

SUPPLEMENTARY TABLE 1

Non-destructive characterisation of mesenchymal stem cell differentiation using LC-MS-based metabolite footprinting

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Supplementary Table 1: Metabolites changed in MSC-conditioned medium compared to fresh medium (blank). ↑ indicates the metabolites that increased in all MSC-conditioned medium (control and OS) compared to their corresponding blanks, and ↓ indicates decreased metabolites. ID confidence: Metabolite identification level according to the metabolomics standards initiative ^{29,30} ; L1 – Level 1, L2 – Level 2.

Exact mass	RT (min)	Formula	Putative metabolite	ID confidence	Identifier (PubChem)	Change compared to blank medium
179.0946	5.30	C ₁₀ H ₁₃ NO ₂	(-)-Salsolinol	L2	91588	↑
358.1410	10.12	C ₂₀ H ₂₂ O ₆	(+)-Pinoresinol	L2	7741	↑
148.0371	10.28	C ₅ H ₈ O ₅	(R)-2-Hydroxyglutarate	L1	43	↑
104.0474	7.05	C ₄ H ₈ O ₃	(R)-3-Hydroxybutanoate	L2	92135	↑
113.0478	10.31	C ₅ H ₇ NO ₂	(S)-1-Pyrroline-5-carboxylate	L2	440162	↑
130.0631	4.76	C ₆ H ₁₀ O ₃	(S)-3-Methyl-2-oxopentanoic acid	L2	47	↑
134.0216	10.80	C ₄ H ₆ O ₅	(S)-Malate	L1	222656	↑
258.1833	4.67	C ₁₄ H ₂₆ O ₄	[FA (14:0/2:0)] Tetradecanedioic acid	L2	13185	↑
224.1777	4.10	C ₁₄ H ₂₄ O ₂	[FA (14:2)] 5,8-Tetradecadienoic acid	L2	5312409	↑
212.0896	10.63	C ₇ H ₁₆ O ₇	[FA (16:0/2:0)] Hexadecanedioic acid	L2	10459	↑
356.2932	3.91	C ₂₁ H ₄₀ O ₄	[FA (21:0/2:0)] Heneicosanedioic acid	L2	9543668	↑
201.1728	7.22	C ₁₁ H ₂₃ NO ₂	[FA amino(11:0)] 11-amino-undecanoic acid	L2	17083	↑
300.2666	3.96	C ₁₈ H ₃₆ O ₃	[FA hydroxy(18:0)] 2S-hydroxy-octadecanoic acid	L2	21145041	↑
437.2911	4.74	C ₂₁ H ₄₄ NO ₆ P	[PE (16:1)] 1-(1Z-hexadecenyl)-sn-glycero-3-phosphoethanolamine	L2	42607469	↑
272.2353	3.96	C ₁₆ H ₃₂ O ₃	16-Hydroxypalmitate	L2	7058075	↑
281.1124	11.00	C ₁₁ H ₁₅ N ₅ O ₄	1-Methyladenosine	L2	27476	↑
136.0637	18.40	C ₇ H ₈ N ₂ O	1-Methylnicotinamide	L2	457	↑

