

Appendix C

A list of putative identification of metabolites in human apocrine sweat. Bold text represents matches found in the HMDB urine database.

m/z	rt (s)	ppm error	MF	Adduct	Metabolites	Class	Ionmode
Amino Acids							
249.0615	84.30	1.73	C11H12N2O2	Na_Na	L-Tryptophan	Amino Acids	pos
369.1512	469.14	0.84	C12H24N2O8	HCOOH	Galactosylhydroxylysine	Sugar Amino Acids	neg
369.1531	504.24	4.47	C12H24N2O9	HCOOH	Galactosylhydroxylysine	Sugar Amino Acids	neg
543.1576	444.30	0.31	C18H34N2O13	NaCl	Glucosylgalactosyl hydroxylysine	Sugar Amino Acids	neg
199.9543	804.54	1.00	C2H7NO3S	KCl	Taurine	Amino Acids	pos
172.0220	67.20	4.48	C3H7NO3	HCOONa	L-Serine	Amino Acids	neg
183.9914	80.16	3.86	C3H7NO6S	H	L-Serine O-sulfate	Amino Acids	neg
164.0296	68.46	1.22	C4H9NO3	Na_Na (HCOONa)	L-Allothreonine;L-Homoserine;L-Threonine	Amino Acids	pos/neg
252.0148	66.48	0.16	C4H9NO5S	HCOONa	L-Methionine sulfone	Amino Acids	pos
191.0406	68.46	1.41	C5H10N2O3	Na_Na	L-Glutamine	Amino Acids	pos
169.0583	385.80	0.35	C5H10N2O3	Na	3-Ureidoisobutyrate	Amino Acids	pos
238.0142	63.84	4.58	C5H11NO2S	Na_HCOONa	L-Methionine	Amino Acids	neg
177.0612	64.56	1.13	C5H12N2O2	Na_Na (HCOONa)	L-Ornithine	Amino Acids	pos/neg
191.0768	64.56	0.84	C6H14N2O2	Na_Na	L-Lysine	Amino Acids	pos
185.9932	76.80	3.71	C5H7NO3	NaCl	Pyroglutamic acid	Amino Acids	neg
231.9888	66.48	1.64	C5H9NO2	NaClx2	L-Proline	Amino Acids	pos
220.0669	66.54	0.05	C6H13N3O3	Na_Na	L-Citrulline	Amino Acids	pos
200.0408	64.56	0.95	C6H9N3O2	Na_Na (HCOONa)	L-Histidine	Amino Acids	pos/neg
240.0486	81.12	2.92	C7H11NO4	HCOONa	(2S,5S)-5-Carboxymethylproline or related compounds	Amino Acids	neg
144.1019	430.92	0.21	C7H13NO2	H	Proline Betaine	Amino Acids	pos
252.9794	81.12	2.10	C8H8N2O3	KCl	Nicotinurate	Cyclic Amino Acids	neg
226.0454	74.28	1.86	C9H11NO3	Na_Na	L-Tyrosine	Amino Acids	pos
307.0345	81.00	2.41	C9H16N2OSS	Na_Na	N-Acetylcystathionine	Amino Acids	neg
Di/Polypeptides							
293.1468	404.58	4.09	C10H17N3O6	NH3	Norophthalmic acid	Polypeptides	pos
319.1248	87.96	2.38	C11H20N2O3	Na_HCOONa (HCOOH)	L-isoleucyl-L-proline;L-leucyl-L-proline	Polypeptides	pos/neg
319.1240	146.64	0.03	C11H20N2O3	Na_HCOONa (HCOOH)	L-leucyl-L-proline	Polypeptides	pos/neg
273.1454	169.86	0.73	C11H20N2O3	HCOOH	L-isoleucyl-L-proline;L-leucyl-L-proline	Polypeptides	neg
273.1452	200.76	1.32	C11H20N2O3	HCOOH	L-leucyl-L-proline	Polypeptides	neg
273.1453	232.32	0.99	C11H20N2O3	HCOOH	L-leucyl-L-proline	Polypeptides	neg
277.1224	682.08	1.30	C11H22N2O4S	H	Pantetheine	Polypeptides	neg
363.1782	414.48	1.82	C16H22N6O4	H	Thyrotropin releasing hormone	Polypeptides	pos
533.2586	383.58	4.01	C22H40N8O5	K	Postin	Polypeptides	neg
581.2786	418.26	3.72	C22H40N8O5	HCOOK	Postin	Polypeptides	pos
177.0331	463.98	4.69	C5H10N2O3S	H	Cys-Gly;Cysteine-S-Acetamide	Polypeptides	neg
187.0716	424.98	4.17	C7H12N2O4	H	L-glycyl-L-hydroxyproline;N-Acetylglutamine	Polypeptides	neg
233.0509	191.58	3.86	C7H12N2O4	Na_Na	L-glycyl-L-hydroxyproline;N-Acetylglutamine	Polypeptides	pos
Polyamines							
239.1647	428.52	1.38	C10H26N4	K	Spermine	Polyamines	neg
301.1766	388.14	3.32	C12H28N4O2	NaCl	N1-Acetylspermine	Polyamines	pos
331.2094	422.16	4.29	C14H30N4O2	Na_Na	N1,N12-Diacetylspermine	Polyamines	pos
Quaternary Amines							
338.2300	465.90	0.47	C17H33NO4	Na	Decanoylcarnitine;O-Decanoyl-L-carnitine	Quaternary Amines	pos
330.2639	444.30	3.39	C18H35NO4	H	4,8-dimethylnonanoyl carnitine	Quaternary Amines	pos
344.2793	457.86	0.58	C19H37NO4	H	Dodecanoylcarnitine	Quaternary Amines	pos
372.3106	478.02	0.64	C21H41NO4	H	Tetradecanoylcarnitine	Quaternary Amines	pos
398.3263	485.88	0.45	C23H43NO4	H	trans-Hexadec-2-enoyl carnitine	Quaternary Amines	pos
430.3164	425.28	0.33	C23H43NO6	H	Hexadecanedioic acid mono-L-carnitine ester	Quaternary Amines	pos
400.3421	501.54	0.05	C23H45NO4	H	L-Palmitoylcarnitine	Quaternary Amines	pos
414.3581	508.68	0.77	C24H47NO4	H	Heptadecanoyl carnitine	Quaternary Amines	pos
424.3422	491.70	0.16	C25H49NO4	H	Linolealidyl carnitine;Linoleyl carnitine	Quaternary Amines	pos
448.3396	508.68	0.25	C25H47NO4	Na	Elaidic carnitine or related compounds	Quaternary Amines	pos
428.3739	518.04	1.05	C25H49NO4	H	Stearoylcarnitine	Quaternary Amines	pos
584.4885	696.00	1.71	C33H65NO4	HCOOH	Hexacosanoyl carnitine	Quaternary Amines	neg
356.0420	66.54	0.42	C9H15N3O2S	HCOONa	Ergothioneine	Quaternary Amines	pos
Carbohydrates							
365.1060	70.44	4.41	C12H22O11	Na	Alpha-Lactose;D-Maltose;Melibiose;Sucrose	Carbohydrates	pos
382.1343	458.82	2.25	C14H23NO11	H	N-Acetyl-9-O-lactoylneuraminic acid	Carbohydrates	pos
485.1127	587.46	3.59	C15H26N2O12	NaCl	Chitobiose	Carbohydrates	pos
201.0374	83.46	3.38	C6H12O6	Na	D-Fructose;D-Galactose;D-Glucose;D-Mannose;Myoinositol	Carbohydrates	neg
253.0140	169.44	4.58	C7H14O5S	Na_Na	4-Methylthio-Alpha-D-Mannose;O1-Methyl-4-Deoxy-4-Thio-Alpha-D-Glucose;O1-Methyl-4-Deoxy-4-Thio-Beta-D-Glucose	Amino ketones	neg
Fatty Acids and Conjugates							
173.1535	604.14	0.58	C10H20O2	H	2-methyl nonanoic acid or related compounds	Fatty Acids and Conjugates	pos
173.1536	648.06	0.23	C10H20O2	H	3-methyl-nonanoic acid or related compounds	Fatty Acids and Conjugates	pos
173.1536	703.80	0.23	C10H20O2	H	7-methyl-nonanoic acid or related compounds	Fatty Acids and Conjugates	pos
173.1536	739.08	0.29	C10H20O2	H	2-methyl nonanoic acid or related compounds	Fatty Acids and Conjugates	pos
185.1535	440.52	0.43	C11H20O2	H	11-Undecanoyl carnitine;2-hendecenoic acid or related compounds	Fatty Acids and Conjugates	pos
213.1848	461.64	0.42	C13H24O2	H	12-tridecenoic acid;2-methyl-2-dodecenoic acid or related compounds	Fatty Acids and Conjugates	pos
295.1885	601.20	1.05	C14H28O2	HCOONa	Myristic acid	Fatty Acids;	neg
311.1974	459.72	0.64	C16H25NO4	NH3	10E-heptadecenoic acid;10-methyl-9-hexadecenoic acid or related compounds	Fatty Acids and Conjugates	neg
251.2005	446.22	0.20	C16H26O2	H	4,7,10-hexadecatrienoic acid or related compounds	Fatty Acids and Conjugates	pos
255.2318	476.16	0.04	C16H30O2	H	Palmitoleic acid	Fatty Acids and Conjugates	pos
253.2169	615.90	1.66	C16H30O2	H	10-hexadecenoic acid or related compounds	Fatty Acids and Conjugates	neg
297.1817	447.96	1.01	C16H30O2	Na_Na	Palmitoleic acid	Fatty Acids and Conjugates	neg
274.2739	448.20	0.55	C16H32O2	NH3 (Na_Na)	Palmitic acid	Fatty Acids and Conjugates	pos/neg
255.2325	656.88	1.92	C16H32O2	H	13-methyl-pentadecanoic acid or related compounds	Fatty Acids and Conjugates	neg
267.2326	641.82	1.27	C17H32O2	H	10E-heptadecenoic acid or related compounds	Fatty Acids and Conjugates	neg
311.1427	562.86	2.67	C18H26O2	K	13E-octadecene-9,11-dienoic acid or related compounds	Fatty Acids and Conjugates	neg
279.2318	438.66	0.25	C18H30O2	H	Alpha-Linolenic acid	Fatty Acids	pos
311.2215	466.44	0.58	C18H30O4	H	(9Z,11E,14Z)-(13S)-hydroperoxyoctadeca-(9,11,14)-trienoate or related compounds	Fatty Acids and Conjugates	pos
