

## Appendix B

A list of putative identification of metabolites present in the *in vitro* ASG5 cell line sweat samples.

m/z	rt (s)	ppm error	MF	Adduct	Metabolites	Class
<b>Carbohydrates</b>						
365.105	599.05	1.78	C12H22O11	Na	1-alpha-D-Galactosyl-myo-inositol or related compounds	Carbohydrates
689.2125	682.00	0.73	C24H42O21	Na	1,1-kestotetraose or related compounds	Carbohydrates
291.0692	444.26	2.71	C9H16O9	Na	2(alpha-D-Mannosyl)-D-glycerate or related compounds	Carbohydrates
<b>Amines</b>						
232.1532	523.19	4.87	C11H21NO4	H	3-(1-Aminoethyl)Nonanedioic Acid;Isobutyryl-L-carnitine;N(alpha)-t-Butoxycarbonyl-L-leucine;O-Butanoylcarnitine	Quaternary Amines
282.2785	108.51	2.23	C18H35NO	H	Oleamide	Fatty amides
131.1175	482.98	2.97	C6H14N2O	H	epsilon-aminocaproamide or related compounds	Polyamines
137.0708	576.19	1.02	C7H8N2O	H	N-Methylnicotinamide or related compounds	Cyclic Amines
<b>Amino Acids</b>						
291.1288	658.24	3.81	C10H18N4O6	H	Argininosuccinic acid;N(omega)-(L-Arginino)succinate	Amino Acids
294.2411	113.38	2.58	C16H33NO2	Na	2-amino-hexadecanoic acid or related compounds	Amino fatty acids
126.0222	606.65	1.98	C2H7NO3S	H	Taurine	Amino Acids
90.0544	613.64	6.22	C3H7NO2	H	L-Alanine	Amino Acids
134.0454	625.87	4.55	C4H7NO4	H	L-Aspartate	Amino Acids
133.0608	639.57	0.23	C4H8N2O3	H	L-Asparagine	Amino Acids
132.0764	613.03	2.73	C4H9N3O2	H	Creatine	Amino Acids
120.0651	617.18	3.50	C4H9NO3	H	L-Threonine	Amino Acids
147.0759	626.82	3.54	C5H10N2O3	H	L-Glutamine	Amino Acids
150.0577	532.21	4.20	C5H11NO2S	H	L-Methionine	Amino Acids
116.0703	585.59	2.67	C5H9NO2	H	L-Proline	Amino Acids
148.0602	621.57	1.62	C5H9NO4	H	L-Glutamate	Amino Acids
130.0861	593.70	1.15	C6H11NO2	H	N4-Acetylaminobutanol or related compounds	Amino Acids
132.1017	504.56	1.51	C6H13NO2	H	L-Isoleucine;L-Leucine	Amino Acids
147.1125	597.33	2.04	C6H14N2O2	H	L-Leucyl-Hydroxylamine	Amino Acids
175.1183	637.50	3.71	C6H14N4O2	H	L-Arginine	Amino Acids
139.0495	556.97	5.11	C6H6N2O2	H	Urocanic acid or related compound	Amino Acids
146.117	700.58	3.83	C7H15NO2	H	2-amino-heptanoic acid or related compounds	Amino fatty acids
138.0551	564.84	1.01	C7H7NO2	H	2-nitrotoluene or related compounds	Amino Acids derivative
152.0702	214.03	2.70	C8H9NO2	H	(E)-4-Hydroxyphenylacetaldehyde-oxime or related compound	Amino Acids
182.0805	553.37	3.68	C9H11NO3	H	L-Tyrosine	Amino Acids
220.117	523.81	0.59	C9H17NO5	H	Pantothenic acid	Amino Acids
<b>Bile Acids</b>						
433.248	512.78	0.30	C24H38O3	NaCl	(20S)-3beta-Hydroxychol-5-en-24-oiic Acid or related compounds	Bile acids and derivatives
391.284	103.24	0.69	C24H38O4	H	(22E)-3alpha,12alpha-Dihydroxy-5beta-chol-22-en-24-oiic Acid or related compounds	Bile acids and derivatives
516.3008	174.38	3.60	C26H45NO7S	H	Taurallocholic acid or related compounds	Bile acids and derivatives
549.341	118.52	2.24	C32H41N3O4	NH3	3-Amino-N-[4-[2-(2,6-Dimethyl-Phenoxy)-Acetylamino]-3-Hydroxy-1-Isobutyl-5-Phenyl-Pentyl]-Benzamide or related compounds	Bile acids and derivatives
<b>Glycerol</b>						
482.3598	466.40	1.43	C24H52NO6P	H	1-O-Hexadecyl-lyso-sn-glycero-3-phosphocholine	Glycerophosphocholines
508.3765	464.47	0.71	C26H54NO6P	H	PC(O-18:1(11Z)/0:0) or related compounds	Glycerophosphocholines
575.3111	503.62	4.94	C27H53O8P	K	PA(12:0/12:0)	Glycerophosphates
606.3647	469.69	2.23	C29H58NO6P	NaCl	PC(O-3:1(1E)/O-18:1(9Z))[S] or related compounds	Glycerophosphocholines
