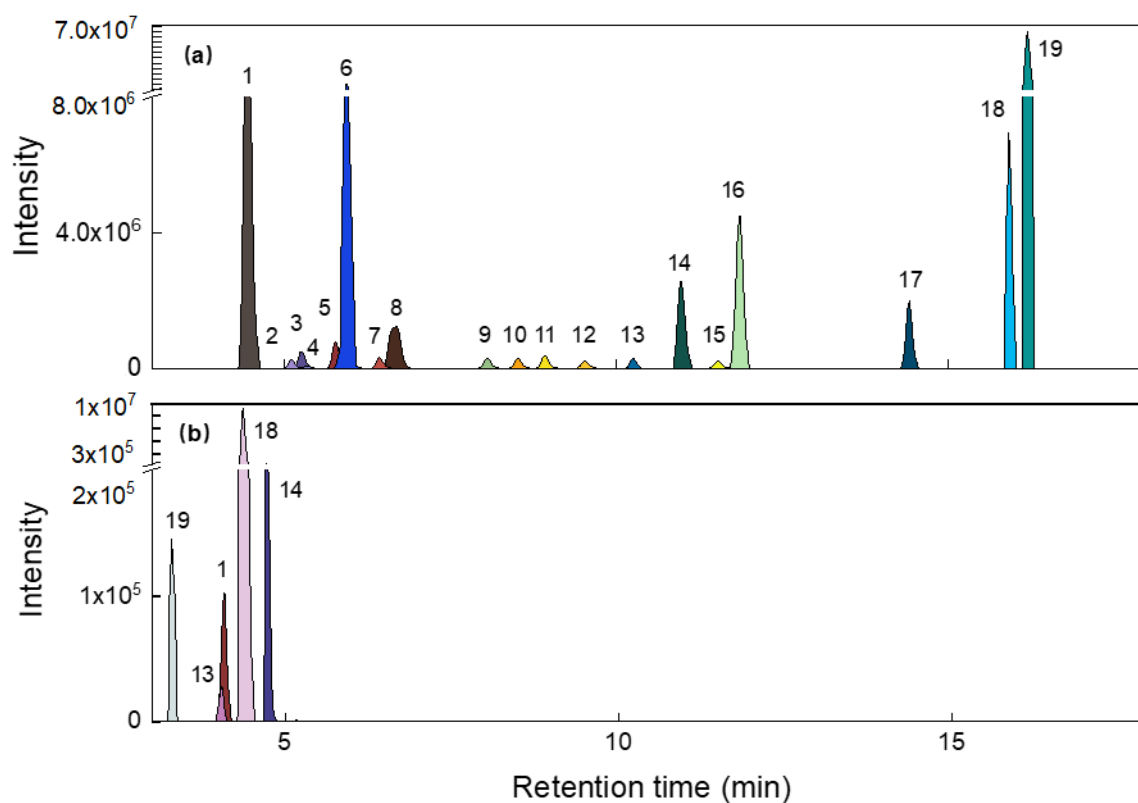


Figure S3. Illustration of database matching. After IsoMS filtration, each of these can be matched to multiple suspect candidates with the chemical mass (under different MS tolerances) included in our database. The exact match between a specific suspect feature and its chemical identity will need to be confirmed using synthetic reference standards.

Suspects after IsoMS filtration

sample	RT	mz_light
suspect 1	349	378.1139
suspect 2	335	386.1015
suspect 3	343	400.1199
suspect 4	358	416.1175
suspect 5	365	428.1283
suspect 8	377	522.0883

Data processing principle

1. Identify suspect compounds by mass matches under different MS tolerances
2. MS2 matches with literature and database



Suspect candidates in the database

ppm	Name	Adduct	Accurate Mass	MZ_light	CAS	Formula
10	Methyl 4-hydroxybenzoate	M+H	152.0473	386.1056	99-76-3	C ₈ H ₈ O ₃
10	3-Hydroxyphenylacetic acid	M+H	152.0473	386.1056	621-37-4	C ₈ H ₈ O ₃
10	Ortho-Hydroxyphenylacetic acid	M+H	152.0473	386.1056	614-75-5	C ₈ H ₈ O ₃
10	p-Hydroxyphenylacetic acid	M+H	152.0473	386.1056	156-38-7	C ₈ H ₈ O ₃
10	Vanillin	M+H	152.0473	386.1056	121-33-5	C ₈ H ₈ O ₃
39	N-Methyl-2-pyridone-5-carboxamide	M+H	152.0585	386.1169	701-44-0	C ₇ H ₈ N ₂ O ₂
39	N-Methyl-4-pyridone-3-carboxamide	M+H	152.0585	386.1169	769-49-3	C ₇ H ₈ N ₂ O ₂

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