316.2983	4.43	C ₁₉ H ₄₀ O ₃	1-O-Hexadecyl-sn-glycerol	L2	72733	↑
214.0244	9.68	C ₅ H ₁₁ O ₇ P	2-Deoxy-D-ribose 5-phosphate	L2	45934311	↑
246.0506	10.47	C ₆ H ₁₅ O ₈ P	2-Deoxyglucose-6-phosphate	L2	46878412	↑
278.152	4.05	C ₁₆ H ₂₂ O ₄	2-Ethylhexyl phthalate	L2	20393	↑
112.0161	11.85	C ₅ H ₄ O ₃	2-Furoate	L2	6919	↑
150.035	5.30	C ₅ H ₁₀ O ₃ S	2-hydroxy-4-methylthiobutanoate	L2	21262170	↑
151.0495	8.33	C ₅ H ₅ N ₅ O	2-Hydroxyadenine	L2	76900	↑
206.0426	11.27	C ₇ H ₁₀ O ₇	2-Hydroxybutane-1,2,4-tricarboxylate	L2	28371	↑
120.0059	11.54	C ₃ H ₄ O ₅	2-Hydroxymalonate	L2	45	↑
160.0371	10.05	C ₆ H ₈ O ₅	2-Oxadipate	L2	71	↑
100.0161	5.10	C ₄ H ₄ O ₃	Unknown			↑
145.0375	7.93	C ₅ H ₇ NO ₄	2-Oxoglutaramate	L2	48	↑
146.0215	10.66	C ₅ H ₆ O ₅	2-Oxoglutarate	L1	51	↑
326.2825	3.94	C ₂₀ H ₃₈ O ₃	2-Oxophytanate	L2	25201496	↑
173.0477	5.30	C ₁₀ H ₇ NO ₂	2-Quinolinecarboxylic acid	L2	7124	↑
166.0629	5.05	C ₉ H ₁₀ O ₃	3-(3-Hydroxy-phenyl)-propanoic acid	L2	91	↑
182.0579	7.15	C ₉ H ₁₀ O ₄	3-(4-Hydroxyphenyl)lactate	L2	9378	↑
180.0423	7.03	C ₉ H ₈ O ₄	3-(4-Hydroxyphenyl)pyruvate	L1	979	↑
192.0805	8.73	C ₁₉ H ₂₈ O ₆ S	3b-16a-Dihydroxyandrostenonesulfate	L2	22833522	↑
84.0211	10.22	C ₄ H ₄ O ₂	3-Butynoate	L2	137547	↑
162.0528	9.68	C ₆ H ₁₀ O ₅	3-Ethylmalate	L2	21145023	↑
241.0079	10.06	C ₆ H ₁₁ NO ₅ S ₂	3-Mercaptolactate-cysteinedisulfide	L2	193536	↑
116.0474	5.18	C ₅ H ₈ O ₃	3-Methyl-2-oxobutanoic acid	L1	49	↑
165.0650	8.56	C ₆ H ₇ N ₅ O	3-Methylguanine	L2	76292	↑
145.0851	11.05	C ₅ H ₁₁ N ₃ O ₂	4-Guanidinobutanoate	L2	500	↑
177.0637	9.44	C ₆ H ₁₁ NO ₅	4-Hydroxy-4-methylglutamate	L2	102515406	↑

156.0536	8.33	C ₆ H ₈ N ₂ O ₃	4-Imidazolone-5-propanoate	L2	23615203	↑
159.0531	8.42	C ₆ H ₉ NO ₄	4-Methylene-L-glutamate	L2	6971046	↑
145.1102	9.77	C ₇ H ₁₅ NO ₂	4-Trimethylammoniobutanoate	L1	134	↑
246.0852	8.59	C ₉ H ₁₄ N ₂ O ₆	5-6-Dihydrouridine	L2	94312	↑
210.0529	5.29	C ₁₀ H ₁₀ O ₅	Unknown			↑
191.0584	10.00	C ₁₀ H ₉ NO ₃	5-Hydroxyindoleacetate	L1	1826	↑
118.0631	5.31	C ₅ H ₁₀ O ₃	5-Hydroxypentanoate	L2	5459830	↑
257.0361	9.59	C ₁₀ H ₁₁ NO ₅ S	5-Hydroxytryptophol sulfate	L2	44237265	↑
257.1011	8.08	C ₁₀ H ₁₅ N ₃ O ₅	5-Methylcytidine	L2	92918	↑
125.0590	8.62	C ₅ H ₇ N ₃ O	5-Methylcytosine	L2	65040	↑
116.0470	7.66	C ₅ H ₈ O ₃	Unknown			↑
179.0807	7.72	C ₇ H ₉ N ₅ O	7-Aminomethyl-7-carbaguanine	L2	171	↑
282.0964	7.65	C ₁₁ H ₁₄ N ₄ O ₅	8-Oxocoformycin	L2	25202745	↑
289.0950	5.32	C ₁₅ H ₁₅ NO ₅	Acronycidine	L2	95708	↑
176.0546	10.43	C ₄ H ₈ N ₄ O ₄	Allantoate	L2	5287444	↑
161.0510	5.15	C ₆ H ₁₁ NO ₂ S	Allylcysteine	L2	23437571	↑
88.0525	5.32	C ₄ H ₈ O ₂	Butanoic acid	L2	264	↑
230.1417	7.03	C ₁₄ H ₁₈ N ₂ O	Unknown			↑
103.1000	10.21	C ₅ H ₁₃ NO	Choline	L2	305	↑
183.0662	10.15	C ₅ H ₁₄ NO ₄ P	Choline phosphate	L1	1014	↑
202.0478	11.29	C ₈ H ₁₀ O ₆	Cis-(homo)2aconitate	L2	25244889	↑
174.0164	11.70	C ₆ H ₆ O ₆	Cis-Aconitate	L2	643757	↑
192.0270	11.88	C ₆ H ₈ O ₇	Citrate	L2	311	↑
243.0855	9.59	C ₉ H ₁₃ N ₃ O ₅	Cytidine	L1	6175	↑
111.0433	9.55	C ₄ H ₅ N ₃ O	Cytosine	L1	597	↑
228.0746	7.65	C ₉ H ₁₂ N ₂ O ₅	Deoxyuridine	L1	13712	↑
210.0376	11.53	C ₆ H ₁₀ O ₈	D-Glucarate	L2	33037	↑
196.0583	9.73	C ₆ H ₁₂ O ₇	D-Gluconic acid	L1	10690	↑