665.4133	471.96	0.83	C32H58NO10P	NH3	1-Palmitoyl-2-(5-keto-8-oxo-6-octenyl)-sn-glycero-3-phosphatidylcholine	Glycerophosphates
694.4177	481.95	1.12	C33H66NO8P	NaCl	PC(10:0/15:0)[U] or related compounds	Glycerophosphocholines
704.5168	130.30	4.61	C35H74NO6P	HCOONa	PE-NMe2(O-14:0/O-14:0)	Glycerophosphocholines
647.4851	112.18	0.93	C36H66O5	HCOONa	DG(15:0/18:2(9Z,12Z)/0:0) or related compounds	Glycerolipids
676.4928	383.12	2.42	C36H70NO8P	H	PC(10:0/18:1(9Z)) or related compounds	Glycerophosphocholines
678.5077	394.42	1.31	C36H72NO8P	H	PC(10:0/18:0) or related compounds	Glycerophosphocholines
718.5324	129.42	4.59	C36H76NO6P	HCOONa	PC(O-14:0/O-14:0)	Glycerophosphocholines
610.5413	103.58	1.34	C37H68O5	NH3	DG(14:0/20:2(11Z,14Z)/0:0) or related compounds	Glycerolipids
754.5299	382.13	4.49	C37H78NO6P	Na_HCOONa	PE(O-16:0/O-16:0)	Glycerophosphoethanolamines
663.4711	113.23	2.19	C38H68O5	NaCl	DG(15:0/20:3(5Z,8Z,11Z)/0:0) or related compounds	Glycerolipids
704.5228	380.02	3.90	C38H74NO8P	H	PC(12:0/18:1(9Z)) or related compounds	Glycerophosphocholines
706.5389	390.41	1.12	C38H76NO8P	H	PC(11:0/19:0) or related compounds	Glycerophosphocholines
706.5414	441.72	4.66	C38H76NO8P	H	PC(10:0/20:0) or related compounds	Glycerophosphocholines
692.5574	395.09	2.08	C38H78NO7P	H	PC(O-14:0/16:0)	Glycerophosphocholines
638.5733	104.49	2.38	C39H72O5	NH3	DG(14:0/22:2(13Z,16Z)/0:0) or related compounds	Glycerolipids
701.5597	448.85	0.74	C39H74NO6P	NH3	1-tetradecanyl-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphoethanolamine	Glycerophosphoethanolamines
718.5387	219.08	4.18	C39H76NO8P	H	16:0-18:1-PE or related compounds	Glycerophosphocholines
728.5542	420.27	3.06	C39H80NO7P	Na	PE(O-18:0/16:0)[U]	Glycerophosphoethanolamines
766.5288	190.92	1.33	C39H82NO6P	KCl	PE-NMe2(O-16:0/O-16:0)	Glycerophosphoethanolamines
782.5612	402.65	4.32	C39H82NO6P	Na_HCOONa	PE-NMe2(O-16:0/O-16:0)	Glycerophosphoethanolamines
709.4405	475.27	4.92	C40H64O5	HCOOK	DG(17:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	Glycerolipids
730.5351	399.98	0.82	C40H76NO8P	H	PC(14:0/18:2(11Z,14Z)) or related compounds	Glycerophosphocholines
780.5472	342.59	4.83	C40H84NO6P	KCl	PC(O-12:0/O-20:0)[U] or related compounds	Glycerophosphocholines
742.5404	197.93	4.77	C41H76NO8P	H	18:0-18:3-PE or related compounds	Glycerophosphates
770.5654	361.64	2.08	C41H82NO8P	Na	PC(10:0/23:0) or related compounds	Glycerophosphocholines
824.4862	252.37	2.89	C42H76NO10P	K	18:0-18:3-PS or related compounds	Glycerophosphoserines
788.5418	324.67	0.79	C42H78NO10P	H	18:0-18:2-PS or related compounds	Glycerophosphoserines
826.4996	497.21	0.16	C42H78NO10P	K	PS(18:0/18:2(9Z,12Z)) or related compounds	Glycerophosphoserines
770.5506	366.21	1.43	C42H79NO8	Na_Na	Galactosylceramide (d18:1/18:1(9Z));Glucosylceramide (d18:1/9Z-18:1)	Glycolipids
784.5799	406.43	3.49	C42H84NO8P	Na	PC(10:0/24:0) or related compounds	Glycerophosphocholines
776.5909	398.33	0.41	C42H86NO6P	Na_Na	PC(O-16:0/O-18:1(9Z))[U] or related compounds	Glycerophosphocholines
772.5976	385.56	0.58	C42H88NO6P	K	PC(O-16:0/O-18:0)	Glycerophosphocholines
753.4658	480.16	2.44	C43H66O5	Na_HCOONa	DG(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0) or related compounds	Glycerolipids
775.4798	481.19	2.17	C43H73O6P	NaCl	DG(17:0/22:4(7Z,10Z,13Z,16Z)/0:0)[iso2] or related compounds	Glycolipids
