Electronic Supplementary Information

Investigating the intracellular effects of hyperbranched polycation-DNA complexes on lung cancer cells using LC-MS-based metabolite profiling

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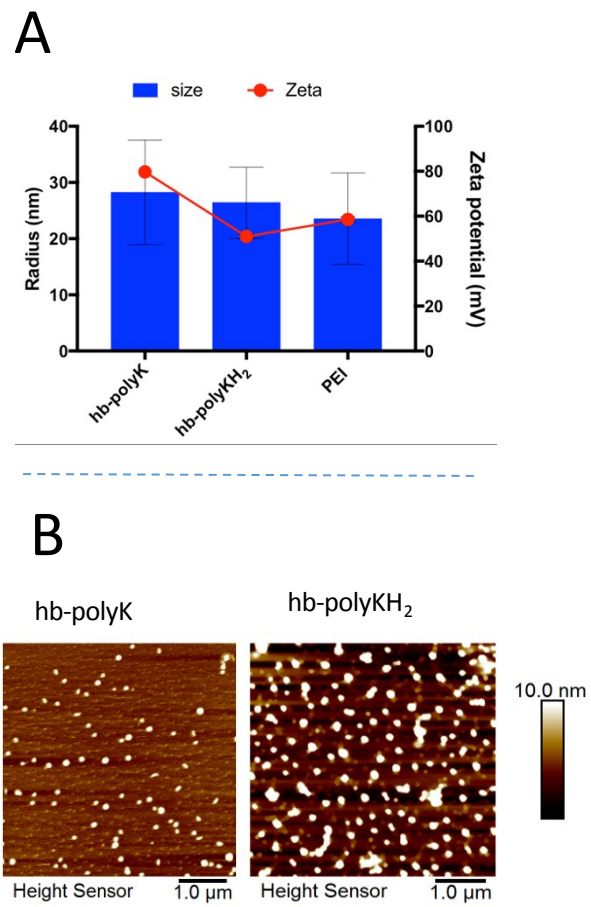

Figure S1 the physicochemical characterization of the polyplexes prepared in HEPES buffer (0.1 mM, pH 7.4) at N/P of 10, the size and zeta potential measurements (A) and the AFM images (B).

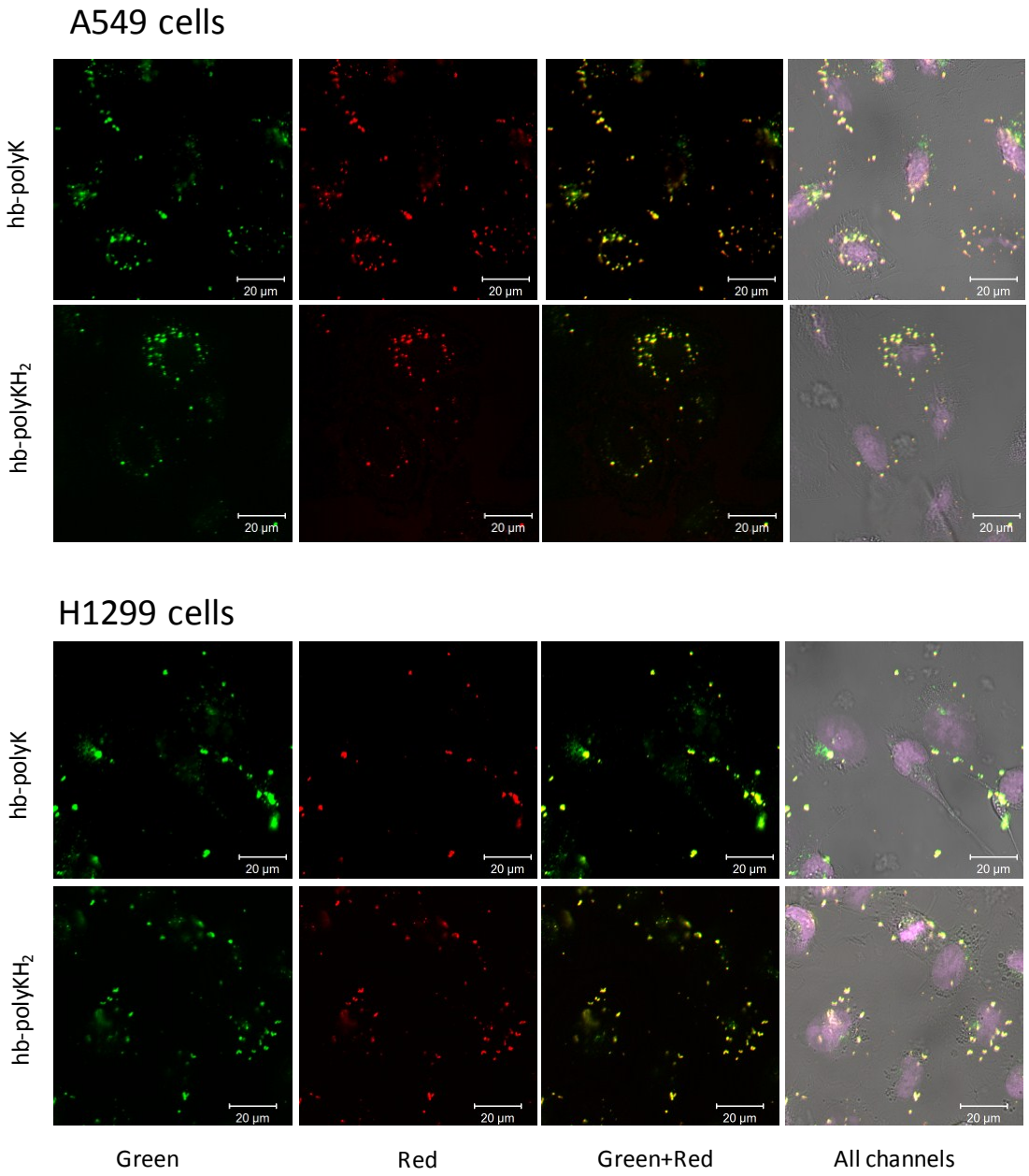

Figure S2 Confocal images show the uptake of hb-polyK and histidine containing hb-polyKH$_2$ complexes in A549 and H1299 cells. Areas in green are FITC-labelled polymers, area in red are Cy3-labelled plasmid, regions in yellow are