341.2444	488.82	0.64	C19H38O2	Na_Na	(+)-16-methyl stearic acid or related compounds	Fatty Acids	neg
347.2200	633.30	1.04	C18H32O2	HCOONa	10E,12E-octadecadienoic acid or related compounds	Fatty Acids and Conjugates	neg
325.2115	634.44	2.03	C18H32O2	Na_Na	Linoleic acid	Fatty Acids and Conjugates	pos
295.2276	443.04	0.95	C18H32O3	H	13S-hydroxyoctadecadienoic acid	Fatty Acids;	neg
313.2371	474.30	0.67	C18H32O4	H	(9Z,11E,13E)-13-Hydroperoxyoctadeca-9,11-dienoic acid or related compounds	Fatty Acids	pos
283.2631	499.50	0.32	C18H34O2	H	Oleic acid	Fatty Acids	pos
281.2483	509.04	1.07	C18H34O2	H	(11E)-Octadecenoic acid or related compounds	Fatty Acid	neg
283.2632	663.66	0.32	C18H34O2	H	Oleic acid	Fatty Acids	pos
327.2273	667.62	1.74	C18H34O2	Na_Na (H)	(11E)-Octadecenoic acid;(6Z)-Octadecenoic acid or related compounds	Fatty Acids	pos/neg
327.2286	479.10	1.59	C18H36O2	Na_Na	Stearic acid	Fatty Acids	neg
399.1968	477.06	2.08	C18H36O2S	HCOOK	2-mercaptopentadecanoic acid	Fatty Acids and Conjugates	pos
325.2373	481.86	0.03	C19H32O4	H	methyl 15-hydroperoxy-9Z,12Z,16E-octadecatrienoate or related compounds	Fatty Acids and Conjugates	pos
374.2539	400.68	0.53	C19H32O6	NH3	methyl 10,12-dihydroperoxy-8E,13E,15Z-octadecatrienoate or related compounds	Fatty Acids and Conjugates	pos
327.2529	485.88	0.15	C19H34O4	H	11-methoxy-12,13-epoxy-9-octadecenoic acid or related compounds	Fatty Acids and Conjugates	pos
369.1955	443.70	1.65	C19H36O2	KCl	10E-nonadecenoic acid or related compounds	Fatty Acids and Conjugates	neg
339.2286	488.82	0.91	C19H36O2	Na_Na	10E-nonadecenoic acid;10-methylene-octadecanoic acid or related compounds	Fatty Acids and Conjugates	neg

297.2790	513.18	0.64	C19H36O2	H	10E-nonadecenoic acid;10-methylene-octadecanoic acid;10Z-nonadecenoic acid or related compounds	Fatty Acids and Conjugates	pos	
371.2116	465.72	2.51	C19H38O2	KCl	(+)-16-methyl stearic acid;"(2R,6S,10S)-pristanate";11-methyl-octadecanoic acid or related compounds	Fatty Acids and Conjugates	neg	
316.3212	478.02	0.76	C19H38O2	NH3	(+)-16-methyl stearic acid;"(2R,6S,10S)-pristanate";11-methyl-octadecanoic acid or related compounds	Fatty Acids and Conjugates	pos	
305.2473	448.14	0.62	C20H32O2	H	Arachidonic acid	Fatty Acids	pos	
307.2640	686.28	0.94	C20H36O2	H	11,14-eicosadienoic acid or related compounds	Fatty Acids and Conjugates	neg	
311.2943	528.90	0.42	C20H38O2	H	13-eicosenoic acid or related compounds	Fatty Acids and Conjugates	pos	
357.2644	484.86	0.56	C20H38O5	H	11,13-dimethoxy-12-hydroxy-9-octadecenoic acid;"13,14-Dihydro PGF-1a"; or related compounds	Fatty Acids and Conjugates	neg	
369.2069	488.34	0.57	C22H28O2	HCOOH	4,7,10,13-Docosatetraenoic acid or related compounds	Fatty Acids and Conjugates	neg	
329.2473	455.88	0.58	C22H32O2	H	Docosahexanoic acid	Fatty Acids and Conjugates	pos/neg	
381.2754	531.84	0.87	C22H42O2	Na_Na	(13Z)-Docosenoic acid or related compounds	Fatty Acids and Conjugates	neg	
383.2911	533.82	1.12	C22H44O2	Na_Na	19-methyl-heneicosanoic acid;3-methyl-heneicosanoic acid;Docosanoic acid;Isobehenic acid	Fatty Acids and Conjugates	neg	
465.3456	801.42	1.01	C23H49N2O5P	H	Sphingosyl-phosphocholine;"2,4,6-trimethyl-2,15-tetracosadienoic acid";	Fatty Acids and Conjugates	pos	
425.2574	592.38	4.63	C23H44O2	KCl	14E-tricosenoic acid or related compounds	Fatty Acids and Conjugates	neg	
409.3039	460.80	3.44	C24H44O2	Na_Na	5,9-tetracosadienoic acid	Fatty Acids and Conjugates	pos	
187.0717	75.90	1.87	C8H16O2	Na_Na	Caprylic acid	Fatty Acids and Conjugates	neg	
187.0717	169.44	4.01	C8H16O2	Na_Na	Caprylic acid	Fatty Acids and Conjugates	neg	
187.0710	203.52	1.98	C8H16O2	Na_Na	Caprylic acid	Fatty Acids and Conjugates	neg	
187.0709	234.24	2.46	C8H16O2	Na_Na	Caprylic acid	Fatty Acids and Conjugates	neg	
187.0717	388.14	4.01	C8H16O2	Na_Na	Caprylic acid	Fatty Acids and Conjugates	neg	
271.0246	169.86	4.02	C9H16O2	NaClx2	2-amyl 3-butenic acid;2E-nonenic acid or related compounds	Fatty Acids and Conjugates	neg	
271.0245	200.76	4.46	C9H16O2	NaClx2	2-amyl 3-butenic acid;2E-nonenic acid or related compounds	Fatty Acids and Conjugates	neg	
271.0247	374.22	3.91	C9H16O2	NaClx2	2-amyl 3-butenic acid;2E-nonenic acid or related compounds	Fatty Acids and Conjugates	neg	
Fatty aldehydes								
167.1430	440.52	0.30	C11H18O	H	2,5-undecadienal	Fatty aldehydes	pos	
209.1898	466.44	0.81	C14H24O	H	5,8-tetradecadienal	Fatty aldehydes	pos	
240.2321	462.54	0.37	C15H26O	NH3	^(1E,4S,5E,7R)-Germacra-1(10) or related compounds	Fatty aldehydes	pos	
270.2794	458.88	0.96	C17H32O	NH3	14-Methyl-8E-hexadecenal or related compounds	Fatty aldehydes	pos	
309.2431	561.06	1.20	C18H32O	HCOOH	9,12-octadecadienal	Fatty aldehydes	pos	
367.2159	576.72	4.49	C20H38O	KCl	11Z-Eicosenal	Fatty aldehydes	neg	
169.0609	169.44	0.71	C8H14O	Na_Na	2-octenal or related compounds	Fatty aldehydes	neg	
Fatty alcohols								
205.1587	430.92	0.24	C14H20O	H	13-tetradecen-2,4-diy-n-1-ol	Fatty alcohols	pos	
253.2139	562.02	0.43	C14H30O2	Na	2,2,9,9-tetramethyl-undecan-1,10-diol	Fatty alcohols	pos	
297.2398	599.22	0.74	C15H32O	HCOONa	3S,7S-dimethyl-2S-tridecanol	Fatty alcohols	pos	
258.2794	454.92	1.12	C16H32O	NH3	1,2-Epoxyhexadecane;11Z-hexadecen-1-ol or related compounds	Fatty alcohols	pos	
311.2554	626.88	0.90	C16H34O	HCOONa	14-methyl-1-pentadecanol;1-Hexadecanol;"3S,7S-dimethyl-2S-tetradecanol"	Fatty alcohols	pos	
343.1316	555.12	2.94	C17H22O2	HCOOK	"1,9Z,16-heptadecatrien-4,6-diy-n-3,8-diol";"5,8,11-heptadecatriynoic acid";Cicutoxin;;	Fatty alcohols	pos	
325.2711	587.46	0.65	C17H36O	HCOONa	14-methyl-1-hexadecanol	Fatty alcohols	pos	
313.2494	480.78	1.63	C18H38O	Na_Na	3S,7S-dimethyl-2-hexadecanol;Octadecanol	Fatty alcohols	neg	
371.2705	465.72	1.83	C20H42O2	NaCl	1,2-eicosanediol; 13-methyl-1,2-nonadecanediol	Fatty alcohols	neg	
371.2895	465.72	3.21	C21H44O2	Na_Na	1,2-heneicosanediol;"13-methyl-1,2-eicosanediol";"15-methyl-1,2-eicosanediol";	Fatty alcohols	pos/neg	
143.0452	463.98	1.47	C6H12O	Na_Na	2E-hexenol;2-Oxohexane; or Unsaturated alcohol	Fatty alcohols	neg	
145.0609	424.98	1.24	C6H14O	Na_Na	3-Methylpentan-1-ol;Hexan-1-ol	Fatty alcohols	neg	
Hydroxy-oxo fatty acids								
263.1618	430.92	0.04	C14H24O3	Na	(1R,2R)-3-oxo-2-pentyl-cyclopentanebutanoic acid or related compounds	Hydroxy fatty acids	pos	
285.1434	501.54	1.05	C14H24O3	Na_Na	6(R)-hydroxy-tetradeca-2E,8Z-dienoate or related compounds	Hydroxy fatty acids	pos	
287.1611	374.22	2.23	C14H28O3	Na_Na	10-hydroxy-tetradecanoic acid or related compounds	Hydroxy fatty acids	neg	
301.1410	558.18	0.53	C16H22O4	Na	2-Ethylhexyl phthalate;3'-carboxy-alpha-chromanol;4-prenylphlorisovalerophenone;Alpha-CEHC;Dibutyl phthalate;Diisobutyl phthalate	Hydroxy fatty acids	pos	
265.1806	442.20	1.28	C16H26O3	H	(2E,6E)-(10R,11S)-10,11-Epoxy-3,7,11-trimethyltrideca-2,6-dienoic acid or related compounds	Hydroxy fatty acids	neg	