763.5828	355.45	2.66	C43H82O5	HCOOK	DG(16:1(9Z)/24:0/0:0) or related compounds	Glycerolipids
763.5885	364.87	4.81	C43H82O5	HCOOK	DG(16:0/24:1(15Z)/0:0) or related compounds	Glycerolipids
824.5581	385.15	3.52	C44H84NO8P	K	PC(14:0/22:2(13Z,16Z)) or related compounds	Glycerophosphocholines
774.5427	179.11	2.48	C45H76NO7P	H	PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/dm18:1(11Z)) or related compounds	Glycerophosphoethanolamines
763.6	360.23	2.96	C45H84O5	NaCl	DG(18:1(11Z)/24:1(15Z)/0:0) or related compounds	Glycerolipids
806.5843	136.27	2.36	C45H86NO6P	K	1-(10-methylhexadecanyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine	Glycerophosphocholines
822.5794	143.75	2.53	C45H86NO7P	H	PE(22:1(13Z)/dm18:1(11Z)) or related compounds	Glycerophosphocholines
808.5851	336.63	3.04	C46H82NO8P	K	PC(16:0/22:5(4E,7E,10E,13E,16E))[U] or related compounds	Glycerophosphocholines
812.6202	340.75	2.45	C46H86NO8P	H	PC(16:0/22:3(13Z,16Z,19Z))[U] or related compounds	Glycerophosphocholines
763.6155	364.36	4.13	C46H86O5	Na_Na	DG(21:0/22:2(13Z,16Z)/0:0)[iso2]	Glycerolipids
730.5395	364.07	1.90	C47H68O5	NH3	DC(2:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)'	Glycerophosphocholines
834.6022	329.38	2.31	C48H84NO8P	H	PC(18:0/22:6(4E,7E,10E,13E,16E,19E))[U] or related compounds	Glycerophosphocholines
894.6423	146.39	0.86	C48H91NO8	HCOOK	Galactosylceramide (d18:1/24:1(15Z)) or related compounds	Glycolipids
792.7049	124.71	3.32	C49H90O6	NH3	TG(16:1(9Z)/14:0/16:1(9Z))[iso3]	Glycerolipids
915.6705	102.32	4.93	C53H92O6	Na_HCOONa	TG(16:1(9Z)/16:1(9Z)/18:3(9Z,12Z,15Z))[iso3] or related compounds	Triacylglycerols
929.6858	102.78	4.47	C56H92O6	HCOONa	TG(16:1(9Z)/17:2(9Z,12Z)/20:5(5Z,8Z,11Z,14Z,17Z))[iso6] or related compounds	Triacylglycerols
<b>Fatty Acids</b>						
184.1325	193.79	3.80	C10H14O2	NH3	1-(3,4-dimethylphenyl)ethane-1,2-diol or related compounds	Fatty Acids and Conjugates
202.1799	492.63	1.24	C11H20O2	NH3	11-Undecanofactone or related compounds	Fatty Acids and Conjugates

208.1328	436.45	1.92	C12H17NO2	H	2-sec-Butylphenyl N-methylcarbamate;3-(Dimethylamino)propyl benzoate;"3,4-Methylenedioxy-N-ethylamphetamine	Fatty Acids and Conjugates
229.1535	680.98	1.61	C12H24O	Na_Na	10-dodecen-1-ol or related compounds	Fatty alcohols
241.1542	555.30	1.95	C13H24O	Na_Na	2-tridecanol	Fatty aldehydes
239.1049	691.73	2.09	C14H16O2	Na	10E,12E-tetradecadiene-4,6-diynoic acid	Fatty Acids and Conjugates
235.206	113.43	1.57	C16H26O	H	4,6,11-hexadecatrienal	Fatty aldehydes
268.2271	110.85	0.00	C16H26O2	NH3	4,7,10-hexadecatrienoic acid or related compounds	Fatty Acids and Conjugates
254.2471	312.60	2.87	C16H28O	NH3	10,12-hexadecadienal or related compounds	Fatty aldehydes
256.263	109.00	1.87	C16H30O	NH3	6E,11Z-hexadecadien-1-ol or related compounds	Fatty alcohols
261.2201	115.22	4.71	C16H30O	Na	10-propyl-5,9-tridecadien-1-ol or related compounds	Fatty alcohols
258.2781	254.89	3.99	C16H32O	NH3	1,2-Epoxyhexadecane;11Z-hexadecen-1-ol or related compounds	Fatty alcohols
274.2733	263.19	2.73	C16H32O2	NH3	13-methyl-heptadecanoic acid or related compounds	Fatty Acids and Conjugates
288.2889	239.09	2.77	C17H34O2	NH3	(+)-14-methyl palmitic acid;10-methyl-hexadecanoic acid or related compounds	Fatty Acids and Conjugates
275.1998	112.20	2.73	C18H26O2	H	13E-octadecene-9,11-diynoic acid or related compounds	Fatty Acids and Conjugates