assigned to overlaid Cy3-labelled plasmid and FITC-labelled polymers, and areas in purple correspond to DRAQ5 stained nuclei

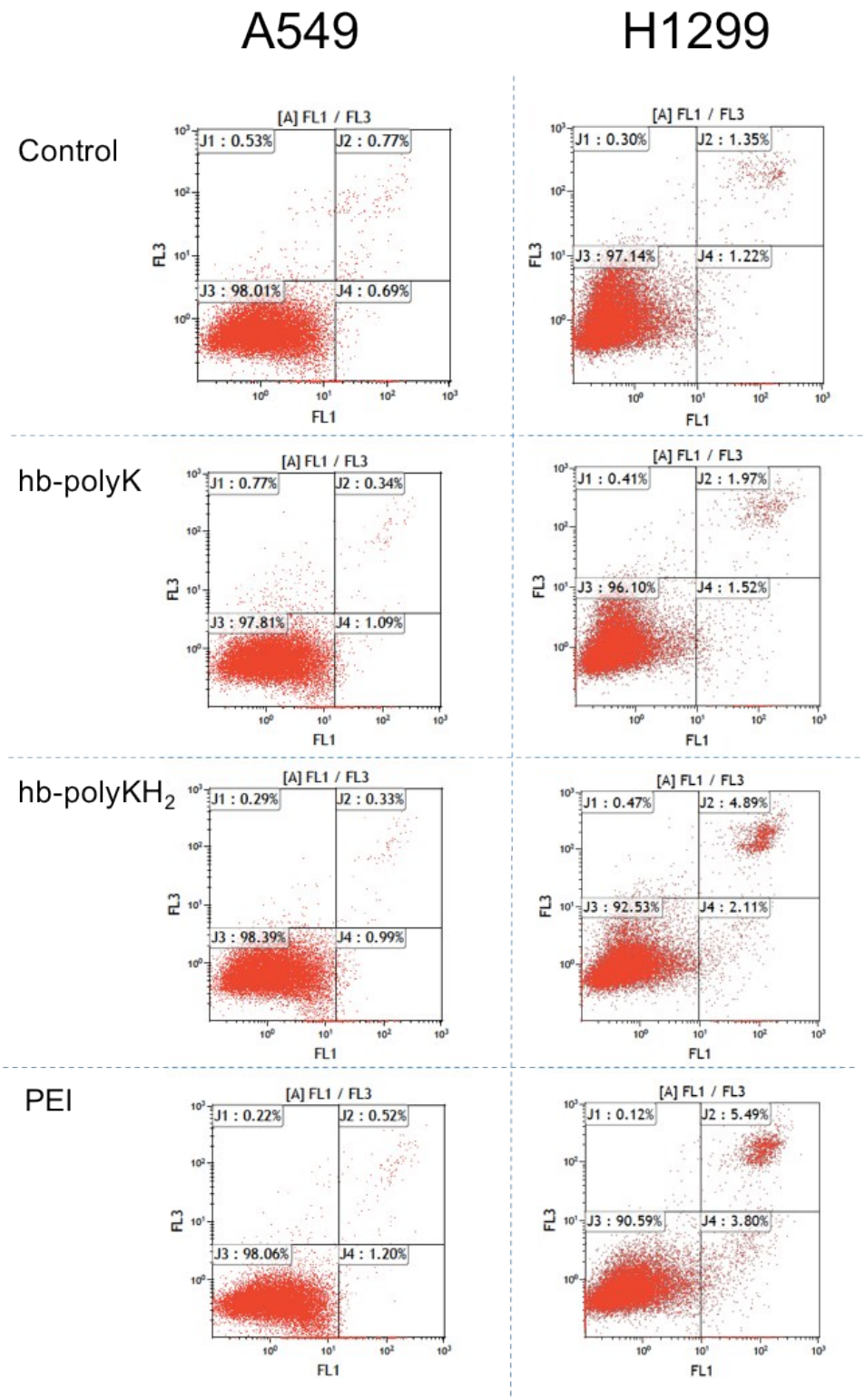

Figure S3 Flow cytometry analysis of Annexin-V/PI apoptosis assays to measure the apoptotic and dead cells in A549 and H1299 cells after four hour treatment with polyplexes of hb-polyK, hb-polyKH2 and PEI (the control group with FBS-free medium), and then 20 hour of incubation without fully supplemented medium. The percentages of live, apoptotic, and dead cells were calculated from FL1/FL3. Annexin-V-FITC was used to detect apoptotic cells, and propidium iodide (PI) was used to detect dead cells. J1~ necrotic cells, J2 ~ dead cells, J3 ~ live cells, and J4 ~ apoptotic cell.