265.1804	549.78	1.96	C16H26O3	H	(9R,13R)-1a,1b-dinor-10,11-dihydro-12-oxo-15-phytoenoic acid or related compounds	Hydroxy fatty acids	neg	
337.1985	444.30	0.68	C16H28O3	HCOONa	(1R,2R)-3-oxo-2-pentyl-cyclopentanehexanoic acid;"(1S,2S)-3-oxo-2-pentyl-cyclopentanehexanoic acid	Hydroxy fatty acids	pos	
291.1929	446.22	0.41	C16H28O3	Na	(1S,2S)-3-oxo-2-pentyl-cyclopentanehexanoic acid or related compounds	Hydroxy fatty acids	pos	
313.1767	404.40	0.57	C16H30O3	Na_Na	(+)-12-hydroxy-9Z-hexadecenoic acid;10-keto palmitic acid or related compounds	Hydroxy fatty acids	neg	
269.2119	510.30	1.19	C16H30O3	H	10-keto palmitic acid or related compounds	Hydroxy fatty acids	neg	
269.2119	570.84	1.08	C16H30O3	H	10-oxo-14-methyl-pentadecanoic acid or related compounds	Hydroxy fatty acids	neg	
315.1924	424.98	0.57	C16H32O3	Na_Na	11-hydroxy palmitic acid or related compounds	Hydroxy fatty acids	neg	
271.2277	598.26	0.70	C16H32O3	H	14-hydroxy palmitic acid or related compounds	Hydroxy fatty acids	neg	
355.2097	567.90	1.32	C16H32O4	HCOONa	10,16-Dihydroxyhexadecanoic acid or related compounds	Hydroxy fatty acids	neg	
309.2043	627.54	1.39	C16H32O4	Na	3,12-dihydroxy palmitic acid or related compounds	Hydroxy fatty acids	neg	
367.2106	467.94	1.20	C17H32O4	HCOONa	2-methyl-hexadecanedioic acid or related compounds	Hydroxy fatty acids	neg	
369.2253	443.70	1.44	C17H34O4	HCOONa	MG(0:0/14:0/0:0);MG(14:0/0:0/0:0)	Hydroxy fatty acids	neg	
369.2254	487.26	1.19	C17H34O4	HCOONa	MG(0:0/14:0/0:0);MG(14:0/0:0/0:0)	Hydroxy fatty acids	neg	
347.1828	430.92	3.31	C18H28O5	Na	12-oxo-14,18-dihydroxy-9Z,13E,15Z-octadecatrienoic acid	Oxo fatty acids	pos	
293.2121	435.36	0.34	C18H30O3	H	(9R,13R)-10,11-dihydro-12-oxo-15-phytoenoic acid or related compounds	Hydroxy fatty acids	neg	
319.2245	548.52	1.19	C18H32O3	Na (H)	(1R,2R)-3-oxo-2-pentyl-cyclopentaneoctanoic acid or related compounds	Hydroxy fatty acids	pos/neg	
341.2080	450.36	1.85	C18H34O3	Na_Na	(6R,7S)-6,7-Epoxyoctadecanoic acid;(9Z)-(12S)-Hydroxyoctadecenoic acid;10-hydroxy-8-octadecenoic acid or related compounds	Hydroxy fatty acids	neg	
297.2431	572.82	1.45	C18H34O3	H	10R-hydroxy-8E-octadecenoic acid or related compounds	Hydroxy fatty acids	neg	
299.2588	565.02	1.30	C18H36O3	H	(R)-2-Hydroxystearate or related compounds	Hydroxy fatty acids	neg	
315.2535	518.10	1.78	C18H36O4	H	(9R,10R)-Dihydroxyoctadecanoic acid or related compounds	Hydroxy fatty acids	pos	
385.2562	536.70	0.39	C18H36O4	HCOONa	(9S,10S)-9,10-Dihydroxyoctadecanoate or related compounds	Hydroxy fatty acids	pos	
383.2413	588.42	0.50	C18H36O4	HCOONa	10,11-dihydroxy stearic acid or related compounds	Hydroxy fatty acids	neg	
337.2357	679.98	3.83	C18H36O4	Na	11,12-dihydroxy stearic acid or related compounds	Hydroxy fatty acids	neg	
399.2373	571.86	2.35	C18H36O5	HCOONa	18-hydroxy-9S,10R-dihydroxy-stearic acid; 9,10,18-trihydroxystearate or related compounds	Hydroxy fatty acids	neg	
371.2407	495.60	0.78	C18H36O6	Na	Sativic acid	Hydroxy fatty acids	pos	
371.2320	465.72	3.85	C19H38O3	NaCl	19-hydroxy-nonadecanoic acid;2-hydroxy-nonadecanoic acid	Hydroxy fatty acids	neg	
369.2751	518.10	0.16	C21H42O2	Na_Na	(+)-18-methyl-eicosanoic acid;19-methyl-eicosanoic acid;"2,6-dimethyl-nonadecanoic acid";Heneicosanoic acid;Homophytanic acid	Methyl branched fatty acids	neg	
372.3476	505.38	1.13	C22H42O3	NH3	10-oxo-docosanoic acid or related compounds	Oxo fatty acids	pos	
400.3789	536.70	0.92	C24H46O3	NH3	24-hydroxy-10Z-tetracosenoic acid;2-hydroxy-15Z-tetracosenoic acid;3-oxo-tetracosanoic acid;Hydroxynervonic acid	Hydroxy fatty acids	pos	
133.0865	577.68	4.51	C6H12O3	H	5-Hydroxyhexanoic acid;Hydroxyisocaproic acid	Hydroxy Acids	pos	
Eicosanoids								
303.2317	448.14	0.43	C20H30O2	H	(+)-Pimelic acid or related compounds	Eicosanoids	pos	

319.2276	452.82	4.39	C20H32O3	H	(15S)-15-Hydroxy-5,8,11-cis-13-trans-eicosatetraenoate or related compounds	Eicosanoids	neg	
321.2432	455.22	0.84	C20H34O3	H	12-HETrE;12R-HETrE; 15-oxo-11Z,13E-eicosadienoic acid or related compounds	Eicosanoids	neg	
356.2793	459.72	0.73	C20H34O4	NH3	10,11-dihydro-12-epi-leukotriene B4;"11,12-DHET";11-deoxy-PGE1;11-deoxy-PGF2a;11-deoxy-PGF2beta;12-keto-tetrahydro-Leukotriene B4;"14,15-DHET";"15-hydroperoxyeicosa-8Z,11Z,13E-trienoate";"5,6-DHET";"5,6-dihydroxy-8,11,14-eicosatrienoic acid";"6,7-dihydro-12-epi-leukotriene B4";"8,9-DHET";"8,9-dihydroxy-5,11,14-eicosatrienoic acid";Aphidicolin;S 1033;Zoapatanol;;	Eicosanoids	pos	
339.2530	489.78	0.12	C20H34O4	H	10,11-dihydro-12-epi-leukotriene B4;"11,12-DHET";11-deoxy-PGE1;11-deoxy-PGF2a;11-deoxy-PGF2beta;12-keto-tetrahydro-Leukotriene B4;"14,15-DHET";"15-hydroperoxyeicosa-8Z,11Z,13E-trienoate";"5,6-DHET";"5,6-dihydroxy-8,11,14-eicosatrienoic acid";"6,7-dihydro-12-epi-leukotriene B4";"8,9-DHET";"8,9-dihydroxy-5,11,14-eicosatrienoic acid";Aphidicolin;S 1033;Zoapatanol	Eicosanoids	pos	
583.1303	463.56	0.65	C20H36O12	NaCl*2	3'-O-N-Octanoyl-a-D-Glucopyranosyl-B-D-Fructofuranoside;"N-Octanoyl-B-D-Fructofuranosyl-a-D-Glucopyranoside,Sucrose Monocaproylate"	Eicosanoids	neg	
369.2634	443.70	3.25	C20H36O3	HCOOH	11(R)-HEDE or related compounds	Eicosanoids	neg	
369.2634	490.74	3.41	C20H36O3	HCOOH	11S-HEDE or related compounds	Eicosanoids	neg	
Fatty amides								
256.2632	448.14	0.94	C16H33NO	H	Palmitic amide	Fatty amides	pos	
294.2405	552.24	0.37	C16H33NO2	Na	N-(Tetradecanoyl)-ethanolamine/2-amino-hexadecanoic acid	Fatty amides/Amino fatty acid	pos	
282.2790	474.30	0.60	C18H35NO	H	Elaidoylamide;Oleamide	Fatty amides	pos	
348.2874	610.02	0.37	C20H39NO2	Na	N-Oleoylethanolamine	Fatty amides	pos	
374.3031	597.24	0.45	C22H41NO2	Na	Anandamide (20:2, n-6)	Fatty amides	pos	
382.3068	494.88	0.16	C22H45NO	Na_Na	Docosanamide	Fatty amides	neg	
430.2857	511.26	2.00	C22H45NO2	KCl	Eicosanoyl-EA	Fatty amides	pos	
504.2398	429.72	0.10	C25H43NO2	NaClx2	"(-)-N-(1R-methyl-2-hydroxy-ethyl) alpha,alpha-dimethylarachidonoyl amine" or related compounds	Fatty amides	neg	
512.3043	483.78	4.57	C25H51NO2	NaClx2	Tricosanoyl-EA	Fatty amides	neg	
510.2523	469.80	5.00	C29H43NO2	KCl	(+/-)N-(1-methyl-2-hydroxy-2-phenyl-ethyl) arachidonoyl amine	Fatty amides	neg	
Fatty acyl glycosides								
545.3663	542.58	0.64	C26H52O7	HCOONa	1-O-alpha-D-glucopyranosyl-1,2-eicosandiol	Fatty acyl glycosides	pos	
671.3632	571.62	1.16	C32H58O13	Na	25-O-(2"-beta-D-glucopyranosyl-beta-D-glucopyranosyl)-25-hydroxy-11E-eicosenoic acid	Fatty acyl glycosides	neg	
691.3669	599.22	2.94	C32H62O8	NaClx2	1-(O-alpha-D-glucopyranosyl)-3-keto-(1,25R)-hexacosanediol	Fatty acyl glycosides	pos	
655.4203	600.24	1.57	C34H66O9	K	1-(O-alpha-D-glucopyranosyl)-25-keto-(1,3R,27R)-octacosanetriol or related compounds	Fatty acyl glycosides	neg	
Carboxylic acids								
307.1886	592.38	1.50	C16H30O4	Na	10-hydroxy-16-oxo-hexadecanoic acid;"2,3-Dihydroxycyclopentaneundecanoic acid";"9-hydroxy-16-oxo-hexadecanoic acid;Hexadecanedioic acid	Dicarboxylic acids	neg	