298.2727	115.34	4.53	C18H32O2	NH3	10E,12E-octadecadienoic acid or related compounds	Fatty Acids
284.2942	273.47	2.04	C18H34O	NH3	11-Octadecenal or related compounds	Fatty alcohols
300.2906	297.59	3.00	C18H34O2	NH3	(11E)-Octadecenoic acid or related compounds	Fatty Acids and Conjugates
304.262	109.01	3.06	C18H35NO	Na	Oleamide	Fatty amides
302.3048	255.27	1.82	C18H36O2	NH3	(+)-Isostearic acid;10-methyl-heptadecanoic acid or related compounds	Fatty Acids and Conjugates
302.3048	314.89	1.82	C18H36O2	NH3	15-methyl-heptadecanoic acid or related compounds	Fatty Acids and Conjugates
316.3203	229.21	2.18	C19H38O2	NH3	(+)-16-methyl stearic acid;11-methyl-octadecanoic acid or related compounds	Fatty Acids and Conjugates
330.3358	248.00	2.54	C20H40O2	NH3	17-methyl-nonadecanoic acid or related compounds	Fatty Acids and Conjugates
340.32	241.18	2.91	C21H38O2	NH3	12Z,15Z-heneicosadienoic acid or related compounds	Fatty Acids and Conjugates
342.3362	239.30	1.29	C21H40O2	NH3	12Z-heneicosenoic acid or related compounds	Fatty Acids and Conjugates
358.3678	241.70	0.39	C22H44O2	NH3	19-methyl-heneicosanoic acid or related compounds	Fatty Acids and Conjugates
480.3083	429.95	0.31	C25H43NO2	Na_HCOONa	(-)-N-(1R-methyl-2-hydroxy-ethyl) alpha.alpha.-dimethylarachidonoyl amine or related compounds	Fatty amides
677.5591	446.20	0.12	C38H76O9	H	1-(O-Alpha-D-glucopyranosyl)-(1,3R,29S,31R)-dotriacontanetetraol	Fatty acyl glycosides
704.5297	441.47	2.19	C40H73N3O4	Na_Na	N-ornithinyl-35-aminobacteriohopane-32,33,34-triol	Hopanooids
782.4773	493.77	4.95	C41H73NO8	KCl	bacteriohopane-32,33,34-triol-35-cyclitol;bacteriohopanetetrol cyclitol	Hopanooids
87.0443	657.38	2.76	C4H6O2	H	1,4-Lactone or related compounds	Fatty Acids
89.0595	161.09	2.36	C4H8O2	H	2-Methylpropanoate or related compounds	Fatty Acids
160.1325	718.21	4.37	C8H14O2	NH3	2-ethyl-3E-hexenoic acid or related compounds	Fatty Acids and Conjugates
156.1376	111.09	4.42	C9H14O	NH3	(3Z,6Z)-nonadienal or related compounds	Fatty aldehydes
155.106	119.97	4.19	C9H14O2	H	2,6-nonadienoic acid or related compounds	Fatty Acids
172.1325	120.17	4.07	C9H14O2	NH3	2,6-nonadienoic acid or related compounds	Fatty Acids and Conjugates
146.0594	496.09	4.38	C9H7NO	H	1(2H)-Isoquinolinone or related compounds	Fatty aldehydes
<b>Hydroxy acids</b>						
250.0928	166.87	0.80	C10H19NO2S2	H	S-Acetyldihydroliipoamide	Lipoamides and Derivatives
223.1071	510.95	2.78	C11H11NO3	NH3	5-Methoxyindoleacetate;Indolelactate	Indoles and Indole Derivatives
239.1047	605.62	1.25	C11H20O3	K	2-hydroxy-10-andecanoic acid or related compounds	Hydroxy fatty acids
226.1438	435.97	0.13	C12H16O3	NH3	12-oxo-5E,8E,10Z-dodecatrienoic acid or related compounds	Oxo fatty acids
304.2852	148.51	1.94	C17H34O3	NH3	17-hydroxy-heptadecanoic acid or related compounds	Hydroxy fatty acids
304.2858	187.96	3.91	C17H34O3	NH3	2-hydroxy-heptadecanoic acid or related compounds	Hydroxy fatty acids
310.2375	115.40	0.52	C18H28O3	NH3	(-)-8-hydroxy-11E,17-octadecadien-9-ynoic acid or related compounds	Hydroxy fatty acids
332.3145	181.15	4.24	C19H38O3	NH3	19-hydroxy-nonadecanoic acid; 2-hydroxy-nonadecanoic acid	Hydroxy fatty acids
387.2633	112.88	0.85	C20H40O3	NaCl	20-hydroxy-eicosanoic acid;2-hydroxy-eicosanoic acid;3-hydroxy-eicosanoic acid;L-2-hydroxyphytanate	Hydroxy fatty acids
137.045	294.53	4.01	C4H8O5	H	D-threonic acid	Hydroxy fatty acids