260.0298	10.88	C ₆ H ₁₃ O ₉ P	D-Glucose 6-phosphate	L1	439958	↑
194.0426	10.81	C ₆ H ₁₀ O ₇	D-Glucuronate	L2	94715	↑
393.1211	8.93	C ₂₂ H ₁₉ NO ₆	Dihydromacarpine	L2	440631	↑
335.0631	8.32	C ₉ H ₁₄ N ₅ O ₇ P	Dihydroneopterin phosphate	L2	25245170	↑
181.0408	8.85	C ₅ H ₁₁ NO ₄ S	Unknown			↑
276.0958	10.99	C ₁₀ H ₁₆ N ₂ O ₇	GammaGlutamylglutamicacid	L2	92865	↑
90.0318	7.09	C ₃ H ₆ O ₃	Glyceraldehyde	L2	751	↑
92.0474	8.77	C ₃ H ₈ O ₃	Glycerol	L1	753	↑
246.0505	8.84	C ₆ H ₁₅ O ₈ P	Glycerophosphoglycerol	L2	439964	↑
75.0321	11.26	C ₂ H ₅ NO ₂	Glycine	L1	750	↑
188.1274	17.21	C ₇ H ₁₆ N ₄ O ₂	Homoarginine	L2	9085	↑
262.0148	11.26	C ₉ H ₁₀ O ₇ S	Homovanillicacidsulfate	L2	29981063	↑
111.9926	9.83	CH ₅ O ₄ P	Hydroxymethylphosphonate	L2	21680357	↑
109.0198	10.90	C ₂ H ₇ NO ₂ S	Hypotaurine	L2	107812	↑
154.0377	8.13	C ₆ H ₆ N ₂ O ₃	Imidazol-5-yl-pyruvate	L2	23615390	↑
159.0684	5.95	C ₁₀ H ₉ NO	Indole-3-acetaldehyde	L2	800	↑
274.1319	5.32	C ₁₅ H ₁₈ N ₂ O ₃	Indole-3-acetyl-valine	L2	25200807	↑
205.0739	7.01	C ₁₁ H ₁₁ NO ₃	Indolelactate	L2	92904	↑
203.0583	6.96	C ₁₁ H ₉ NO ₃	Indolepyruvate	L2	5460337	↑
129.0427	7.77	C ₅ H ₇ NO ₃	L-1-Pyrroline-3-hydroxy-5-carboxylate	L2	1059	↑
117.0427	7.34	C ₄ H ₇ NO ₃	L-2-Amino-3-oxobutanoic acid	L2	440033	↑
161.0688	10.05	C ₆ H ₁₁ NO ₄	L-2-Aminoadipate	L1	6992111	↑
89.0477	10.78	C ₃ H ₇ NO ₂	L-Alanine	L1	5950	↑
166.0477	9.49	C ₅ H ₁₀ O ₆	L-Arabinonate	L2	5459849	↑
132.0534	10.76	C ₄ H ₈ N ₂ O ₃	L-Asparagine	L1	6267	↑
133.0376	10.35	C ₄ H ₇ NO ₄	L-Aspartate	L1	5460294	↑
175.0957	11.13	C ₆ H ₁₃ N ₃ O ₃	L-Citrulline	L1	9750	↑