299.2215	464.46	0.70	C17H30O4	H	8E-Heptadecenedioic acid	Dicarboxylic acids	pos	
369.3013	443.70	0.87	C22H42O4	H	Di(2-ethylhexyl) adipate;Docosanedioic acid	Dicarboxylic acids	neg	
393.2978	577.68	0.79	C22H42O4	Na	Di(2-ethylhexyl) adipate;Docosanedioic acid	Dicarboxylic acids	pos	
402.3577	499.50	0.10	C23H44O4	NH3	Tricosanedioic acid	Dicarboxylic acids	pos	
416.3737	513.18	0.65	C24H46O4	NH3	Tetracosanedioic acid	Dicarboxylic acids	pos	
444.4049	554.22	0.36	C26H50O4	NH3	Hexacosanedioic acid	Dicarboxylic acids	pos	
543.2937	615.90	4.58	C26H50O4	NaClx2	Hexacosanedioic acid	Dicarboxylic acids	pos	
449.3599	788.94	0.56	C26H50O4	Na	Hexacosanedioic acid	Dicarboxylic acids	pos	
193.0351	64.56	0.05	C6H8O7	H	Citric acid;Isocitric acid	Tricarboxylic Acids	pos	
Steroids and Derivatives								
339.1573	571.44	3.45	C18H22O2	HCOONa	Estrone	Steroids and Steroid Derivatives	pos	
355.1528	562.02	1.63	C18H22O3	HCOONa (HCOOK)	2-Hydroxyestrone	Steroids and Steroid Derivatives	pos/neg	
357.1473	566.94	2.86	C18H24O2	HCOOK	17a-Estradiol; Estradiol	Steroids and Steroid Derivatives	pos	
277.2162	434.82	0.14	C18H28O2	H	19-Norandrosterone; 19-Noretiocholanolone	Steroids and Steroid Derivatives	pos	
371.1626	573.84	4.58	C19H26O2	HCOOK	Androstenedione	Steroids and Steroid Derivatives	pos	
273.2213	441.54	0.11	C19H28O	H	3-Oxo-delta1-steroid; 5a-Androst-3-en-17-one	Steroids and Steroid Derivatives	pos	
373.1986	442.38	0.13	C19H28O3	HCOONa	11-Ketotiocholanolone;16a-Hydroxydehydroisandrosterone;;	Steroids and Steroid Derivatives	pos	
361.2349	485.88	0.17	C19H32O2	HCOONa	Androstanediol	Steroids and Steroid Derivatives	pos	
311.2007	566.04	4.37	C21H28O2	H	16-Dehydroprogesterone or related compounds	Steroids and Steroid Derivatives	neg	
383.1636	429.00	4.31	C21H28O4	K	11-Dehydrocorticosterone or related compounds	Steroids and Steroid Derivatives	pos	
383.1837	581.58	1.77	C21H28O5	Na	Aldosterone;Cortisone	Steroids and Steroid Derivatives	pos	
385.1787	583.80	3.06	C21H30O4	K	Cortisolone	Steroids and Steroid Derivatives	pos	
401.2297	455.88	0.77	C21H32O3	HCOONa	16-a-Hydroxypregnenolone;21-Hydroxypregnenolone;;	Steroids and Steroid Derivatives	pos	
417.2248	438.66	0.34	C21H32O4	HCOONa	11b,21-Dihydroxy-5b-pregnane-3,20-dione or related compounds	Steroids and Steroid Derivatives	pos	
403.2455	463.56	0.67	C21H34O3	HCOONa	Tetrahydrodeoxycorticosterone	Steroids and Steroid Derivatives	pos	
419.2403	444.30	0.17	C21H34O4	HCOONa	5a-Tetrahydrocorticosterone;"5beta-Pregnane-3alpa,17alpa,20alpa-triol-11-one";"9-deoxy-9-methylene-PGE2;Tetrahydrocorticosterone	Steroids and Steroid Derivatives	pos	
384.2743	430.92	0.39	C21H34O5	NH3	5a-Tetrahydrocortisol;Cortolone;Tetrahydrocortisol	Steroids and Steroid Derivatives	pos	
367.2484	467.94	4.93	C21H36O5	H	Beta-Cortol;Cortol	Steroids and Steroid Derivatives	neg	
377.1968	567.96	2.44	C21H28O6	H (HCOOH)	18-Oxocortisol	Steroids and Steroid Derivatives	pos/neg	
504.2750	476.10	0.67	C26H45NO	NaClx2	25-Azacholesterol	Steroids and Steroid Derivatives	pos	
455.3346	659.76	0.75	C26H46O6	H	27-norcholestanehexol	Steroids and Steroid Derivatives	pos	
511.2906	447.96	1.27	C27H44O9	H	(24R)-11alpa,20,24-trihydroxyecdysone;"(25R)-11alpa,20,26-trihydroxyecdysone";"(25S)-11alpa,20,26-trihydroxyecdysone";;	Cholesterol and derivatives	neg	
417.3455	513.18	3.07	C27H48	Na_Na	5beta-cholestane	Cholesterol and derivatives	pos	
454.3897	544.56	1.28	C27H48O4	NH3	3alpa,7alpa,12alpa,26-Tetrahydroxy-5beta-cholestane or related compounds	Steroids and Steroid Derivatives	pos	
497.2937	527.88	4.28	C30H48O	KCl	4alpa,14alpa-dimethyl-24-methylene-cholest-7,9(11)-dien-3beta-ol	Ergosterols and C24-methyl derivatives	neg	
466.3895	548.52	0.99	C28H48O4	NH3	Teasterone;Typhasterol	Ergosterols and C24-methyl derivatives	pos	
459.3559	526.92	4.03	C29H50O	Na_Na	Beta-Sitosterol	Steroids and Steroid Derivatives	pos	
541.3406	619.20	4.53	C29H52O	NaCl_HCOONa	23R,24R-dimethylcholestan-3b-ol or related compounds	Ergosterols and C24-methyl derivatives	neg	
553.2842	549.78	4.18	C33H38N4O4	H	Integresine	Steroids and Steroid Derivatives	neg	
693.5314	712.62	4.79	C44H74O2	NaCl	episteryl palmitoleate;fecosteryl palmitoleate;;	Ergosterols and C24-methyl derivatives	pos	
733.5092	504.24	2.13	C46H76O2	KCl	ergosteryl oleate	Ergosterols and C24-methyl derivatives	neg	
Bile acids								
473.2511	518.04	3.63	C22H33NO9	NH3	(23R)-23-Hydroxy-3,7-dioxo-5beta-cholan-24-oic Acid or related compounds	Bile acids and derivatives	pos	
414.3210	464.46	0.84	C23H40O5	NH3	24-Nor-5beta-choleane-3alpa,7alpa,12alpa,22,23-pentol;PGF2alpa isopropyl ester	Bile acids and derivatives	pos	
367.2293	467.94	3.89	C24H32O3	H	3-Oxochola-1,4,6-trien-24-oic Acid	Bile acids and derivatives	neg	
383.2236	588.42	0.42	C24H32O4	H	(22E)-12alpa-Hydroxy-3-oxochola-1,4,22-trien-24-oic Acid or related compounds	Bile Acids	neg	
399.2181	571.86	0.80	C24H32O5	H	3,7,12-Trioxo-5beta-cho-1-en-24-oic Acid or related compounds	Bile Acids	neg	
355.2630	474.30	0.42	C24H34O2	H	5beta-Chola-3,8(14),11-trien-24-oic Acid	Bile acids and derivatives	pos	
369.2441	443.70	1.65	C24H34O3	H	(20S,22E)-3beta-Hydroxychola-5,16,22-trien-24-oic Acid or related compounds	Bile Acids	neg	
373.2735	474.30	0.56	C24H36O3	H	(20S)-3beta-Hydroxychola-5,16-dien-24-oic Acid or related compounds	Bile acids and derivatives	pos	
449.2541	520.02	0.82	C24H36O5	HCOOH	(23R)-23-Hydroxy-3,7-dioxo-5beta-cholan-24-oic Acid or related compounds	Bile Acids	neg	

413.2662	752.82	0.31	C24H38O4	Na	(22E)-3alpha,12alpha-Dihydroxy-5beta-chole-22-en-24-oiic Acid or related compounds	Bile acids and derivatives	pos	
445.2558	453.96	2.31	C24H38O6	Na	(3r,5r)-7-(1r,2r,6s,8r,8as)-2,6-Dimethyl-8-([(2r)-2-Methylbutanoyl]Oxy)-1,2,6,7,8,8a-Hexahydronaphthalen-1-Yl)-3,5-Dihydroxyheptanoic Acid or related compounds	Bile acids and derivatives	pos	
391.2847	512.22	1.69	C24H40O4	H	Chenodeoxycholic acid;Deoxycholic acid;Hyodeoxycholic acid;Isoursodeoxycholic acid;Ursodeoxycholic acid	Bile Acids	neg	
431.2766	474.30	0.39	C24H40O5	Na	(22R)-3alpha,7alpha,22-Trihydroxy-5beta-cholelan-24-oiic Acid or related compounds	Bile acids and derivatives	pos	
407.2796	477.06	4.32	C24H40O5	H	1b,3a,12a-Trihydroxy-5b-choleanoic acid;Cholic acid;Hyocholic acid;Ursocholic acid	Bile Acids	neg	
450.3209	457.86	1.11	C26H43NO5	H	Chenodeoxycholic acid glycine conjugate	Acyl Glycines;Bile Acids	pos	
494.2848	476.10	0.99	C26H43NO5	Na_Na	3alpha,12alpha-Dihydroxy-5beta-cholelan-24-oylglycine or related compounds	Acyl Glycines;Bile Acids	pos/neg	
516.2936	476.70	1.30	C26H43NO5	HCOONa	Chenodeoxycholic acid glycine conjugate	Acyl Glycines;Bile Acids	neg	
464.3010	447.54	1.68	C26H43NO6	H	Glycocholic acid	Acyl Glycines;Bile Acids	neg	
488.2986	449.16	0.63	C26H43NO6	Na	Glycocholic acid	Acyl Glycines;Bile Acids	pos	