133.0855	160.75	3.16	C6H12O3	H	(R)-3-Hydroxyhexanoic acid or related compounds	Hydroxy Acids
219.0051	638.54	1.46	C9H8O4	K	2,4-Dihydroxy-Trans Cinnamic Acid or related compounds	Hydroxy Acids
<b>Isoprenoids</b>						
368.4239	220.63	3.15	C25H50	NH3	4-pentacosene;6-pentacosene;9-pentacosene;C25 Monocyclic highly branched isoprenoid;C25:1 Highly branched isoprenoid	Isoprenoids
447.3383	114.34	4.25	C30H48	K	4,4'-Diapophytoene;"4,4'-Diapophytoene/ Dehydroqualene"	Isoprenoids
489.3617	113.79	1.37	C30H54	KCl	Tetrahydroqualene	Isoprenoids
489.35	114.72	1.74	C35H46	Na	4'-Apo-3,4-didehydrolycopene/ (4-Apo-3',4'-didehydrolycopene)	Isoprenoids
<b>Phospholipids</b>						
468.3079	465.94	1.17	C22H46NO7P	H	LysoPC(14:0);PC(0:0/14:0) or related compounds	Phospholipids
494.3238	464.08	0.61	C24H48NO7P	H	1-16:1-LysoPC or related compounds	Phospholipids
480.3443	456.83	1.12	C24H50NO6P	H	LysoPC(dml16:0);PC(O-16:(11Z)/0:0) or related compounds	Phospholipids
496.3401	463.31	0.71	C24H50NO7P	H	LysoPC(16:0) or related compounds	Phospholipids
520.3404	461.86	1.25	C26H50NO7P	H	LysoPC(18:2(9Z,12Z)) or related compounds	Phospholipids
544.3384	461.39	1.95	C28H50NO7P	H	LysoPC(20:4(SZ,8Z,11Z,14Z)) or related compounds	Phospholipids
692.4062	212.33	4.87	C33H64NO8P	NaCl	PE(14:0/14:1(9Z)) or related compounds	Phospholipids
688.4941	208.14	4.27	C37H70NO8P	H	PE(14:0/18:2(9Z,12Z)) or related compounds	Phospholipids
674.5119	197.75	0.00	C37H72NO7P	H	PE(14:0/dml8:1(11Z)) or related compounds	Phospholipids
690.5069	210.44	3.62	C37H72NO8P	H	PE(14:0/18:1(11Z)) or related compounds	Phospholipids
675.5451	450.32	2.32	C37H75N2O6P	H	SM(dl18:1/14:0)	Phospholipids
736.4311	223.45	0.39	C38H68NO8P	K	PE(15:0/18:4(6Z,9Z,12Z,15Z)) or related compounds	Phospholipids
738.4443	488.35	3.71	C38H70NO8P	K	PE(15:0/18:3(6Z,9Z,12Z)) or related compounds	Phospholipids
702.5098	372.47	4.26	C38H72NO8P	H	PC(14:1(9Z)/16:1(9Z)) or related compounds	Phospholipids
700.5287	193.51	1.66	C39H74NO7P	H	PE(16:1(9Z)/dml8:1(11Z)) or related compounds	Phospholipids
716.5237	204.02	1.73	C39H74NO8P	H	16:0-18:2-PE or related compounds	Phospholipids
702.5441	198.47	1.30	C39H76NO7P	H	PE(18:1(11Z)/dml16:0) or related compounds	Phospholipids
702.5408	421.81	3.40	C39H76NO7P	H	PE(16:0/dml8:1(9Z)) or related compounds	Phospholipids
702.5442	507.59	1.44	C39H76NO7P	H	1-Hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycerol-3-phosphonoethanolamine or related compounds	Phospholipids
728.5561	520.51	0.45	C39H80NO7P	Na	PE(O-18:0/16:0)[U]	Phospholipids
728.526	348.01	4.86	C40H74NO8P	H	PC(14:0/18:3(6Z,9Z,12Z)) or related compounds	Phospholipids
716.5567	438.82	2.99	C40H78NO7P	H	PC(14:0/dml8:1(9Z)) or related compounds	Phospholipids
732.554	371.08	3.62	C40H78NO8P	H	PC(16:0/16:1(9Z)) or related compounds	Phospholipids
732.5537	408.42	3.21	C40H78NO8P	H	PC(14:0/18:1(9Z)) or related compounds	Phospholipids
732.5549	443.06	4.85	C40H78NO8P	H	PC(14:0/18:1(9E))[U] or related compounds	Phospholipids
732.5547	503.26	4.57	C40H78NO8P	H	PC(14:0/18:1(11Z)) or related compounds	Phospholipids
718.5741	378.11	0.54	C40H80NO7P	H	PC(14:0/dml18:0) or related compounds	Phospholipids
722.5098	186.64	3.78	C41H72NO7P	H	PE(18:4(6Z,9Z,12Z,15Z)/dml8:1(11Z)) or related compounds	Phospholipids
782.4689	493.25	0.51	C41H72NO8P	Na_Na	PE(14:0/22:5(4Z,7Z,10Z,13Z,16Z)) or related compounds	Phospholipids