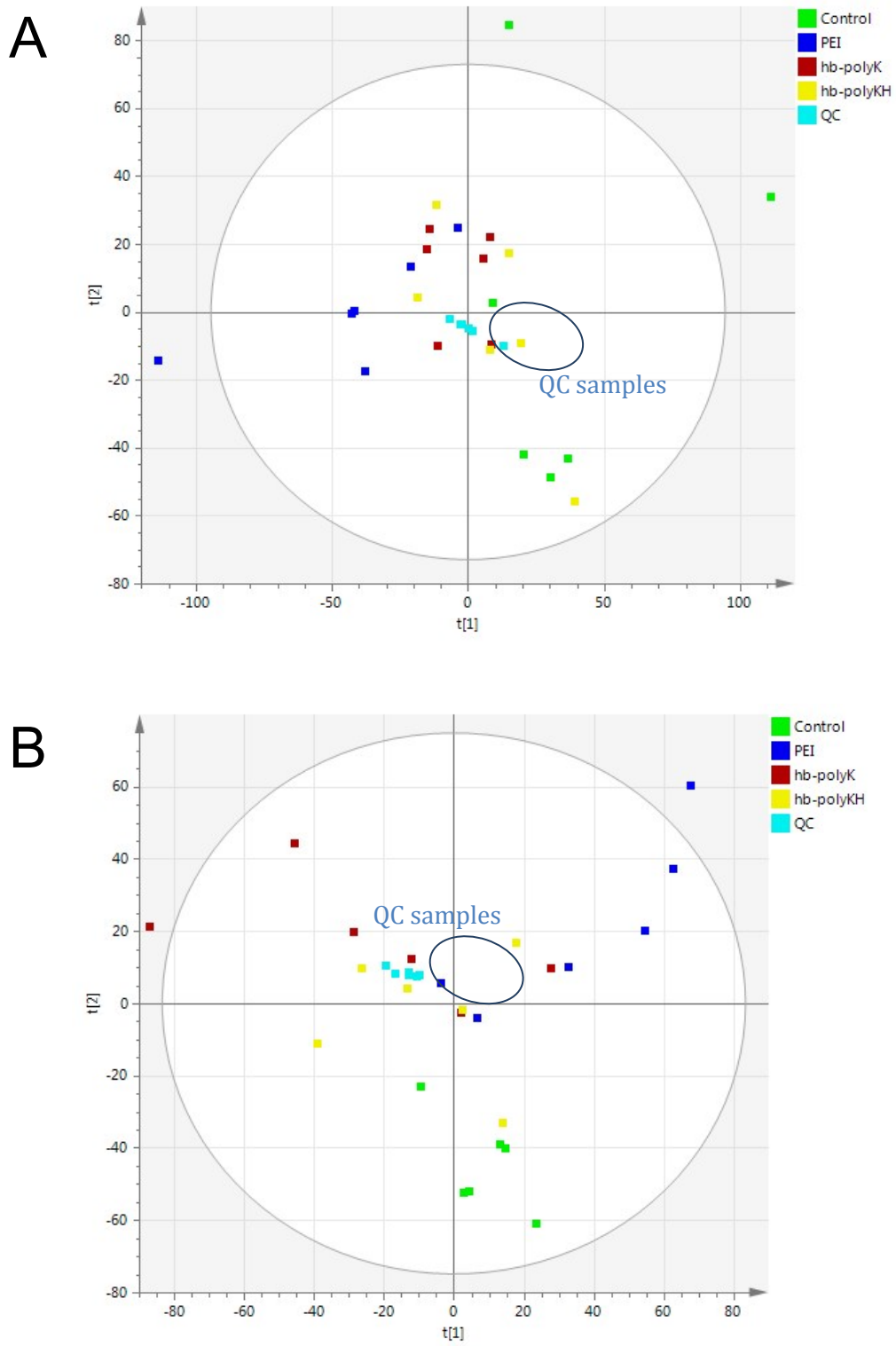

Figure S4: PCA scores plots of A) A549 cells samples (R2X=0.563, Q2=0.147) and B) H1299 cells samples (R2X=0.622, Q2=0.333) after four hour treatment with polyplexes of hb-polyK, hb-polyKH2 and PEI (the control group with FBS-free medium), and then 20 hour of incubation without fully supplemented medium. Both of the PCA plots couldn't separate between the different treatment groups, however the clustering of the repeatedly injected pooled QC samples indicating that the LC-MS system was stable throughout the run, this is confirmed by the fact that more than 70% of the detected features from the QC samples had CV of less than 30%.

Table S1: The metabolites that were changed significantly in A549 cells after the treatment with polyplexes, IDC: metabolite identification level according to the metabolomics standards initiative L1 – Level 1, L2 – Level 2.