482.3475	453.96	4.73	C27H44O6	NH3	3alpha,6alpha,7alpha,12alpha-Tetrahydroxy-5beta-cholest-24-en-26-oiic acid;3-Epicypsone;Ecdysone;Ponasterone A	Bile acids and derivatives	pos	
468.3681	478.02	0.58	C27H46O5	NH3	3a,7a,12a-Trihydroxy-5b-cholestanoic acid or related compounds	Bile acids and derivatives	pos	
484.3633	459.72	0.06	C27H46O6	NH3	1beta,3alpha,7alpha,12alpha-Tetrahydroxy-5beta-cholestan-26-oiic acid or related compounds	Bile acids and derivatives	pos	
686.3416	488.34	3.26	C32H51NO12	HCOOH	(3a,5b,7a,12a)-24-[[carboxymethyl]amino]-1,12-dihydroxy-24-oxocholan-3-yl-b-D-Glucopyranosiduronic acid	Bile Acids	neg	
Vitamins and derivatives								
393.2099	86.04	1.04	C22H32O4S	H	(6RS)-22-oxo-23,24,25,26,27-pentanorvitamin D3 6,19-sulfur dioxide adduct / (6RS)-22-oxo-23,24,25,26,27-pentanocholecalciferol 6,19-sulfur dioxide adduct	Vitamin D2 and derivatives	pos	
415.1918	443.04	3.78	C22H34O4S	Na	(6RS)-22-hydroxy-23,24,25,26,27-pentanorvitamin D3 6,19-sulfur dioxide adduct / (6RS)-22-hydroxy-23,24,25,26,27-pentanocholecalciferol 6,19-sulfur dioxide adduct	Vitamin D2 and derivatives	neg	
597.3108	561.06	1.19	C37H48O3	NaCl	1alpha,25-dihydroxy-25,25-diphenyl-26,27-dinorvitamin D3 / 1alpha,25-dihydroxy-25,25-diphenyl-26,27-dinorcholecalciferol	Vitamin D2 and derivatives	neg	
469.3142	620.76	1.26	C23H44O5	HCOONa	1,2-Didecanoylglycerol	Vitamin D2 and derivatives	pos	
501.2882	476.70	3.49	C29H48O2	KCl	(22alpha)-hydroxy-isofucosterol;"(24R,24R)-Fucosterol epoxide or related compounds	Vitamin D2 and derivatives	neg	
453.2883	612.96	1.32	C28H44O	NaCl	(5E)-isovitamin D2 / (5E)-isogocalciferol or related compounds	Vitamin D2 and derivatives	neg	
422.3263	481.86	0.43	C25H40O4	NH3	11'-carboxy-gamma-chromanol or related compounds	Vitamin D2 and derivatives	pos	
452.3368	464.46	0.49	C26H42O5	NH3	(24R)-1alpha,24,25-trihydroxy-22-oxavitamin D3 / (24R)-1alpha,24,25-trihydroxy-22-oxocholecalciferol or related compounds	Vitamin D2 and derivatives	pos	
460.2728	429.00	3.17	C26H43NO	KCl	25-azavitamin D3 / 25-azacholecalciferol;;	Vitamin D2 and derivatives	pos	
455.2678	583.50	4.70	C27H42O2	NaCl	(22E)-1alpha-hydroxy-22,23-didehydrovitamin D3 / (22E)-1alpha-hydroxy-22,23-didehydrocholecalciferol or related compounds	Vitamin D2 and derivatives	neg	
509.2575	390.90	3.28	C26H43O4P	NaCl	24-(dimethoxyphosphoryl)-25,26,27-trinorvitamin D3 / 24-(dimethoxyphosphoryl)-25,26,27-trinorcholecalciferol or related compounds	Vitamin D2 and derivatives	pos	
464.3367	463.56	0.67	C27H42O5	NH3	(23R)-1alpha,23,25-trihydroxy-24-oxavitamin D3 / (23R)-1alpha,23,25-trihydroxy-24-oxocholecalciferol or related compounds	Vitamin D2 and derivatives	pos	
511.2728	545.52	1.55	C27H43F	NaCl_HCOONa	3-Fluoro-9,10-secocholesta-5,7,10(19)-triene	Vitamin D3 and derivatives	neg	
485.2726	734.22	1.24	C27H44O4S	Na	(6R)-25-hydroxyvitamin D3 6,19-sulfur dioxide adduct / (6R)-25-hydroxycholecalciferol 6,19-sulfur dioxide adduct or related compounds	Vitamin D2 and derivatives	neg	
466.3525	470.34	0.39	C27H44O5	NH3	(23S,25R)-1alpha,23,25,26-tetrahydroxyvitamin D3 / (23S,25R)-1alpha,23,25,26-tetrahydroxycholecalciferol or related compounds	Vitamin D2 and derivatives	pos	
452.3735	518.04	0.11	C27H46O4	NH3	(10R)-1alpha,19,25-trihydroxy-10,19-dihydrovitamin D3 / (10R)-1alpha,19,25-trihydroxy-10,19-dihydrocholecalciferol or related compounds	Vitamin D2 and derivatives	pos	
409.3103	780.12	3.35	C28H42O2	H	calicoferol D or related compounds	Vitamin D3 and derivatives	neg	
553.2653	575.70	4.57	C28H45ClO3	Na_HCOONa	11alpha-(chloromethyl)-1alpha,25-dihydroxyvitamin D3 / 11alpha-(chloromethyl)-1alpha,25-dihydroxycholecalciferol;;	Vitamin D3 and derivatives	neg	
487.2770	575.70	4.10	C28H46O2	KCl	(22alpha)-hydroxy-campest-4-en-3-one or related compounds	Vitamin D3 and derivatives	neg	
499.2940	585.48	4.27	C29H46O3	NaCl	(22E)-1alpha,25-dihydroxy-26,27-dimethyl-22,23-didehydrovitamin D3 / (22E)-1alpha,25-dihydroxy-26,27-dimethyl-22,23-didehydrocholecalciferol or related compounds	Vitamin D2 and derivatives	neg	
492.3680	478.02	0.73	C29H46O5	NH3	18-acetoxy-1alpha,25-dihydroxyvitamin D3 / 18-acetoxy-1alpha,25-dihydroxycholecalciferol	Vitamin D2 and derivatives	pos	
497.3147	617.04	0.72	C30H48O2	NaCl	26,27-Dihomo-1alpha-hydroxy-24-epivitamin D2;"26,27-Dihomo-1alpha-hydroxyvitamin D2;"4,4-Dimethyl-14a-formyl-5a-cholesta-8,24-dien-3b-ol;"4,4-dimethyl-14alpha-formyl-5alpha-cholesta-8,24-dien-3beta-ol"	Vitamin D2 and derivatives	neg	
479.3195	662.52	0.69	C27H43FO3	HCOOH	(10E)-19-fluoro-1alpha,25-dihydroxyvitamin D3 / (10E)-19-fluoro-1alpha,25-dihydroxycholecalciferol or related compounds	Vitamin D2 and derivatives	neg	
509.3297	662.52	4.59	C32H46O5	H	11-(3-acetoxy-1-propynyl)-1alpha,25-dihydroxy-9,11-didehydrovitamin D3 / 11-(3-acetoxy-1-propynyl)-1alpha,25-dihydroxy-9,11-didehydrocholecalciferol	Vitamin D2 and derivatives	neg	
597.3098	398.76	1.64	C34H50O4	KCl	1alpha-hydroxy-18-[m-(1-hydroxy-1-ethylpropyl)-benzyloxy]-23,24,25,26,27-pentanorvitamin D3 / 1alpha-hydroxy-18-[m-(1-hydroxy-1-ethylpropyl)-benzyloxy]-23,24,25,26,27-pentanocholecalciferol	Vitamin D2 and derivatives	pos	
Prostaglandins								
349.1986	427.08	0.32	C18H30O5	Na	2,3-dinor-6-keto-prostaglandin F1 a or related compounds	Prostanoids	pos	
365.1939	410.46	0.99	C18H30O6	Na	2,3-dinor, 6-keto-PGF 1alpha;"2,3-Dinor-TXB2	Prostaglandins	pos	
375.2142	446.22	4.34	C20H32O5	Na	13,14-Dihydro-15-keto-PGE2;20-Hydroxy-leukotriene B4;Prostaglandin E2;Thromboxane A2	Prostanoids	pos	
373.1998	465.72	4.80	C20H32O5	Na	(13E)-11alpha-Hydroxy-9,15-dioxoprost-13-enoate or related compounds	Prostanoids	neg	
391.2089	429.00	0.92	C20H32O6	Na	11-Dehydro-thromboxane B2	Prostanoids	pos	
393.2247	425.28	0.13	C20H34O6	Na	10,11-dihydro-20-dihydroxy-LTB4;19(R)-hydroxy-PGE1 or related compounds	Prostaglandins	pos	
341.2686	503.40	0.12	C20H36O4	H	11-deoxy-PGF1a;11-deoxy-PGF1b;15S-HpEDE;PGE1 alcohol;PGF2alpha alcohol	Prostaglandins	pos	
353.2385	568.92	0.76	C20H40	KCl	8-Isoprostane	Prostanoids	neg	
368.2793	459.72	0.71	C21H34O4	NH3	11-deoxy-11-methylene-PGD2 or related compounds	Prostaglandins	pos	
351.2529	487.80	0.31	C21H34O4	H	3alpha,11beta,17alpha-Trihydroxy-5beta-pregnan-20-one or related compounds	Prostaglandins	pos	
426.2052	581.94	1.13	C23H33NO4	K	17-phenyl-trinor-PGF2alpha amide	Prostaglandins	pos	
517.2413	520.02	3.48	C23H40O7	Na_HCOONa	1(3)-glyceryl-PGF2alpha;2-glyceryl-PGF2alpha	Prostaglandins	neg	
428.3008	429.00	0.37	C23H41NO6	H	PGF2alpha-dihydroxypropanylamine	Prostaglandins	pos	
554.2462	445.32	0.97	C23H41NO6	NaCl_HCOONa	PGF2alpha-dihydroxypropanylamine	Prostaglandins	pos	
Leukotrienes								
440.2449	438.66	1.32	C23H37NOSS	H	11-trans-LTE4;Leukotriene E4	Leukotrienes	pos	
462.2284	440.52	0.19	C23H37NOSS	Na (Na)	(7E,9E,11Z,14Z)-(5S,6R)-6-(cystein-S-yl)-5-hydroxyicoso-7,9,11,14-tetraenoate;"11-trans-LTE4;Leukotriene E4;	Leukotrienes	pos/neg	