297.0455	9.93	C ₈ H ₁₅ N ₃ O ₅ S ₂	L-Cysteinyglycinedisulfide	L2	22833544	↑
174.0163	8.04	C ₆ H ₆ O ₆	L-Dehydroascorbate	L2	440667	↑
254.0396	10.67	C ₇ H ₁₄ N ₂ O ₄ S ₂	L-Djenkolic acid	L2	68134	↑
163.0480	11.06	C ₅ H ₉ NO ₅	L-erythro-4-Hydroxyglutamate	L2	440854	↑
120.0423	7.90	C ₄ H ₈ O ₄	L-Erythrulose	L2	5460032	↑
131.0583	10.61	C ₅ H ₉ NO ₃	L-Glutamate 5-semialdehyde	L2	193305	↑
161.0688	5.75	C ₆ H ₁₁ NO ₄	L-Glutamate methylester	L2	68662	↑
165.0460	9.61	C ₅ H ₁₁ NO ₃ S	L-Methionine S-oxide	L2	158980	↑
115.0633	9.82	C ₅ H ₉ NO ₂	L-Proline	L1	145742	↑
114.0793	8.67	C ₅ H ₁₀ N ₂ O	L-proline amide	L2	3765327	↑
133.0197	7.03	C ₄ H ₇ NO ₂ S	Unknown			↑
273.1000	4.88	C ₁₅ H ₁₅ NO ₄	L-Thyronine	L2	5461103	↑
104.0110	10.54	C ₃ H ₄ O ₄	Malonate	L1	9084	↑
72.0210	8.76	C ₃ H ₄ O ₂	Methylglyoxal	L1	880	↑
146.0215	11.92	C ₅ H ₆ O ₅	Methyloxaloacetate	L2	440890	↑
180.0634	11.75	C ₆ H ₁₂ O ₆	Myo-Inositol	L1	892	↑
246.1328	10.41	C ₉ H ₁₈ N ₄ O ₄	N2-(D-1-Carboxyethyl)-L-arginine	L2	6992007	↑
218.1266	10.35	C ₉ H ₁₈ N ₂ O ₄	N2-(D-1-Carboxyethyl)-L-lysine	L2	193187	↑
203.0795	9.49	C ₈ H ₁₃ NO ₅	N2-Acetyl-L-aminoadipate	L2	443992	↑
311.1230	7.73	C ₁₂ H ₁₇ N ₅ O ₅	N2-N2-Dimethylguanosine	L2	92919	↑
174.1005	9.84	C ₇ H ₁₄ N ₂ O ₃	N5-Ethyl-L-glutamine	L2	439378	↑
295.1282	5.36	C ₁₂ H ₁₇ N ₅ O ₄	N6,N6-Dimethyladenosine	L2	440004	↑
188.1161	9.50	C ₈ H ₁₆ N ₂ O ₃	N6-Acetyl-L-lysine	L1	6991978	↑
131.0582	7.04	C ₅ H ₉ NO ₃	N-Acetyl-beta-alanine	L2	76406	↑
237.0849	11.88	C ₈ H ₁₅ NO ₇	N-Acetyl-D-glucosaminat	L2	16126799	↑
189.0637	9.61	C ₇ H ₁₁ NO ₅	N-Acetyl-L-glutamate	L1	70914	↑
177.0459	5.31	C ₆ H ₁₁ NO ₃ S	N-Formyl-L-methionine	L2	439750	↑
123.0320	5.35	C ₆ H ₅ NO ₂	Nicotinate	L2	937	↑