Mass	Polarity	Mass error (PPM)	RT	FORMULA	Putative metabolite	IDC	Pathway	Control	Poly PEI	Poly K	Poly KH
89.0477	+	0.247308	11.01	C3H7NO2	L-Alanine	L1	Amino Acid Metabolism	1.00	0.70	1.00	1.00
90.0317	-	0.417857	7.42	C3H6O3	Lactate	L1	Carbohydrate Metabolism	1.00	0.52	0.78	0.90
100.0525	+	0.399236	11.04	C5H8O2	Tiglic acid	L2	Lipids: Fatty Acyls	1.00	0.38	0.60	0.83
101.0841	+	0.625395	16.84	C5H11NO	Betaine aldehyde	L2	Amino Acid Metabolism	1.00	0.58	0.73	0.85
103.0633	+	-0.17921	11.02	C4H9NO2	4-Amino-butanoate	L2	Amino Acid Metabolism	1.00	0.49	0.61	0.86
103.0997	+	-0.18211	10.23	C5H13NO	Choline	L2	Amino Acid Metabolism	1.00	0.74	0.83	0.76
104.0474	-	0.090649	7.42	C4H8O3	3-Hydroxy-butanoate	L2	Lipid Metabolism	1.00	0.75	1.17	1.02
111.9926	-	0.523104	9.68	CH5O4P	Hydroxymethylphosphonate	L2	Amino Acid Metabolism	1.00	0.58	0.57	0.84
113.0477	-	0.319435	10.03	C5H7NO2	1-Pyrroline-5-carboxylate	L2	Amino Acid Metabolism	1.00	0.55	0.89	0.53
113.0589	+	0.111963	8.47	C4H7N3O	Creatinine	L1	Amino Acid Metabolism	1.00	0.61	0.97	0.86
117.0426	-	0.260081	7.44	C4H7NO3	2-Amino-3-oxobutanoic acid	L2	Amino Acid Metabolism	1.00	0.51	0.89	1.06
117.0789	+	-0.42807	9.67	C5H11NO2	Valine	L1	Amino Acid Metabolism	1.00	0.62	0.89	0.88
122.0479	+	-0.63014	9.7	C6H6N2O	Isonicotineamide	L2	-	1.00	0.49	0.51	0.94
123.9927	+	1.019145	10.08	C2H5O4P	Phosphonoacetaldehyde	L2	Amino Acid Metabolism	1.00	0.71	0.86	0.86
125.0147	+	0.021564	10.7	C2H7NO3S	Taurine	L1	Lipid Metabolism	1.00	0.62	0.87	0.88
126.0084	-	1.323157	9.7	C2H7O4P	Ethylphosphate	L2	-	1.00	0.42	0.69	0.76
126.0429	-	-0.37997	7.49	C5H6N2O2	Thymine	L1	Nucleotide Metabolism	1.00	6.09	7.59	1.88
126.043	+	0.318535	8.67	C5H6N2O2	Imidazole-4-acetate	L1	Amino Acid Metabolism	1.00	0.41	0.76	1.10
128.0586	+	0.513835	10.85	C5H8N2O2	5,6-Dihydrothymine	L2	Nucleotide Metabolism	1.00	0.59	0.88	0.93
129.0427	-	0.67742	5.48	C5H7NO3	1-Pyrroline-4-hydroxy-2-carboxylate	L2	Amino Acid Metabolism	1.00	0.44	0.56	0.49
130.063	-	0.108729	9.68	C6H10O3	4-Methyl-2-oxopentanoate	L2	Amino Acid Metabolism	1.00	0.52	0.82	0.80
130.1106	+	0.1079	16.69	C6H14N2O	N-Acetylputrescine	L2	Amino Acid Metabolism	1.00	0.43	0.60	0.81
131.0582	-	-0.09926	5.3	C5H9NO3	4-Amino-5-oxopentanoate	L2	Metabolism of Cofactors and Vitamins	1.00	0.49	0.71	0.86
131.0583	+	0.81444	10.58	C5H9NO3	Glutamate 5-semialdehyde	L2	Amino Acid Metabolism	1.00	0.65	0.80	0.90
131.0695	+	0.181322	10.77	C4H9N3O2	Creatine	L1	Amino Acid Metabolism	1.00	0.59	0.85	1.03
131.0946	+	0.113021	9.05	C6H13NO2	Leucine	L2	Amino Acid Metabolism	1.00	0.60	0.84	0.85
134.0216	+	-0.1023	10.44	C4H6O5	Malate	L1	Carbohydrate Metabolism	1.00	0.69	0.92	1.00
135.0545	+	-0.32059	8.53	C5H5N5	Adenine	L1	Nucleotide Metabolism	1.00	0.74	0.56	0.78
136.0524	-	0.096993	5.15	C8H8O2	Phenylacetic acid	L2	Amino Acid Metabolism	1.00	0.68	0.78	0.82
137.0476	-	-0.38995	7.35	C7H7NO2	Anthranilate	L2	Amino Acid Metabolism	1.00	6.11	6.55	1.54
140.0585	+	-0.21461	7.43	C6H8N2O2	Methylimidazoleacetic acid	L2	Amino Acid Metabolism	1.00	0.57	0.92	0.90
141.0193	+	1.080585	10.68	C2H8NO4P	Ethanolamine phosphate	L1	Amino Acid Metabolism	1.00	1.47	1.59	1.22

145.0375	-	-0.3444	7.42	C5H7NO4	4-Oxoglutaramate	L2	Amino Acid Metabolism	1.00	0.53	0.68	1.05
145.0851	+	-0.23836	11.07	C5H11N3O2	4-Guanidinobutanoate	L2	Amino Acid Metabolism	1.00	0.58	0.88	0.92