442.2621	446.22	0.18	C23H39NOSS	H	Leukotriene E3	Leukotrienes	pos/neg	
517.2351	429.72	2.20	C25H40N2O6S	Na	11-trans-LTD4;"14,15-LTD4";Leukotriene D4	Leukotrienes	neg	

Porphyrins									
580.1019	468.66	0.90	C25H27N3O6	NaClx2		Biotripyrrin-a;Biotripyrrin-b	Porphyrins		neg
589.2993	585.48	1.63	C33H40N4O6	H		D-Urobilin	Porphyrins		pos
569.3151	377.16	4.99	C34H40N4O4	H		Adouetine Y;Crenatine A:Protoporphyrinogen IX	Porphyrins		pos
567.2999	551.40	4.00	C34H40N4O4	H		Adouetine Y;Crenatine A:Protoporphyrinogen IX	Porphyrins		neg
Isoprenoids									
285.2210	448.14	0.95	C20H28O	H		retinal; 11-cis-3,4-dihydroretinol or related compounds	isoprenoids		pos
653.3361	379.14	2.77	C40H50O4	NaCl		4-Keto-4'-hydroxyalloxanthin; 7,8-Didehydroastaxanthin	Isoprenoids		pos
679.3389	417.72	2.49	C40H52O4	HCOOK		3R,3'S-astaxanthin or related compounds	Isoprenoids		neg
655.3396	411.78	2.37	C40H52O5	Na_Na		4-Oxomylloxanthin	Isoprenoids		neg
657.3676	387.00	0.82	C40H54O4	NaCl		4,4'-Dihydroxydiatoxanthin;4-Ketomylxol;7-Methylhexoxanthine;Halocynthiaxanthin;Mylloxanthin	Isoprenoids		pos
641.3521	571.62	1.93	C40H56O2	KCl		(3R,3'R,13-cis)-b,b-Carotene-3,3'-diol or related compounds	isoprenoids		neg
637.4225	657.84	3.09	C40H56O2	HCOONa		Lutein	isoprenoids		pos
643.3900	614.88	1.76	C40H56O3	NaCl		Antheraxanthin;Caloxanthin;Capsanthin;Cucurbitaxanthin A;Desoxyxanthin;Flavoxanthin;Loroxanthin/ 19-Hydroxylutein;"Lutein 5,6-epoxide";Micromonal;Mylxol;; Anhydrotetradolol	Isoprenoids		pos
623.3976	613.92	2.73	C41H58O	NaCl		1'-Hydroxy-gamma-carotene glucoside or related compounds	isoprenoids		neg
789.4253	572.34	0.10	C46H68O6	KCl			Isoprenoids		neg
Sulphates/Sulphonates									
321.0765	384.06			HCOOH	C10H16N2O5S	HCOOH	Biotin sulfone	Biotin and Derivatives	neg
413.1370	464.40	0.29	C19H28O5S	Na_Na	C19H28O5S	Na_Na	DHEA sulfate; Testosterone sulfate	Steroids and Steroid Derivatives	pos
367.1576	467.94	2.37	C19H28O5S	H	C19H28O5S	H	3beta-Hydroxyandrost-5-en-17-one 3-sulfate; Testosterone sulfate	Steroids and Steroid Derivatives	neg
735.3234	467.94				C19H28O5S	H	3beta-Hydroxyandrost-5-en-17-one 3-sulfate; Testosterone sulfate	Steroids and Steroid Derivatives	neg
425.1174	468.66	4.00	C19H28O5S	NaCl	C19H28O5S	NaCl	DHEA sulfate; Testosterone sulfate	Steroids and Steroid Derivatives	neg
435.1454	471.30	1.13	C19H28O5S	HCOONa	C19H28O5S	HCOONa	DHEA sulfate; Testosterone sulfate	Steroids and Steroid Derivatives	neg
435.1451	503.46	1.70	C19H28O5S	HCOONa	C19H28O5S	HCOONa	(15S)-15-Hydroxy-5,8,11-cis-13-trans-icosatetraenoate or related compounds	Steroids and Steroid Derivatives	neg
367.1579	504.24	2.21	C19H28O5S	H	C19H28O5S	H	DHEA sulfate;Testosterone sulfate	Steroids and Steroid Derivatives	neg
367.1581	535.74	1.72	C19H28O5S	H	C19H28O5S	H	3beta-Hydroxyandrost-5-en-17-one 3-sulfate; Testosterone sulfate	Steroids and Steroid Derivatives	neg
383.1531	388.44	0.68	C19H28O6S	H	C19H28O6S	H	3b,16a-Dihydroxyandrostene sulfate; "(11Z)-8,18-ethanoretinol";14'-apo-beta-Carotenal;Desogestrel;;	Steroids and Steroid Derivatives	neg
383.1531	420.60	0.60	C19H28O6S	H	C19H28O6S	H	3b,16a-Dihydroxyandrostene sulfate	Steroids and Steroid Derivatives	neg
383.1528	466.86	1.41	C19H28O6S	H	C19H28O6S	H	3b,16a-Dihydroxyandrostene sulfate	Steroids and Steroid Derivatives	neg
437.1605	442.08	2.31	C19H30O5S	HCOONa	C19H30O5S	HCOONa	Androsterone sulfate	Steroids and Steroid Derivatives	neg
369.1734	487.26	0.57	C19H30O5S	H	C19H30O5S	H	5a-Dihydrotestosterone sulfate;5alpha-dihydrotestosterone sulfate;Androsterone sulfate	Steroids and Steroid Derivatives	neg
437.1609	490.08	1.53	C19H30O5S	HCOONa	C19H30O5S	HCOONa	5a-Dihydrotestosterone sulfate;5alpha-dihydrotestosterone sulfate;Androsterone sulfate	Steroids and Steroid Derivatives	neg
369.1735	520.02	0.81	C19H30O5S	H	C19H30O5S	H	5a-Dihydrotestosterone sulfate;5alpha-dihydrotestosterone sulfate;Androsterone sulfate	Steroids and Steroid Derivatives	neg
369.1734	679.98	0.41	C19H30O5S	H	C19H30O5S	H	5a-Dihydrotestosterone sulfate;5alpha-dihydrotestosterone sulfate;Androsterone sulfate	Steroids and Steroid Derivatives	neg
445.1200	734.16	1.26	C19H30O5S	KCl	C19H30O5S	KCl	Androsterone sulfate	Steroids and Steroid Derivatives	pos
395.1893	509.04	0.68	C21H32O5S	H	C21H32O5S	H	Pregnenolone sulfate	Steroids and Steroid Derivatives	neg
512.2681	495.66	1.29	C26H43NO7S	H	C26H43NO7S	H	Sulfoglycolithocholate;Sulfolithocholyglycine;;	Bile Acids	neg
506.2895	384.24	3.02	C26H45NO5S	Na (HCOONa)	C26H45NO5S	Na (HCOONa)	Lithocholytaurine;Taurolithocholate	Bile Acids	pos/neg
498.2893	444.18	3.23	C26H45NO6S	H	C26H45NO6S	H	Tauroursodeoxycholic acid	Bile Acids	neg
522.2864	476.10	0.92	C26H45NO6S	Na	C26H45NO6S	Na	chenodeoxycholytaurine;Taurochenodeoxycholate;Tauroursodeoxycholic acid;Tauroursodeoxycholic acid	Bile acids and derivatives	pos/neg
498.2887	476.70	4.40	C26H45NO6S	H	C26H45NO6S	H	Tauroursodeoxycholic acid	Bile Acids	neg
514.2834	444.18	1.93	C26H45NO7S	H	C26H45NO7S	H	Taurocholic acid	Bile Acids	neg
552.2423	75.12	3.71	C26H45NO7S	K	C26H45NO7S	K	Taurallocholic acid;Tauro-b-muricholic acid;Taurocholate;Taurohochocholate;Tauroursocholic acid;Aldosterone 18-glucuronide	Bile Acids	neg
465.3037	648.36	0.99	C27H46O4S	H	C27H46O4S	H	Cholesterol sulfate	Steroids and Steroid Derivatives	neg
519.2527	484.80	4.80	C27H46O5S	K	C27H46O5S	K	26-hydroxycholesterol 3-sulfate	Steroids and Steroid Derivatives	neg
481.2987	568.92	1.23	C27H46O5S	H	C27H46O5S	H	26-hydroxycholesterol 3-sulfate	Steroids and Steroid Derivatives	neg
Glucuronides									
465.2494	573.78	2.36	C25H36O8	H	C25H36O8	H	Testosterone glucuronide	Glucuronides	pos
465.2487	456.72	1.53	C25H38O8	H	C25H38O8	H	Androsterone glucuronide	Glucuronides	neg
481.2436	423.24	0.46	C25H38O9	H	C25H38O9	H	11beta-hydroxyandrost-5-en-17-one 3-glucuronide	Glucuronides	neg
467.2646	443.16	0.86	C25H40O8	H	C25H40O8	H	17-hydroxyandrostane-3-glucuronide;18-acetoxy-PGF2alpha-11-acetate methyl ester;"3,17-Androstenediol glucuronide";3-alpha-androstenediol glucuronide	Glucuronides	neg
554.2581	76.32	2.63	C27H36O11	NH3	C27H36O11	NH3	Aldosterone 18-glucuronide	Glucuronides	pos
563.2459	455.88	0.64	C29H38O11	H	C29H38O11	H	Eriocapin	Glucuronides	pos
613.3206	561.06	0.16	C30H48O10	HCOOH	C30H48O10	HCOOH	"(3a,5b,7a)-2,3-carboxy-7-hydroxy-24-norcholan-3-yl-b-D-Glucopyranosiduronic acid";6alpha-Glucuronosylhydroxycholelate;Deoxycholic acid 3-glucuronide	Glucuronides	neg
609.3400	486.84	1.36	C34H52O8	Na	C34H52O8	Na	25-hydroxyvitamin D2 25-(beta-glucuronide) / 25-hydroxyergocalciferol 25-(beta-glucuronide);25-hydroxyvitamin D2-25-glucuronide;25-hydroxyvitamin D2 25-(beta-glucuronide)	Glucuronides	neg
Sphingoid/Sphingolipid									
226.2170	504.24	2.61	C14H29NO	H	C14H29NO	H	Halaminol A	Sphingoid bases	neg
266.2093	513.24	0.94	C14H29NO2	Na	C14H29NO2	Na	(4E,d14:1) sphingosine;2-amino-tetradecanoic acid	Sphingoid bases	pos