516.0412	9.89	C ₂₁ H ₁₆ N ₄ O ₈ S ₂	Nitrocefin	L2	44123393	↑
75.0321	5.17	C ₂ H ₅ NO ₂	Nitroethane	L2	6587	↑
249.0310	12.10	C ₈ H ₁₁ NO ₆ S	Norepinephrinesulfate	L2	123747	↑
281.1124	7.21	C ₁₁ H ₁₅ N ₅ O ₄	O6-Methyl-2'-deoxyguanosine	L2	73317	↑
161.0688	8.64	C ₆ H ₁₁ NO ₄	O-Acetyl-L-homoserine	L2	25244888	↑
217.1314	8.08	C ₁₀ H ₁₉ NO ₄	O-Propanoylcarnitine	L2	107738	↑
156.0171	7.93	C ₅ H ₄ N ₂ O ₄	Orotate	L1	967	↑
288.0595	8.99	C ₁₀ H ₁₂ N ₂ O ₈	Orotidine	L1	92751	↑
97.9771	10.61	H ₃ O ₄ P	Orthophosphate	L2	1061	↑
219.0743	9.61	C ₈ H ₁₃ NO ₆	O-Succinyl-L-homoserine	L2	439406	↑
89.9954	11.83	C ₂ H ₂ O ₄	Oxalate	L1	971	↑
266.0904	9.93	C ₁₂ H ₁₄ N ₂ O ₅	p-aminobenzoyl glutamate	L2	25202539	↑
342.1461	10.62	C ₂₀ H ₂₂ O ₅	Unknown			↑
173.9986	4.89	C ₆ H ₆ O ₄ S	Unknown			↑
193.0739	5.17	C ₁₀ H ₁₁ NO ₃	Phenylacetyl glycine	L2	68144	↑
164.0474	4.77	C ₉ H ₈ O ₃	Phenylpyruvate	L1	997	↑
79.9663	10.97	[PO ₃] ₃ ⁻	Phosphite	L2	22497	↑
303.1684	5.34	C ₁₄ H ₂₅ NO ₆	Pimelylcarnitine	L2	91825640	↑
74.0367	7.09	C ₃ H ₆ O ₂	Propanoate	L2	1032	↑
154.0031	8.57	C ₃ H ₇ O ₅ P	Propanoyl phosphate	L2	1034	↑
72.0210	10.40	C ₃ H ₄ O ₂	Propenoate	L2	6581	↑
244.0700	9.61	C ₉ H ₁₂ N ₂ O ₆	Pseudouridine	L2	15047	↑
297.1073	8.56	C ₁₁ H ₁₅ N ₅ O ₅	Psicofuranin	L2	65086	↑
326.1512	9.80	C ₂₀ H ₂₂ O ₄	Pulverochromenol	L2	441982	↑
229.0376	11.28	C ₁₂ H ₇ NO ₄	Resazurin	L2	11077	↑
221.0355	8.67	C ₇ H ₁₁ NO ₅ S	S-(3-oxo-3-carboxy-n-propyl)cysteine	L2	21252272	↑
210.0739	10.49	C ₇ H ₁₄ O ₇	Sedoheptulose	L2	102926	↑

426.0880	10.92	C ₁₃ H ₂₂ N ₄ O ₈ S ₂	S-glutathionyl-L-cysteine	L2	10455148	↑
174.0528	7.12	C ₇ H ₁₀ O ₅	Unknown			↑
257.1029	10.21	C ₈ H ₂₀ NO ₆ P	Sn-glycero-3-Phosphocholine	L1	657272	↑
215.0558	10.77	C ₅ H ₁₄ NO ₆ P	Sn-glycero-3-Phosphoethanolamine	L2	444183	↑
118.0267	10.09	C ₄ H ₆ O ₄	Succinate	L1	1110	↑
311.1008	7.24	C ₁₄ H ₁₇ NO ₇	Taxiphyllin	L2	107721	↑
272.0831	9.17	C ₁₁ H ₁₆ N ₂ O ₄ S	Thienamycin	L2	441128	↑
147.0353	7.01	C ₅ H ₉ NO ₂ S	Thiomorpholine 3-carboxylate	L2	440159	↑
242.0905	7.07	C ₁₀ H ₁₄ N ₂ O ₅	Thymidine	L1	5789	↑
126.0429	7.09	C ₅ H ₆ N ₂ O ₂	Thymine	L1	1135	↑
112.0273	8.46	C ₄ H ₄ N ₂ O ₂	Uracil	L2	1174	↑
168.0283	9.38	C ₅ H ₄ N ₄ O ₃	Urate	L1	1175	↑
244.0696	8.58	C ₉ H ₁₂ N ₂ O ₆	Uridine	L1	6029	↑
138.0429	8.37	C ₆ H ₆ N ₂ O ₂	Urocanate	L2	736715	↑
228.1110	9.96	C ₁₀ H ₁₆ N ₂ O ₄	(S)-ATPA	L2	2253	↑
467.3012	5.06	C ₂₂ H ₄₆ NO ₇ P	PC (14:0)] 1-tetradecanoyl-sn-glycero-3-phosphocholine	L2	460604	↑
465.3218	4.69	C ₂₃ H ₄₈ NO ₆ P	[PC (15:1)] 1-(1Z-pentadecenyl)-sn-glycero-3-phosphocholine	L2	24779524	↑
87.0320	10.93	C ₃ H ₅ NO ₂	2-Aminoacrylate	L2	123991	↑
88.0162	7.03	C ₃ H ₄ O ₃	3-Oxopropanoate	L2	9543142	↑
153.0092	11.27	C ₃ H ₇ NO ₄ S	L-Cysteine sulfinat	L2	1549098	↑
162.0164	8.47	C ₅ H ₆ O ₆	4-Hydroxy-2-oxoglutarate	L2	599	↑
114.0430	7.04	C ₄ H ₆ N ₂ O ₂	5,6-Dihydrouracil	L2	649	↑
175.0634	4.32	C ₁₀ H ₉ NO ₂	5-Hydroxyindoleacetaldehyde	L2	74688	↑
158.0439	10.91	C ₄ H ₆ N ₄ O ₃	Allantoin	L1	204	↑
176.0321	10.39	C ₆ H ₈ O ₆	Ascorbate	L1	54670067	↑
240.1222	11.21	C ₁₀ H ₁₆ N ₄ O ₃	Beta-Alanyl-N(pi)-methyl-L-histidine	L2	112072	↑