724.5276	184.40	3.41	C41H74NO7P	H	PE(18:3(6Z,9Z,12Z)/dml8:1(11Z)) or related compounds	Phospholipids
726.5429	189.44	2.92	C41H76NO7P	H	PE(18:2(9Z,12Z)/dml8:1(11Z)) or related compounds	Phospholipids
728.5606	191.66	2.42	C41H78NO7P	H	PE(18:1(11Z)/dml8:1(11Z));PE(18:1(11Z)/dml8:1(9Z)) or related compounds	Phospholipids
744.5539	166.55	0.19	C41H78NO8P	H	PE(14:0/22:2(13Z,16Z)) or related compounds	Phospholipids
744.5557	202.25	2.61	C41H78NO8P	H	18:0-18:2-PE or related compounds	Phospholipids
744.5551	395.76	1.80	C41H78NO8P	H	PC(15:0/18:2(9Z,12Z)) or related compounds	Phospholipids
756.5543	353.49	3.90	C42H78NO8P	H	PC(14:0/20:3(SZ,8Z,11Z)) or related compound	Phospholipids
756.5505	438.70	1.12	C40H80NO8P	Na	PC(10:0/22:0) or related compounds	Phospholipids
775.5495	109.36	1.50	C42H79O10P	H	PG(18:0/18:2(9Z,12Z)) or related compounds	Phospholipids
742.5756	342.73	4.74	C42H80NO7P	H	PC(16:1(9Z)/dml18:1(11Z)) or related compounds	Phospholipids
758.5702	358.48	1.04	C42H80NO8P	H	PC(14:0/20:2(11Z,14Z)) or related compounds	Phospholipids
744.5895	352.48	0.86	C42H82NO7P	H	PC(16:0/dml18:1(11Z)) or related compounds	Phospholipids
760.585	365.23	3.10	C42H82NO8P	H	PC(14:1(9Z)/20:0) or related compounds	Phospholipids
760.583	428.20	0.47	C42H82NO8P	H	PC(14:0/20:1(11Z)) or related compounds	Phospholipids
746.6046	373.88	1.59	C42H84NO7P	H	PC(16:0/dml18:0) or related compounds	Phospholipids
780.4597	237.21	2.69	C43H68NO8P	Na	PE(18:4(6Z,9Z,12Z,15Z)/20:5(SZ,8Z,11Z,14Z,17Z)) or related compounds	Phospholipids
750.5424	184.27	2.16	C43H76NO7P	H	PE(20:4(SZ,8Z,11Z,14Z)/dml18:1(11Z)) or related compounds	Phospholipids
768.5906	335.00	3.73	C44H82NO7P	H	PC(18:2(9Z,12Z)/dml18:1(11Z)) or related compounds	Phospholipids
784.5877	347.40	3.38	C44H82NO8P	H	PC(14:1(9Z)/22:2(13Z,16Z)) or related compounds	Phospholipids
770.6083	344.05	3.26	C44H84NO7P	H	PC(18:1(11Z)/dml18:1(11Z)) or related compounds	Phospholipids

824.5595	342.49	3.54	C44H84NO8P	K	PC(14:0/22:2(13Z,16Z)) or related compounds	Phospholipids
786.5984	381.69	2.92	C44H84NO8P	H	PC(14:1(9Z)/22:1(13Z)) or related compounds	Phospholipids
786.6028	427.54	2.67	C44H84NO8P	H	PC(16:0/20:2(11E,14E)) [U] or related compounds	Phospholipids
786.5982	451.86	3.18	C44H84NO8P	H	PC(18:1(10Z)/18:1(10Z)) or related compounds	Phospholipids
786.6026	505.34	2.42	C44H84NO8P	H	PC(18:0/18:2(2E,4E)) or related compounds	Phospholipids
786.6042	594.01	4.45	C44H84NO8P	H	PC(18:0/18:2(6Z,9Z)) or related compounds	Phospholipids
786.6028	675.87	2.67	C44H84NO8P	H	PC(18:0/18:2(10Z,12Z)) or related compounds	Phospholipids
772.618	360.33	4.45	C44H86NO7P	H	PC(18:0/dm18:1(11Z)) or related compounds	Phospholipids
776.5602	182.06	4.66	C45H78NO7P	H	PE(22:5(4Z,7Z,10Z,13Z,16Z)/dm18:1(11Z)) or related compounds	Phospholipids
810.6021	333.87	4.70	C46H84NO8P	H	20:2-18:2-PC or related compounds	Phospholipids
836.596	141.97	3.62	C46H88NO7P	K	PC(20:1(11Z)/dm18:1(11Z)) or related compounds	Phospholipids
814.634	426.34	2.46	C46H88NO8P	H	PC(14:1(9Z)/24:1(15Z)) or related compounds	Phospholipids
850.6111	140.03	2.92	C47H90NO7P	K	PE(24:1(15Z)/dm18:1(11Z)) or related compounds	Phospholipids
880.6235	146.68	2.25	C48H92NO8P	K	PC(16:1(9Z)/24:1(15Z)) or related compounds	Phospholipids
924.7379	103.23	1.34	C52H104NO8P	Na	PC(18:0/26:0) or related compounds	Phospholipids
188.175	580.12	3.88	C9H21N3O	H	N1-Acetylspermidine or related compounds	Polyamines