310.2354	507.36	0.42	C16H33NO3	Na	C16H33NO3	Na	Prosopimine	Sphingoid bases	pos
368.2192	577.68	4.45	C17H35NO2	HCOOK	C17H35NO2	HCOOK	Anteiso (4E,14-methyl-d17:1) sphingosine";C17 Sphingosine";"iso (4E,15-methyl-d17:1) sphingosine"	Sphingoid bases	neg
288.2898	458.88	0.45	C17H37NO2	H	C17H37NO2	H	C17 Sphinganine	Sphingoid bases	pos
322.2719	474.30	0.78	C18H37NO2	Na	C18H37NO2	Na	Sphinganine	Sphingoid bases	pos
322.2716	597.24	0.03	C18H37NO2	Na	C18H37NO2	Na	Sphinganine	Sphingoid bases	pos
322.2719	474.30	0.78	C18H37NO2	Na	C18H37NO2	Na	Sphinganine	Sphingoid bases	pos
322.2716	597.24	0.03	C18H37NO2	Na	C18H37NO2	Na	Sphinganine	Sphingoid bases	pos
338.2665	450.12	0.21	C18H37NO3	Na	C18H37NO3	Na	4-hydroxysphingosine;6-hydroxysphingosine	Sphingoid bases	pos
286.3106	476.10	0.42	C18H39NO	H	C18H39NO	H	Spisulosine	Sphingoid bases	pos
302.3052	468.42	0.46	C18H39NO2	H	C18H39NO2	H	Sphinganine	Sphingoid bases	pos
302.3052	468.42	0.46	C18H39NO2	H	C18H39NO2	H	Sphinganine	Sphingoid bases	pos
318.3001	448.14	0.38	C18H39NO3	H	C18H39NO3	H	4-hydroxysphinganine;Phytosphingosine	Sphingoid bases	pos
314.3418	499.56	0.22	C20H43NO	H	C20H43NO	H	2-amino-14,16-dimethyltetradecan-3-ol	Sphingoid bases	pos
402.2855	410.46	1.14	C21H39NO6	H	C21H39NO6	H	Myricin;Sphingofungin F	Sphingoid bases	pos
438.3545	528.24	1.92	C23H47NO2	HCOONa	C23H47NO2	HCOONa	Choline stearate;Penazetidine A	Sphingoid bases	pos
552.3096	648.06	4.18	C24H47NO7	Na_HCOONa	C24H47NO7	Na_HCOONa	Galactosylsphingosine;Glucosylsphingosine	Sphingolipids	pos
414.2999	476.10	4.66	C26H36O3	NH3	C26H36O3	NH3	Estradiol 17beta-cyclopentylpropionate;Estradiol cypionate (USP)	Sphingoid bases	pos
563.3770	489.78	4.53	C30H52N2O2	Na_HCOONa	C30H52N2O2	Na_HCOONa	Leucettamol A	Sphingoid bases	pos
534.3213	402.66	4.32	C31H45NO5	Na	C31H45NO5	Na	Scyphostatin A	Sphingoid bases	pos
560.5014	775.32	0.20	C34H67NO3	Na	C34H67NO3	Na	N-Palmitoylsphingosine	Sphingolipids	pos
562.5176	739.08	1.14	C34H69NO3	Na	C34H69NO3	Na	Cer(d18:0/16:0)	Sphingolipids	pos
722.5523	653.88	2.57	C40H77NO8	Na	C40H77NO8	Na	Galactosylceramide (d18:1/16:0);GlcCer(d18:1/16:0);Glucosylceramide (d18:1/16:0)	Sphingolipids	pos
722.5523	687.24	2.57	C40H77NO8	Na	C40H77NO8	Na	Galactosylceramide (d18:1/16:0);GlcCer(d18:1/16:0);Glucosylceramide (d18:1/16:0)	Sphingolipids	pos
722.5522	717.54	2.66	C40H77NO8	Na	C40H77NO8	Na	Galactosylceramide (d18:1/16:0);GlcCer(d18:1/16:0);Glucosylceramide (d18:1/16:0)	Sphingolipids	pos
722.5523	748.86	2.57	C40H77NO8	Na	C40H77NO8	Na	Galactosylceramide (d18:1/16:0);GlcCer(d18:1/16:0);Glucosylceramide (d18:1/16:0)	Sphingolipids	pos

906.6986	739.08	2.01	C50H95NO8	HCOONa	Galactosylceramide (d18:1/26:1(17Z));Glucosylceramide (d18:1/26:1(17Z))	Sphingolipids	pos
Glycerolipids							
381.2979	691.08	0.97	C21H42O4	Na	MG(18:0/0:0/0)	Glycerolipids	pos
396.3105	478.02	0.76	C23H38O4	NH3	1-Arachidonoylglycerol or related compounds	Glycerolipids	pos
401.2661	573.78	0.57	C23H38O4	Na	2-Arachidonoylglycerol or related compounds	Glycerolipids	pos
430.3891	528.90	0.00	C25H48O4	NH3	MG(0:0/22:1(13Z)/0:0);MG(22:1(13Z)/0:0/0:0)	Glycerolipids	pos
471.3659	694.98	4.50	C27H50O6	H	Tricapilin	Glycerolipids	pos
599.4249	679.32	1.52	C33H62O6	Na_Na (NaClx2)	TG(10:0/10:0/10:0)[iso]	Glycerolipids	pos
613.4246	656.88	1.09	C36H64O5	K	DG(15:0/18:3(6Z,9Z,12Z)/0:0) or related compounds	Glycerolipids	neg
669.4655	790.86	3.17	C36H66O5	Na_HCOONa	DG(15:0/18:2(9Z,12Z)/0:0) or related compounds	Glycerolipids	pos
701.3729	569.76	4.65	C37H62O5	NaClx2	DG(14:0/20:5(5Z,8Z,11Z,14Z,17Z)/0:0) or related compounds	Glycerolipids	pos
697.3989	582.54	1.23	C40H64O5	KCl	DG(17:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	Diacylglycerols	neg
713.4774	464.94	1.37	C40H70O5	HCOOK	DG(15:0/22:4(7Z,10Z,13Z,16Z)/0:0) or related compounds	Glycerolipids	neg
723.5552	696.72	2.28	C40H78O5	HCOOK	DG(15:0/22:0:0);DG(16:0/21:0/0:0)[iso2];DG(17:0/20:0/0:0)[iso2]; DG(18:0/19:0/0:0)[iso2];DG(22:0/15:0/0:0)	Glycerolipids	pos
780.5947	700.86	1.59	C42H81NO7	HCOONa	DGTS(16:0/16:0)	Glycerolipids	pos
780.5947	736.14	1.59	C42H81NO7	HCOONa	DGTS(16:0/16:0)	Glycerolipids	pos
780.5950	767.46	1.28	C42H81NO7	HCOONa	DGTS(16:0/16:0)	Glycerolipids	pos
795.5443	550.38	4.45	C43H82O5	NaClx2	DG(16:0/24:1(15Z)/0:0) or related compounds	Glycerolipids	pos
795.5430	636.36	2.84	C43H82O5	NaClx2	DG(16:1(9Z)/24:0/0:0) or related compounds	Glycerolipids	pos
795.5431	775.32	2.99	C43H82O5	NaClx2	DG(18:0/22:1(13Z)/0:0) or related compounds	Glycerolipids	pos
781.5978	769.44	3.33	C46H80O5	HCOONa	DG(21:0/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	Diacylglycerols	pos
791.5926	550.38	0.19	C49H84O5	K	DG(22:5(4Z,7Z,10Z,13Z,16Z)/24:1(15Z)/0:0) or related compounds	Glycerolipids	pos
911.6267	630.54	2.72	C54H92O6	KCl	TG(16:1(9Z)/17:2(9Z,12Z)/18:3(9Z,12Z,15Z))[iso6]; TG(17:2(9Z,12Z)/17:2(9Z,12Z)/17:2(9Z,12Z))	Triacylglycerols	pos
911.6267	710.70	2.72	C54H92O6	KCl	TG(16:1(9Z)/17:2(9Z,12Z)/18:3(9Z,12Z,15Z))[iso6]; TG(17:2(9Z,12Z)/17:2(9Z,12Z)/17:2(9Z,12Z))	Triacylglycerols	pos
945.7081	775.32	0.73	C56H102O6	KCl	TG(16:0/17:0/20:3(8Z,11Z,14Z))[iso6] or related compounds	Triacylglycerols	pos
963.7382	771.36	0.56	C62H100O6	Na	TG(17:0/20:4(8Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso6] or related compounds	Triacylglycerols	pos
Phospholipids							
443.2405	448.14	0.02	C19H39O9P	H	PG(13:0/0:0)	glycerophosphates	pos
454.2930	751.80	0.48	C21H44NO7P	H	1-16:0-lysoPE:PC(13:0/0:0);PE(16:0/0:0)	glycerophosphates	pos
531.2572	575.70	1.36	C22H43O12P	H	PI(13:0/0:0)	glycerophosphates	pos
516.2876	444.18	2.79	C24H50NO6P	K	LysoPC(dm16:0);PC(O-16:1(11Z)/0:0) or related compounds	glycerophosphocholines	neg
617.2943	557.28	0.16	C25H49O12P	HCOOH	PI(16:0/0:0)	glycerophosphates	neg
616.2625	189.54	0.47	C27H44NO7P	Na_HCOONa	LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)); LysoPE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	glycerophosphoethanolamines	pos
543.3197	586.44	1.36	C27H46NO7P	NH3	LysoPE(0:0/22:5(4Z,7Z,10Z,13Z,16Z)) or related compounds	glycerophosphoethanolamines	neg
691.3055	566.94	2.10	C27H53O12P	Na_HCOONa (HCOOH)	PI(18:0/0:0)	glycerophosphates	pos/neg
557.3354	598.26	1.26	C28H48NO7P	NH3	LysoPC(20:5(8Z,8Z,11Z,14Z,17Z))	glycerophosphocholines	neg
625.3041	420.18	1.28	C28H55O8P	KCl	PA(12:0/13:0)	glycerophosphates	pos
710.3937	603.12	1.77	C33H66NO8P	KCl	PE(16:0/12:0); PC(10:0/15:0)[U] or related compounds	glycerophosphoethanolamines	neg
712.3601	408.24	0.48	C34H62NO10P	K	PS(14:1(9Z)/14:1(9Z))	glycerophosphoserines	neg
745.3991	571.62	1.14	C37H69O8P	KCl	16:0-18:2-PA;PA(16:0/18:2(9Z,12Z)); Phosphatidyl ethanol	glycerophosphates	neg
752.4275	679.32	4.28	C37H76NO7P	KCl	PE(0-16:0/16:0); PC(O-14:0/15:0) or related compounds	glycerophosphoethanolamines	pos
752.5147	542.64	3.89	C38H78NO8P	Na_Na	PS(O-16:0/O-16:0)[U] or related compounds	glycerophosphoserines	neg