145.1102	+	-0.31882	9.85	C7H15NO2	4-Trimethylammoniobutanoate	L1	Amino Acid Metabolism	1.00	0.64	0.96	1.08
146.0215	-	-0.36396	10.29	C5H6O5	2-Oxoglutarate	L1	Carbohydrate Metabolism	1.00	0.42	0.68	0.88
146.0691	+	-0.5994	10.71	C5H10N2O3	Glutamine	L1	Amino Acid Metabolism	1.00	1.26	1.12	0.93
147.0532	-	-0.00964	7.44	C5H9NO4	O-Acetyl-L-serine	L2	Amino Acid Metabolism	1.00	0.47	0.84	1.16
148.0371	-	-0.22135	10.05	C5H8O5	Xylonolactone	L2	Carbohydrate Metabolism	1.00	0.64	0.77	0.97
150.0527	-	-0.65371	8.56	C5H10O5	Ribose	L2	Carbohydrate Metabolism	1.00	2.28	3.96	1.53
152.0684	-	-0.30823	9.87	C5H12O5	Xylitol	L2	Carbohydrate Metabolism	1.00	0.49	0.87	1.14
156.0535	+	-0.10662	8.26	C6H8N2O3	4-Imidazolone-5-propanoate	L2	Amino Acid Metabolism	1.00	0.43	0.65	0.98
158.0439	-	-0.48709	10.65	C4H6N4O3	Allantoin	L2	Nucleotide Metabolism	1.00	0.59	0.92	0.70
159.0531	-	-0.39978	5.3	C6H9NO4	N-Methyl-2-oxoglutaramate	L2	-	1.00	0.47	0.59	0.68
159.0896	+	0.369441	9.57	C7H13NO3	5-Acetamidopentanoate	L2	Amino Acid Metabolism	1.00	0.59	0.88	1.03
160.1211	+	-0.33452	16.28	C7H16N2O2	N6-Methyl-L-lysine	L2	Amino Acid Metabolism	1.00	0.59	0.77	0.78
161.0688	+	-0.20004	8.87	C6H11NO4	O-Acetyl-L-homoserine	L2	Amino Acid Metabolism	1.00	0.37	0.80	0.85
161.0688	-	-0.07702	7.41	C6H11NO4	O-Acetyl-L-homoserine	L2	Amino Acid Metabolism	1.00	0.41	0.73	0.90
161.1052	+	-0.24637	9.84	C7H15NO3	Carnitine	L1	Amino Acid Metabolism	1.00	0.63	0.94	1.01
163.0666	+	-0.40217	5.88	C6H13NO2S	homomethionine	L2	Amino Acid Metabolism	1.00	0.52	0.60	0.81
165.0426	-	0.257381	4.89	C8H7NO3	Formylanthranilate	L2	Amino Acid Metabolism	1.00	54.7	33.7	1.18
165.079	+	0.148487	8.49	C9H11NO2	Phenylalanine	L2	Amino Acid Metabolism	1.00	0.61	0.84	0.92
166.0477	-	-0.18446	9.59	C5H10O6	Arabinonate	L2	Carbohydrate Metabolism	1.00	0.46	1.05	0.84
167.0712	-	0.537182	9.17	C5H14NO3P	N-Trimethyl-2-aminoethylphosphonate	L2	Amino Acid Metabolism	1.00	0.59	0.84	0.82
169.0044	-	-0.34971	10.69	C3H7NO5S	Cysteate	L1	Amino Acid Metabolism	1.00	0.64	0.87	0.95
169.0504	+	-0.15033	9.61	C4H12NO4P	Phosphodimethylethanolamine	L2	Lipid Metabolism	1.00	0.43	0.83	0.88
172.0137	-	-0.1157	9.97	C3H9O6P	Glycerol 3-phosphate	L1	Lipid Metabolism	1.00	0.56	0.92	0.79
173.0688	+	-0.03571	5.3	C7H11NO4	N-Acetyl-L-glutamate 5-semialdehyde	L2	Amino Acid Metabolism	1.00	0.57	0.74	1.02
174.0164	-	-0.28792	11.2	C6H6O6	cis-Aconitate	L2	Carbohydrate Metabolism	1.00	0.63	0.70	1.08
174.1368	+	0.056377	15.07	C8H18N2O2	Ne,Ne dimethyllysine	L2	-	1.00	0.48	0.78	0.69
175.048	-	-0.17279	9.72	C6H9NO5	N-Acetyaspartate	L2	Amino Acid Metabolism	1.00	0.66	0.94	0.88
176.0432	-	-0.44438	10.8	C5H8N2O5	N-Carbamoyaspartate	L2	Nucleotide Metabolism	1.00	0.44	0.81	0.96
183.0661	+	0.490828	10.09	C5H14NO4P	Choline phosphate	L1	Lipid Metabolism	1.00	0.77	0.93	0.97
185.9928	-	-0.51588	11.02	C3H7O7P	3-Phospho-D-glycerate	L2	Carbohydrate Metabolism	1.00	0.39	0.59	1.05
189.0637	+	-0.11107	9.47	C7H11NO5	N-Acetyglutamate	L1	Amino Acid Metabolism	1.00	0.31	0.65	0.58
190.059	-	0.240851	10.58	C6H10N2O5	N-Carbamyglutamate	L2	Amino Acid Metabolism	1.00	0.39	0.49	0.92
202.143	+	0.172679	15.51	C8H18N4O2	NG,NG-Dimethyarginine	L2	-	1.00	0.52	0.74	0.81
204.0899	+	0.10895	9.56	C11H12N2O2	Tryptophan	L1	Amino Acid Metabolism	1.00	0.50	0.73	0.83
204.1474	+	0.13242	13.9	C9H20N2O3	3-Hydroxy-N6,N6,N6-trimethyl-L-lysine	L2	Amino Acid Metabolism	1.00	0.50	0.63	1.00