188.175	623.03	3.93	C9H21N3O	H	N8-Acetylspermidine or related compounds	Polyamines
<b>Polypeptides</b>						
273.0825	294.95	1.25	C10H16N2O4	Na_Na	(S)-ATPA;Prolyhydroxyproline	Polypeptides
308.0904	615.60	2.21	C10H17N3O6S	H	Glutathione;Reduced glutathione	Polypeptides
229.1539	541.82	3.36	C11H20N2O3	H	L-isoleucyl-L-proline;L-leucyl-L-proline	Polypeptides
427.0954	664.31	4.40	C13H22N4O8S2	H	Cysteineglutathione disulfide	Polypeptides
613.1595	649.09	0.16	C20H32N6O12S2	H	Glutathione disulfide;Oxidized glutathione	Polypeptides
681.1999	294.13	3.21	C22H42N4O8S2	NaCl_HCOONa	D-Pantethine	Polypeptides
179.0482	614.98	1.62	C5H10N2O3S	H	Cys-Gly;Cysteine-S-Acetamide	Polypeptides
188.1751	477.34	3.40	C9H21N3O	H	N1-Acetylspermidine;N8-Acetylspermidine	Polyamines
<b>Nucleotides and Derivatives</b>						
275.0738	250.68	4.62	C10H12N4O4	Na	Deoxyinosine;Nebularine;Purine Riboside	Nucleoside Analogues
306.0804	507.19	1.57	C10H13N5O5	Na	8-Hydroxy-2'-Deoxyguanosine;8-Hydroxy-deoxyguanosine;Crotonoside;Guanosine;	Nucleoside Analogues
338.0497	548.33	0.12	C10H13N5O6	K	8-Hydroxyguanosine	Nucleoside Analogues
364.0643	642.29	2.69	C10H14N5O8P	H	8-Oxo-2'-Deoxy-Guanosine-5'-Monophosphate or related compounds	Nucleotides
298.0957	156.40	3.82	C11H15N5O3S	H	5-Methylthioadenosine or related compounds	Nucleoside Analogues
565.0832	696.81	0.30	C16H26N2O16P2	H	dTDP-D-galactose or related compounds	Nucleotides
608.0896	610.25	1.23	C17H27N3O17P2	H	UDP-GlcNAc or related compounds	Nucleotides
664.1178	617.75	0.72	C21H27N7O14P2	H	Nicotinamide adenine dinucleotide or related compounds	Nucleotides
113.0341	185.11	4.07	C4H4N2O2	H	Uracil	Pyrimidines and Derivatives
129.0765	524.80	4.57	C4H5N3O	NH3	Cytosine	Pyrimidines and Derivatives
152.0561	508.74	4.93	C4H6O5	NH3	3-Dehydro-L-threonate;Malate	Purines and Purine Derivatives
152.056	642.92	4.27	C4H6O5	NH3	3-Dehydro-L-threonate;Malate	Purines and Purine Derivatives
137.0454	446.55	2.85	C5H4N4O	H	Hypoxanthine	Purines and Purine Derivatives
153.0412	314.70	3.27	C5H4N4O2	H	6,8-Dihydroxypurine;Alloxanthine;Oxypurinol	Purines and Purine Derivatives
136.0617	615.68	0.51	C5H5N5	H	Adenine	Purines and Purine Derivatives
136.0615	252.64	1.98	C5H5N5	H	Adenine	Purines and Purine Derivatives
136.0612	229.73	4.19	C5H5N5	H	Adenine	Purines and Purine Derivatives
136.0621	157.31	2.43	C5H5N5	H	Adenine	Purines and Purine Derivatives
152.0561	461.72	4.93	C5H5N5O	H	2-Hydroxyadenine;8-Hydroxyadenine;Guanine	Purines and Purine Derivatives
129.0657	629.63	1.24	C5H8N2O2	H	5,6-Dihydrothymine or related compounds	Pyrimidines and Derivatives
405.0095	616.31	4.07	C9H14N2O12P2	H	UDP	Nucleotides
<b>Quaternary Amines</b>						
244.1538	126.45	2.17	C12H21NO4	H	Tiglylcarnitine	Quaternary Amines
246.1694	499.59	2.36	C12H23NO4	H	2-Methylbutyrylcarnitine;Isovalerylcarnitine	Quaternary Amines
330.2638	119.83	3.03	C18H35NO4	H	4,8 dimethylnonanoyl carnitine	Quaternary Amines
398.3262	440.68	2.59	C23H43NO4	H	trans-Hexadec-2-enoyl carnitine	Quaternary Amines
400.3418	440.34	0.80	C23H45NO4	H	L-Palmitoylcarnitine	Quaternary Amines
426.357	436.45	1.81	C25H47NO4	H	Elaidic carnitine;octadecenoyl carnitine;Vaccenyl carnitine;;	Quaternary Amines
162.1119	653.66	3.52	C7H15NO3	H	L-Carnitine	Quaternary Amines
204.1222	590.80	4.07	C9H17NO4	H	L-Acetylcarnitine	Quaternary Amines
<b>Sphingoid bases</b>						