226.1066	10.91	C ₉ H ₁₄ N ₄ O ₃	Carnosine	L2	439224	↑
180.0634	10.35	C ₆ H ₁₂ O ₆	D-Fructose	L1	5984	↑
328.2407	3.95	C ₂₂ H ₃₂ O ₂	Docosaehaenoicacid	L2	445580	↑
150.0528	10.69	C ₅ H ₁₀ O ₅	D-Xylulose	L2	5289590	↑
117.0538	11.53	C ₃ H ₇ N ₃ O ₂	Guanidinoacetate	L2	25201830	↑
151.0493	10.14	C ₅ H ₅ N ₅ O	Guanine	L1	764	↑
245.0688	5.14	C ₁₃ H ₁₁ NO ₄	Haplopine	L2	165368	↑
117.0538	11.53	C ₃ H ₇ N ₃ O ₂	Guanidinoacetate	L2	25201830	↑
615.1693	7.17	C ₃₄ H ₃₂ N ₄ O ₄ Fe	Heme	L2	26945	↑
136.0385	8.82	C ₅ H ₄ N ₄ O	Hypoxanthine	L1	790	↑
174.1117	16.85	C ₆ H ₁₄ N ₄ O ₂	L-Arginine	L1	6322	↑
121.0198	10.66	C ₃ H ₇ NO ₂ S	L-Cysteine	L1	5862	↑
240.0240	10.66	C ₆ H ₁₂ N ₂ O ₄ S ₂	L-Cystine	L1	67678	↑
147.0531	10.07	C ₅ H ₉ NO ₄	L-Glutamate	L1	5460299	↑
146.0691	10.71	C ₅ H ₁₀ N ₂ O ₃	L-Glutamine	L1	5961	↑
131.0946	8.95	C ₆ H ₁₃ NO ₂	L-Leucine	L1	6106	↑
149.0510	9.05	C ₅ H ₁₁ NO ₂ S	L-Methionine	L1	6137	↑
105.0426	11.13	C ₃ H ₇ NO ₃	L-Serine	L1	5951	↑
181.0739	10.00	C ₉ H ₁₁ NO ₃	L-Tyrosine	L1	6057	↑
335.1332	10.60	C ₁₂ H ₂₁ N ₃ O ₈	N4-(Acetyl-beta-D-glucosaminy)asparagine	L2	123826	↑
102.0681	5.26	C ₅ H ₁₀ O ₂	Pentanoate	L2	114781	↑
200.9766	11.66	C ₃ H ₇ NO ₅ S ₂	S-Sulfo-L-cysteine	L2	115015	↑
139.9779	12.05	C ₂ H ₄ O ₅ S	Sulfoacetate	L2	31257	↑
125.0147	10.78	C ₂ H ₇ NO ₃ S	Taurine	L1	1123	↑
152.9918	10.65	C ₃ H ₇ NO ₂ S ₂	Thiocysteine	L2	165331	↑
152.0334	9.01	C ₅ H ₄ N ₄ O ₂	Xanthine	L1	1188	↑
284.0758	8.54	C ₁₀ H ₁₂ N ₄ O ₆	Xanthosine	L1	64959	↑