208.0848	+	-0.01681	9.05	C10H12N2O3	Kynurenine	L1	Amino Acid Metabolism	1.00	8.25	7.76	0.74
210.0527	-	-0.39274	5.21	C10H10O5	5-Hydroxyferulate	L2	Biosynthesis of Secondary Metabolites	1.00	0.69	0.91	0.69
211.0358	+	0.131998	9.98	C4H10N3O5P	Phosphocreatine	L2	Amino Acid Metabolism	1.00	0.30	0.69	0.90
218.1266	+	-0.14451	10.42	C9H18N2O4	N2-(D-1-Carboxyethyl)-L-lysine	L2	Amino Acid Metabolism	1.00	0.45	0.63	0.97
219.0742	-	-0.61579	9.4	C8H13NO6	O-Succinyhomoserine	L2	Amino Acid Metabolism	1.00	0.27	0.54	0.59

Mass	Polarity	Mass error (PPM)	RT	FORMULA	Putative metabolite	IDC	Pathway	Control	Poly PEI	Poly K	Poly KH
88.016	-	-0.00068	5.69	C3H4O3	3-Oxopropanoate	L2	Carbohydrate Metabolism	1.00	0.49	0.86	0.78
89.0477	-	-0.01326	10.06	C3H7NO2	beta-Alanine	L2	Nucleotide Metabolism	1.00	0.67	0.63	0.74
89.0477	+	0.20821	11.15	C3H7NO2	Alanine	L1	Amino Acid Metabolism	1.00	0.61	0.55	0.70
103.0997	+	-0.06347	17.54	C5H13NO	Choline	L2	Amino Acid Metabolism	1.00	2.88	1.77	1.81
105.0426	+	0.396434	11.52	C3H7NO3	Serine	L1	Amino Acid Metabolism	1.00	2.25	1.44	1.43
109.0198	+	0.074003	11.25	C2H7NO2S	Hypotaurine	L2	Amino Acid Metabolism	1.00	0.48	0.55	0.72
113.0477	-	0.283662	10.37	C5H7NO2	1-Pyrroline-5-carboxylate	L2	Amino Acid Metabolism	1.00	3.00	1.16	1.79
220.0848	117.0538	+	0.154061	44225	7.52	C11H12N2O3	C3H7NO3	3-Hydroxy-tryptophan	Glycolaldehyde	L2	Amino Acid Metabolism	1.00	1.62	1.00	1.02
222.0674	117.079	+	-0.24604	24017	11.33	C7H14N2O4S	C5H11NO2S	Cystathionine	Betaine	L1	Amino Acid Metabolism	1.00	1.23	0.85	0.97
227.0906	118.063	-	0.068625	32397	7.56	C9H13N3O4	C5H10O3	Deoxycytidine	5-Hydroxypentanoate	L2	Nucleotide Metabolism	Lipids: Fatty Acyls	1.00	0.79	0.68	0.77
231.147	119.058	+	-0.33596	05021	7.77	C10H21NO4	C4H9NO3	Butanoylcarnitine	Threonine	L2	Lipids: Fatty Acyls	Amino Acid Metabolism	1.00	1.67	1.00	1.13
236.0797	125.014	+	-0.12813	05618	8.38	C10H12N2O4	C2H7NO3S	Ethylkynurenine	Taurine	L1	Amino Acid Metabolism	Lipid Metabolism	1.00	0.39	0.49	0.63
240.1473	130.11	+	-0.25949	91578	8.67	C12H20N2O3	C6H14N2O	Spermine	N-Acetylputrescine	L2	Biosynthesis of Secondary Metabolites	Amino Acid Metabolism	1.00	0.53	0.72	0.75
246.0504	131.058	+	-0.35348	37712	9.07	C6H15O8P	C5H9NO3	Glycerophosphoserine	5-Amino-2-oxopentanoic acid	L2	-	L2	Amino Acid Metabolism	1.00	0.65	0.56	0.66
246.1329	131.058	+	0.169951	15717	10.44	C9H18N4O4	C5H9NO3	N2-(D-1-Carboxyethyl)-arginine	N-Acetyl-beta-alanine	L2	Amino Acid Metabolism	Amino Acid Metabolism	1.00	0.63	0.42	0.63
247.142	131.069	+	0.122203	3973	8.86	C11H21NO5	C4H9NO2	Hydroxybutyrylcarnitine	Creatinine	L2	-	L1	Amino Acid Metabolism	1.00	0.44	0.46	0.60
257.1028	131.094	+	0.024194	26989	10.26	C8H20NO6P	C6H13NO2	Glycero-3-Phosphocholine	Isoleucine	L1	Lipid Metabolism	Amino Acid Metabolism	1.00	1.95	1.17	1.24
260.0296	132.053	-	-0.4651	0.062907	10.46	C6H13O9P	C4H8N2O3	Glucose 6-phosphate	Asparagine	L1	Carbohydrate Metabolism	Amino Acid Metabolism	1.00	1.06	0.77	0.93
275.1733	134.021	-	0.207346	085993	8.25	C14H25NO5	C4H6O5	N-(3S-hydroxyhexanoyl)-L-serine	Malate	L2	Lipids: Fatty Acyls	Carbohydrate Metabolism	1.00	0.63	0.53	0.79
301.2979	145.085	+	-0.51462	46629	7.43	C14H39NO2	C5H11N3O2	Spermine	4-Guanidinobutanoate	L2	Lipids: Sphingolipids	Amino Acids	1.00	0.73	0.72	0.83
307.0838	145.11	+	-0.01621	34575	9.82	C12H17N3O6S	C7H15NO2	Cystathione	4-Trimethylammoniobutanoate	L1	Amino Acid Metabolism	Amino Acid Metabolism	1.00	0.90	0.71	0.76