252.2303	113.30	2.10	C14H31NO	Na	Lauryl Dimethylamine-N-Oxide;Xestoinol C;;	Sphingoid bases
310.1746	712.63	4.93	C15H23N3O4	H	Polyproline	Sphingoid bases
442.1864	609.22	4.95	C17H38NO5P	KCl	C17 Sphinganine-1-phosphate	Sphingoid bases
318.2399	110.04	1.38	C18H33NO2	Na	(4E,8E,10E-d18:3)sphingosine;;	Sphingoid bases
320.2555	111.94	1.53	C18H35NO2	Na	(4E,8E,d18:2) sphingosine or related compounds	Sphingoid bases
648.38	200.39	3.87	C32H63NO5S	KCl	N-(tetradecanoyl)-deoxysphing-4-ene-1-sulfonate	Sphingolipids
703.575	449.57	0.26	C39H79N2O6P	H	SM(d18:1/16:0)	Sphingolipids
785.6536	446.72	0.67	C45H89N2O6P	H	SM(d18:1/22:1(13Z))	Sphingolipids
<b>Vitamines</b>						
417.2769	274.31	0.86	C27H38O2	Na	25-hydroxy-16,17,23,23,24,24-hexadehydrovitamin D3 / 25-hydroxy-16,17,23,23,24,24-hexadehydrocholecalciferol or related compounds	Vitamin D2 and derivatives
447.3106	115.06	1.45	C27H42O5	H	(23R)-1alpha,23,25-trihydroxy-24-oxovitamin D3 / (23R)-1alpha,23,25-trihydroxy-24-oxocholecalciferol or related compounds	Vitamin D2 and derivatives
433.3304	103.54	3.67	C27H44O4	H	(20S)-1alpha,20,25-trihydroxyvitamin D3 / (20S)-1alpha,20,25-trihydroxycholecalciferol or related compounds	Vitamin D3 and derivatives
447.3466	103.15	0.60	C28H46O4	H	(20S)-1alpha,20,25-trihydroxy-24a-homovitamin D3 / (20S)-1alpha,20,25-trihydroxy-24a-homocholecalciferol or related compounds	Vitamin D2 and derivatives
503.3072	191.93	3.93	C29H48O2	KCl	(22alpha)-hydroxy-isofoosterol or related compounds	Vitamin D2 and derivatives
461.3626	103.90	0.17	C29H48O4	H	(20S)-14alpha,20,25-trihydroxy-26,27-dimethylvitamin D3 / (20S)-1alpha,20,25-trihydroxy-26,27-dimethylcholecalciferol or related compounds	Vitamin D2 and derivatives
601.3268	506.60	4.31	C36H50O	K	11-(4-acetoxymethylphenyl)-1alpha,25-dihydroxy-9,11-didehydrovitamin D3 / 11-(4-acetoxymethylphenyl)-1alpha,25-dihydroxy-9,11-didehydrocholecalciferol or related compounds	Vitamin D2 and derivatives
725.4475	131.38	0.65	C39H64O12	H	1-Hydroxyvitamin D3 cellobioside;;	Vitamin D3 and derivatives
<b>Miscellaneous</b>						
224.125	193.91	3.17	C10H19NO3	Na	Capryloylglycine	Acyl Glycines
188.0704	496.37	1.12	C11H9NO2	H	Indoleacrylic acid	Indoles and Indole Derivatives
275.1412	408.38	1.53	C15H24O2	K	Capsidiol;dihydroartemisinin;Farnesic acid;Helminthosporol;Hernandulcin;Latia luciferin;Lubimin;Sirenin;;	Alcohols and Polyol
289.1792	103.80	2.14	C18H24O3	H	16,17-Epiestriol or related compounds	Steroids and Steroid Derivatives
300.3246	260.32	4.93	C19H38O	NH3	2-nonadecanone;Pristanal	Aldehydes
357.2622	113.06	3.75	C20H36O5	H	13,14-dihydro PGE1 or related compounds	Prostanoids
478.3214	198.74	4.41	C21H43N5O7	H	Gentamicin	Drug
142.0261	697.79	1.90	C2H8NO4P	H	1-Hydroxy-2-aminoethylphosphonate;Ethanolamine phosphate;;	Acyl Phosphates
604.354	189.84	2.25	C30H52O7P2	NH3	all-trans-Hexaprenyl diphosphate	Alkanes and Alkenes
790.5238	186.10	2.76	C46H73N3O4	NaCl	N-tryptophanyl-35-aminobacteriohopane-32,33,34-triol	Hopanoids
104.1064	573.42	5.67	C5H13NO	H	Choline	Aldehydes
123.0549	152.27	3.17	C6H6N2O	H	Nicotinamide	Cyclic Amines
107.0492	483.94	0.56	C7H6O	H	Benzaldehyde	Aldehydes
187.1076	646.46	0.64	C8H11NO3	NH3	5-Hydroxydopamine or related compounds	Catecholamines and Derivatives
204.0861	610.01	2.55	C8H13NO5	H	N2-acetyl-alpha-aminoadipate or related compounds	Pterins
147.0436	552.77	2.72	C9H6O2	H	Phenylpropionic acid	Alkyl Chlorides