729.3889	567.90	1.00	C39H65O8P	K	PA(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z)) or related compounds	glycerophosphates	pos
765.3679	463.14	3.71	C39H65O8P	KCl	18:3-18:3-PA or related compounds	glycerophosphates	neg
733.5494	587.46	0.50	C39H74NO8P	NH3	PE(14:0/20:2(11Z,14Z)) or related compounds	glycerophosphoethanolamines	pos
760.5789	648.12	4.89	C39H82NO6P	HCOONa	PE-NMe2(O-16:0/O-16:0)	glycerophosphoethanolamines	pos
790.4674	682.08	4.78	C40H70NO8P	HCOONa	PC(14:1(9Z)/18:4(6Z,9Z,12Z,15Z));PC(18:4(6Z,9Z,12Z,15Z)/14:1(9Z));PE(15:0/20:5(5Z,8Z,11Z,14Z,17Z));PE(20:5(5Z,8Z,11Z,14Z,17Z)/15:0)	glycerophosphocholines	neg
796.4550	426.06	3.06	C40H72NO10P	K	16:0-18:3-PS	glycerophosphoserines	pos
842.4243	550.44	4.96	C40H74NO8P	NaClx2	PC(14:0/18:3(6Z,9Z,12Z)); PE(15:0/20:3(5Z,8Z,11Z)) or related compounds	glycerophosphocholines	neg
909.4085	551.34	4.39	C40H75O13P	NaClx2	PI(17:0/14:1(9Z))	glycerophosphoinositols	neg
753.4823	681.30	1.05	C40H75O8P	HCOONa	PA(18:2(9Z,12Z)/19:0); 1-tetradecanyl-2-(8-[3]-ladderane-octanyl)-sn-glycero-3-phospho-(1'-sn-glycerol)	glycerophosphates	pos
774.5945	683.22	4.92	C40H84NO6P	HCOONa	PC(O-12:0/O-20:0)[U];PC(O-14:0/O-18:0)[U];PC(O-16:0/O-16:0);PC(O-20:0/O-12:0)[U]	glycerophosphocholines	pos
738.5050	775.32	0.81	C41H72NO8P	H	PE(14:0/22:5(4Z,7Z,10Z,13Z,16Z)) or related compounds	glycerophosphoethanolamines	pos
743.5705	741.00	1.02	C41H76NO7P	NH3	PE(18:2(9Z,12Z)/dm18:1(11Z)) or related compounds	glycerophosphoethanolamines	pos
796.5443	542.64	0.58	C41H78NO7P	HCOONa	PE(18:1(11Z)/dm18:1(11Z)) or related compounds	glycerophosphoethanolamines	pos
816.6057	701.88	3.93	C42H86NO7P	HCOONa	PC(18:0/O-16:0) or related compounds	glycerophosphocholines	neg
838.4536	476.94	3.05	C43H76NO8P	KCl	20:2-18:3-PE or related compounds	glycerophosphoethanolamines	pos
789.6122	675.42	0.73	C43H82NO8P	NH3	PC(15:0/20:2(11Z,14Z)) or related compounds	glycerophosphoethanolamines	pos
839.5638	474.30	0.64	C43H83O13P	H	PI(16:0/18:0);PI(18:0/16:0)	glycerophosphoinositols	pos
820.5991	585.48	4.16	C43H88NO7P	NaCl	PC(O-16:0/19:0) or related compounds	glycerophosphoethanolamines	pos
830.6205	634.44	4.78	C43H88NO7P	HCOONa	PE(O-16:0/22:0) or related compounds	glycerophosphoethanolamines	pos
830.6209	737.10	4.41	C43H88NO7P	HCOONa	PE(O-18:0/20:0) or related compounds	glycerophosphoethanolamines	pos
817.4409	571.86	3.56	C44H71O9P	Na_Na	1-(6-[5]-ladderane-hexanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycero-3-phospho-(1'-sn-glycerol)	glycerophosphoglycerols	neg
833.4513	573.18	1.82	C44H73O9P	NaCl	1-(6-[3]-ladderane-hexanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycero-3-phospho-(1'-sn-glycerol)	glycerophosphoglycerols	neg
834.6154	612.84	0.74	C44H90NO7P	NaCl	PC(O-14:0/22:0);PC(O-16:0/20:0);PC(O-18:0/18:0);PC(O-20:0/16:0)	glycerophosphocholines	pos
844.6361	699.90	4.87	C44H90NO7P	HCOONa	PC(O-14:0/22:0);PC(O-16:0/20:0);PC(O-18:0/18:0);PC(O-20:0/16:0)	glycerophosphocholines	pos
868.5003	477.06	3.15	C45H82NO8P	KCl	PC(15:0/22:4(7Z,10Z,13Z,16Z)) or related compounds	glycerophosphoethanolamines	neg
846.6154	657.84	4.80	C45H90NO7P	NaCl	PE(22:0/dm18:0);PE(24:0/dm16:0);	glycerophosphoethanolamines	pos
809.6154	699.90	1.57	C46H82NO7P	NH3	PC(20:4(8Z,8Z,11Z,14Z)/dm18:1(11Z)) or related compounds	glycerophosphocholines	pos
809.6156	748.86	1.35	C46H82NO7P	NH3	PC(20:4(8Z,8Z,11Z,14Z)/dm18:1(11Z)) or related compounds	glycerophosphocholines	pos
905.5129	492.72	1.10	C47H81O13P	Na	PI(16:0/22:5(4Z,7Z,10Z,13Z,16Z)) or related compounds	glycerophosphoinositols	neg
908.7015	739.08	4.28	C48H100NO6P	Na_HCOONa	1,2-diphtanyl-sn-glycero-3-phosphocholine;PC(O-20:0/O-20:0)	glycerophosphocholines	pos
848.6309	567.00	4.61	C48H92NO6P	K	1-(2E,6E-phytadienyl)-2-(2E,6E-phytadienyl)-sn-glycero-3-phosphocholine	glycerophosphocholines	pos
848.6313	644.16	2.29	C48H92NO6P	K	1-(2E,6E-phytadienyl)-2-(2E,6E-phytadienyl)-sn-glycero-3-phosphocholine	glycerophosphocholines	pos
899.6350	476.10	0.23	C48H93O11P	Na	1,2-ditetradecanoyl-sn-glycero-3-phospho-(2'-lyso-3'-tetradecanoyl-1'-sn-glycerol)	glycerophosphoglycerols	pos
921.6165	476.10	0.17	C48H93O11P	Na_Na	1,2-ditetradecanoyl-sn-glycero-3-phospho-(2'-lyso-3'-tetradecanoyl-1'-sn-glycerol)	glycerophosphoglycerols	pos/neg
888.6621	659.76	4.29	C48H96NO7P	NaCl	PC(22:0/dm18:0); PC(24:0/dm16:0)	glycerophosphocholines	pos
904.6939	769.38	4.70	C49H100NO7P	NaCl	PC(O-19:0/22:0)	glycerophosphoethanolamines	pos
866.6684	805.50	4.63	C50H94NO8P	H	PC(18:2(9Z,12Z)/24:1(15Z)) or related compounds	glycerophosphocholines	neg
980.6476	803.46	4.07	C50H98NO7P	NaCl_HCOONa	PC(24:0/dm18:1(11Z)) or related compounds	glycerophosphocholines	pos
964.7150	602.16	2.02	C54H104NO8P	K	PC(22:1(13Z)/24:1(15Z)) or related compounds	glycerophosphocholines	neg
Miscellaneous							
151.0478	385.80	0.13	C5H8N2O2	Na	5,6-Dihydrothymine	Pyrimidines and Derivatives	pos
167.0198	73.98	2.51	C6H8N2O	Na_Na	Methylimidazole acetaldehyde;N-Propanoylimidazole	Aldehydes Imidazoles	neg
255.9781	66.54	3.52	C7H8NO5P	K	3-(Phosphonomethyl)Pyridine-2-Carboxylic Acid	Pyridoxals and Derivatives	pos
853.5855	538.68	1.96	C54H82O4	NaCl	Ubiquinone-9	Quinones and Derivatives	pos
853.5854	636.36	2.10	C54H82O4	NaCl	Ubiquinone-9	Quinones and Derivatives	pos
853.5857	712.62	1.75	C54H82O4	NaCl	Ubiquinone-9	Quinones and Derivatives	pos
627.3831	611.94	3.63	C39H58O4	K	Coenzyme Q6;ubiquinone-6	Ubiquinones	neg
511.2729	540.72	2.01	C30H44O2	KCl	2-Phetyl-1,4-naphthoquinone;demethylphyloquinone	Naphthoquinones	pos/neg
310.9307	65.58	1.80	C3H7O7P	NaCl_HCOONa	2-Phosphoglyceric acid;3-Phospho-D-glycerate;D-Glycerate 2-phosphate	Acyl Phosphates	neg
765.3972	443.04	4.49	C40H68O7P2	Na_Na	all-trans-Octaprenyl diphosphate;octaprenyl diphosphate; Prephytoene diphosphate	Acyl Phosphates	neg

308.0255	634.44	3.67	C6H12N3O8P	Na	2-(Formamido)-N1-(5-phospho-D-ribosyl)acetamide	Sugar Phosphates	pos
687.3727	582.54	0.04	C40H60O2	NaClx2	5,6-dihydro-5,6-dihydroxy- γ,γ -Carotene or related compounds	Alcohols and Polyols	neg
611.4239	530.82	2.32	C40H60O2	K	Dihydroparasiloxanthin/ 7,8,7',8'-Tetrahydrozeaxanthin or related compounds	Alcohols and Polyols	pos
611.4236	788.94	1.82	C40H60O2	K	OH-Demethylspheroidene or related compounds	Alcohols and Polyols	pos
368.9881	444.48	2.22	C14H6O8	HCOONa	Ellagic acid	Polyphenols	neg
293.1755	486.84	0.96	C16H24O2	HCOOH	2E,6Z,8Z,12E-hexadecatetraenoic acid or related compounds	Polyphenols	neg
488.2680	475.26	0.08	C18H37N9O4	Na_Na	dynorphin A (6-8)	Solanidines and alkaloid derivatives	pos
416.3524	408.48	0.24	C27H45NO2	H	22-iso-teinemine or related compounds	Solanidines and alkaloid derivatives	pos
581.4545	633.30	3.08	C36H64O4	Na	2-methylbacteriohopane-32,33,34,35-tetrol	Hopanoids	neg
728.5527	646.14	2.81	C40H73N3O4	HCOONa	N-ornithinyl-35-aminobacteriohopane-32,33,34-triol	Hopanoids	pos