304.2404	3.99	C ₂₀ H ₃₂ O ₂	[FA (20:4)] 5Z,8Z,11Z,14Z-eicosatetraenoic acid	L2	444899	↓
467.3015	5.07	C ₂₂ H ₄₆ NO ₇ P	[PC (14:0)] 1-tetradecanoyl-sn-glycero-3-phosphocholine	L2	460604	↓
519.3327	4.90	C ₂₆ H ₅₀ NO ₇ P	[PC (18:2)] 1-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphocholine	L2	11005824	↓
541.3200	4.89	C ₂₈ H ₄₈ NO ₇ P	[PC (20:5)] 1-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-glycero-3-phosphocholine	L2	11757087	↓
567.3318	4.81	C ₃₀ H ₅₀ NO ₇ P	[PC (22:6)] 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycero-3-phosphocholine	L2	10415542	↓
153.0096	10.15	C ₃ H ₇ NO ₄ S	3-Sulfin-L-alanine	L2	439270	↓
176.0321	10.39	C ₆ H ₈ O ₆	Ascorbate	L1	54670067	↓
240.1224	11.21	C ₁₀ H ₁₆ N ₄ O ₃	Beta-Alanyl-N(pi)-methyl-L-histidine	L2	112072	↓
226.1066	10.91	C ₉ H ₁₄ N ₄ O ₃	Carnosine	L2	439224	↓
357.1572	10.69	C ₂₀ H ₂₃ NO ₅	Deacetylcolchicine	L2	25203116	↓
180.0634	10.35	C ₆ H ₁₂ O ₆	D-Fructose	L1	439709	↓
328.2404	3.95	C ₂₂ H ₃₂ O ₂	Docosaehaenoicacid	L2	445580	↓
615.1689	7.17	C ₃₄ H ₃₂ N ₄ O ₄ Fe	Heme	L2	26945	↓
306.2557	3.97	C ₂₀ H ₃₄ O ₂	Icosatrienoic acid	L2	5312529	↓
436.2589	4.84	C ₂₁ H ₄₁ O ₇ P	LPA(0:0/18:1(9Z))	L2	52929749	↓
543.3325	4.87	C ₂₈ H ₅₀ NO ₇ P	LysoPC(20:4(5Z,8Z,11Z,14Z))	L2	24779476	↓
569.3483	4.79	C ₃₀ H ₅₂ NO ₇ P	LysoPC(22:5(4Z,7Z,10Z,13Z,16Z))	L2	53480473	↓
335.1332	10.66	C ₁₂ H ₂₁ N ₃ O ₈	N4-(Acetyl-beta-D-glucosaminyl)asparagine	L2	123826	↓
330.2562	3.96	C ₂₂ H ₃₄ O ₂	Taxa-4(20),11(12)-dien-5alpha-yl acetate	L2	443486	↓
304.2404	3.99	C ₂₀ H ₃₂ O ₂	[FA (20:4)] 5Z,8Z,11Z,14Z-eicosatetraenoic acid	L2	444899	↓

467.3015	5.07	$C_{22}H_{46}NO_7P$	[PC (14:0)] 1-tetradecanoyl-sn-glycero-3-phosphocholine	L2	460604	↓
519.3327	4.90	$C_{26}H_{50}NO_7P$	[PC (18:2)] 1-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphocholine	L2	11005824	↓
541.3200	4.89	$C_{28}H_{48}NO_7P$	[PC (20:5)] 1-(5Z,8Z,11Z,14Z,17Z-eicosapentaenoyl)-sn-glycero-3-phosphocholine	L2	11757087	↓
567.3327	4.81	$C_{30}H_{50}NO_7P$	[PC (22:6)] 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-sn-glycero-3-phosphocholine	L2	10415542	↓