369.2877	146.021	-	-0.58459	23147	5.2	C20H39NO4	C5H6O5	5-Tetradecenoylcarnitine	2-Oxoglutarate	L2	-	L1	Carbohydrate Metabolism	1.00	0.43	0.45	0.61
466.3117	147.053	+	0.090681	69791	4.04	C27H46O4S	C5H9NO4	Cholesterolsulfate	Glutamate	L2	Lipids: Steroids	Amino Acid Metabolism	1.00	0.60	0.39	0.65
612.152	149.051	-	0.050963	039816	10.86	C20H32N6O12S2	C5H11NO2S	Glutathione disulfide	Methionine	L1	Amino Acid Metabolism	Amino Acid Metabolism	1.00	1.77	1.26	1.34
663.1091	151.049	+	-0.00434	27461	9.62	C21H27N7O14P2	C5H5N5	NAD+	Guanine	L2	Energy Metabolism	Nucleoside	0.00	11.63	0.00	0.00
703.515	161.068	+	-0.26307	42558	4.64	C38H74NO8P	C6H11NO2	PC(32:1)	O-Acetyl-L-homoserine	L2	Lipids: Glycerophospholipids	Amino Acid Metabolism	1.00	0.50	0.44	0.70
704.5844	161.105	+	1.648575	11743	4.74	C32H81N2O6P	C7H15NO3	SP(d16:0)	Carnitine	L2	Lipids: Sphingolipids	Amino Acids	1.00	0.68	0.66	0.73
719.5836	165.079	+	0.013402	015858	4.84	C40H82NO7P	C9H11NO2	PC(32:2)	Phenylalanine	L2	Lipids: Glycerophospholipids	Amino Acid Metabolism	1.00	2.20	1.33	1.36
731.5462	169.050	+	-0.38157	15903	4.63	C43H78NO8P	C4H12NO4P	PC(42:1)	Phosphodimethylethanolamine	L2	Lipids: Glycerophospholipids	Lipid Metabolism	1.00	0.73	0.76	0.94
748.5254	172.013	-	0.001225	08564	4.03	C40H77O10P	C3H9O6P	PG(34:1)	Glycerol 3-phosphate	L2	Lipids: Glycerophospholipids	Lipid Metabolism	1.00	1.57	1.55	1.22
774.5412	174.016	-	0.145202	49691	4.02	C42H79O10P	C6H6O6	PG(36:2)	cis-Aconitate	L2	Lipids: Glycerophospholipids	Carbohydrate Metabolism	1.00	0.67	0.52	0.83
174.1004	+	0.004804	10.28	C7H14N2O3	N5-Ethyl-L-glutamine	L2	-	1.00	1.54	1.07	0.96
175.0481	+	0.069856	10.04	C6H9NO5	N-Acetyl-L-aspartate	L2	Amino Acid Metabolism	1.00	0.66	0.64	0.78
175.0957	+	0.019941	11.54	C6H13N3O3	Citrulline	L1	Amino Acid Metabolism	1.00	1.50	0.91	1.12
177.046	+	-0.06226	5.58	C6H11NO3S	N-Formymethionine	L2	Amino Acid Metabolism	1.00	0.88	0.65	0.70
178.0412	+	-0.05819	10.09	C5H10N2O3S	Cys-Gly	L2	Amino Acid Metabolism	1.00	0.57	0.62	0.83
179.0582	-	-0.05216	7.42	C9H9NO3	N-Acetylanthranilate	L2	-	1.00	0.69	0.59	0.72
181.0739	-	0.112349	10.4	C9H11NO3	Tyrosine	L1	Amino Acid Metabolism	1.00	1.72	0.94	1.32
182.0791	-	0.333763	10.65	C6H14O6	Sorbitol	L2	Carbohydrate Metabolism	1.00	1.57	0.77	1.16
183.0661	+	0.429736	10.42	C5H14NO4P	Choline phosphate	L1	Lipid Metabolism	1.00	0.64	0.85	0.87
188.1525	+	0.2506	15.86	C9H20N2O2	N6,N6,N6-Trimethyl-L-lysine	L2	Amino Acid Metabolism	1.00	1.80	0.97	1.23
189.0637	+	-0.05389	9.77	C7H11NO5	N-Acetyl-L-glutamate	L1	Amino Acid Metabolism	1.00	0.80	0.60	0.70
191.0616	+	0.116175	5.32	C7H13NO3S	N-Acetylmethionine	L2	-	1.00	0.72	0.44	0.65
195.0897	+	0.709481	5.65	C10H13NO3	Tyrosine methyl ester	L2	Amino Acid Metabolism	1.00	0.75	0.66	0.86
203.1158	+	0.26164	9.08	C9H17NO4	O-Acetylcarnitine	L1	Amino Acid Metabolism	1.00	0.63	0.48	0.64
204.0899	+	0.051584	9.88	C11H12N2O2	Tryptophan	L1	Amino Acid Metabolism	1.00	2.03	1.25	1.27
231.147	+	-0.114	8.05	C11H21NO4	O-Butanoylcarnitine	L2	Lipids: Fatty Acyls	1.00	0.56	0.58	0.70
243.0854	+	-0.34119	9.91	C9H13N3O5	Glutamyl-beta-cyanoalanine	L2	Amino Acid Metabolism	1.00	3.28	0.82	1.08
244.0882	+	-0.01307	5.65	C10H16N2O3S	Biotin	L2	Metabolism of Cofactors and	1.00	1.52	0.75	0.98

							Vitamins				
244.1059	+	0.062446	10.1	C10H16N2O5	Glu-Pro	L2	Peptide(di-)	1.00	0.56	0.42	0.81
245.1626	+	-0.26101	7.71	C12H23NO4	N-(octanoyl)-L-homoserine	L2	-	1.00	0.77	0.75	0.85
245.1626	+	-0.25621	6.35	C12H23NO4	2-Methylbutyroylcarnitine	L2	-	1.00	0.69	0.63	0.70
246.0504	+	-0.17565	9.37	C6H15O8P	Glycerophosphoglycerol	L2	-	1.00	0.31	0.36	0.54
246.1329	+	0.467084	10.81	C9H18N4O4	N2-(D-1-Carboxyethyl)-L-arginine	L2	Amino Acid Metabolism	1.00	0.87	0.54	0.71
257.1029	+	0.15967	10.62	C8H20NO6P	sn-glycero-3-Phosphocholine	L1	Lipid Metabolism	1.00	1.41	1.41	1.19
267.0967	+	-0.19584	8.45	C10H13N5O4	Adenosine	L1	Nucleotide Metabolism	1.00	1.66	1.40	1.15
281.1124	+	-0.13102	12.23	C11H15N5O4	1-Methyladenosine	L2	-	1.00	1.93	0.88	0.96
299.2824	+	-0.13397	7.33	C18H37NO2	3-dehydrosphinganine	L2	Lipids: Sphingolipids	1.00	1.17	0.69	0.55
301.298	+	-0.2723	7.44	C18H39NO2	Sphinganine	L2	Lipids: Sphingolipids	1.00	1.24	0.64	0.67
307.0838	+	-0.15933	10.1	C10H17N3O6S	Glutathione	L1	Amino Acid Metabolism	1.00	0.55	0.64	0.81
347.063	+	-0.20359	9.66	C10H14N5O7P	AMP	L1	Nucleotide Metabolism	1.00	0.79	0.58	0.82
371.3036	+	0.200741	5.44	C21H41NO4	Tetradecanoylcarnitine	L2	-	1.00	2.12	2.20	1.01
397.3192	+	-0.05176	5.34	C23H43NO4	Hexadec-2-enoylcarnitine	L2	-	1.00	2.48	1.87	1.02
399.3349	+	0.08556	5.3	C23H45NO4	O-Palmitoyl-R-carnitine	L2	Lipids: Fatty Acyls	1.00	3.25	3.05	1.67
425.3505	+	-0.00153	5.23	C25H47NO4	Elaidiccarnitine	L2	-	1.00	3.99	3.41	1.62
427.3662	+	0.097364	5.18	C25H49NO4	Stearoylcarnitine	L2	-	1.00	3.83	5.58	2.07
466.3115	-	-0.29258	4.09	C27H46O4S	Cholesterolsulfate	L2	Lipids: Sterol lipids	1.00	0.87	0.61	0.64
467.3012	+	-0.05581	5.48	C22H46NO7P	PC (14:0)	L2	Lipids: Glycerophospholipids	1.00	1.43	0.68	0.81
481.3534	+	0.347655	5.38	C24H52NO6P	PC (16:2)	L2	Lipids: Glycerophospholipids	1.00	0.76	0.67	0.68
523.2909	+	-0.18379	4.42	C24H46NO9P	PS (18:1)	L2	Lipids: Glycerophospholipids	1.00	1.72	0.73	0.78
525.3067	+	-0.03636	4.4	C24H48NO9P	PS (18:0)	L2	Lipids: Glycerophospholipids	1.00	1.71	0.71	0.73
537.5121	+	0.029172	4.58	C34H67NO3	SP (16:0)	L2	Lipids: Sphingolipids	1.00	1.17	0.81	0.74
598.3119	-	0.09071	4.44	C27H51O12P	PI (18:1)	L2	Lipids: Glycerophospholipids	1.00	1.57	0.69	0.79
600.3277	-	0.454354	4.42	C27H53O12P	PI (18:0)	L2	Lipids: Glycerophospholipids	1.00	1.34	0.80	0.78
674.4886	-	-0.03932	4.11	C37H71O8P	PA(34:1)	L2	Lipids: Glycerophospholipids	1.00	0.64	0.38	0.49
689.4995	+	-0.0279	4.58	C37H72NO8P	PE(32:1)	L2	Lipids: Glycerophospholipids	1.00	0.73	0.58	0.63
705.5306	+	-0.33223	4.8	C38H76NO8P	PC(30:0)	L2	Lipids: Glycerophospholipids	1.00	0.82	0.72	0.85
717.5309	+	0.061038	4.57	C39H76NO8P	PE(34:1)	L2	Lipids: Glycerophospholipids	1.00	0.74	0.61	0.66
719.5833	+	0.539418	4.78	C40H82NO7P	PC (32:2)	L2	Lipids: Glycerophospholipids	1.00	0.80	0.63	0.71
731.5464	+	-0.10583	4.78	C40H78NO8P	PC(32:1)	L2	Lipids: Glycerophospholipids	1.00	0.81	0.73	0.81
733.4892	+	-0.20987	4.16	C38H72NO10P	PS(32:1)	L2	Lipids: Glycerophospholipids	1.00	0.67	0.47	0.66
748.5256	-	0.220898	4.06	C40H77O10P	PG(34:1)	L2	Lipids: Glycerophospholipids	1.00	0.69	0.48	0.68
761.5206	+	-0.06133	4.17	C40H76NO10P	PS(34:1)	L2	Lipids: Glycerophospholipids	1.00	0.76	0.50	0.58
819.6153	+	1.358911	4.7	C48H86NO7P	PC(40:5)	L2	Lipids: Glycerophospholipids	1.00	1.46	1.03	1.05
820.5258	-	0.496579	4.02	C46H77O10P	PG(40:7)	L2	Lipids: Glycerophospholipids	1.00	1.86	1.48	1.41
879.5841	+	0.4514	4.17	C45H86NO13P	PI (36:0)	L2	Lipids: Glycerophospholipids	1.00	0.86	0.55	0.70