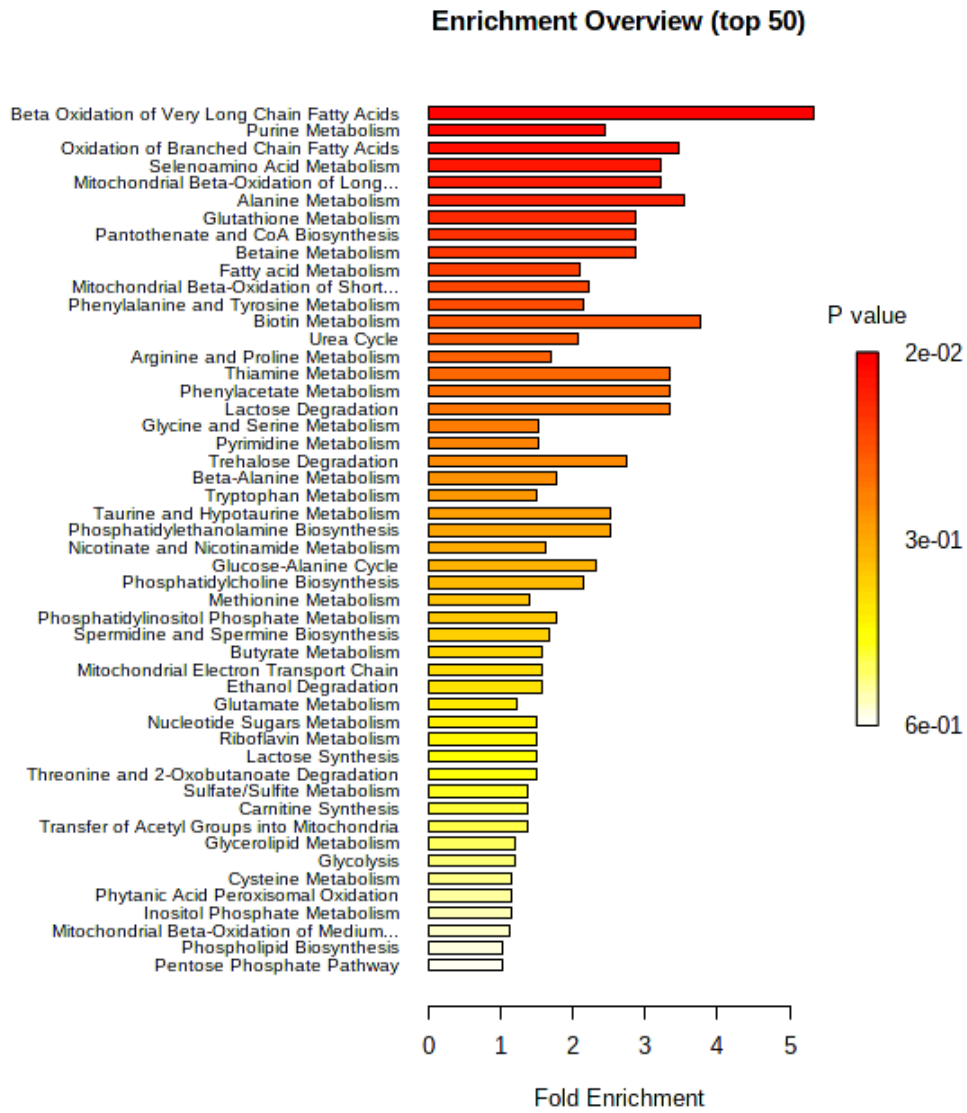


Supplementary materials

(1) 31 tumor abbreviations

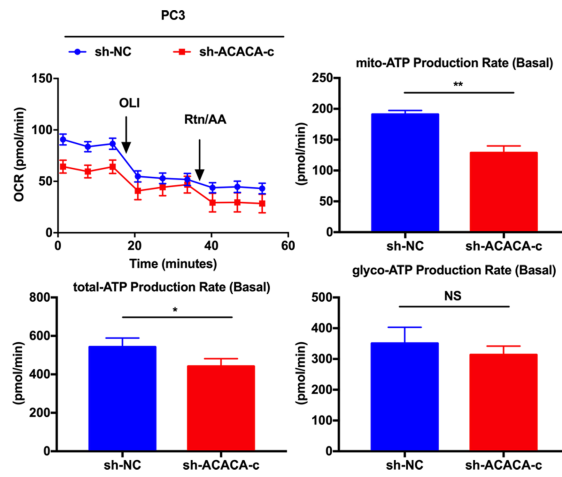
1. ACC Adrenocortical carcinoma
2. BLCA Bladder Urothelial Carcinoma
3. BRCA Breast invasive carcinoma
4. CESC Cervical squamous cell carcinoma and endocervical adenocarcinoma
5. CHOL Cholangiocarcinoma
6. COAD Colon adenocarcinoma
7. DLBC Lymphoid Neoplasm Diffuse Large B-cell Lymphoma
8. ESCA Esophageal carcinoma
9. GBM Glioblastoma multiforme
10. HNSC Head and Neck squamous cell carcinoma
11. KICH Kidney Chromophobe
12. KIRC Kidney renal clear cell carcinoma
13. KIRP Kidney renal papillary cell carcinoma
14. LAML Acute Myeloid Leukemia
15. LGG Brain Lower Grade Glioma
16. LIHC Liver hepatocellular carcinoma
17. LUAD Lung adenocarcinoma
18. LUSC Lung squamous cell carcinoma
19. OV Ovarian serous cystadenocarcinoma
20. PAAD Pancreatic adenocarcinoma
21. PCPG Pheochromocytoma and Paraganglioma
22. PRAD Prostate adenocarcinoma
23. READ Rectum adenocarcinoma
24. SARC Sarcoma
25. SKCM Skin Cutaneous Melanoma
26. STAD Stomach adenocarcinoma
27. TGCT Testicular Germ Cell Tumors
28. THCA Thyroid carcinoma
29. THYM Thymoma
30. UCEC Uterine Corpus Endometrial Carcinoma
31. UCS Uterine Carcinosarcoma

(2) Supplementary Figure 1



Summary Plot for metabolites analysis in DU145-SH and PC3-SH cell lines. Thirty-nine metabolites compounds which were both have changed including up-regulated and down-regulated in DU145-SH and PC3-SH cell lines were input for the Metabolite Set Enrichment Analysis.

(3) Supplementary Figure 2



OCR in the PC3 cells was analyzed by the seahorse XF Real-Time-ATP-Rate kit. ATP production was analyzed in the bar graph.

(4) Supplementary Table 1

Position	No.	Age	Sex	Organ/Anator	Pathology diagnosis	n	m	group	Intensity	area	SCORE	TNM	Grade	Stage	Stage	Type	Tissue ID
A1	1	71	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	2	II		Malignant	Mpr00049
A2	2	66	M	Prostate	Adenocarcinoma	1	1	1	4	2	8	T3N1M1	1	IV	4	Malignant	Mpr00049
A3	3	60	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	3	III	3	Malignant	Mpr00010
A4	4	76	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	1	II	2	Malignant	Mpr00277
A5	5	73	M	Prostate	Adenocarcinoma	0	0	0	4	2	8	T2NM0	2	IIA	2	Malignant	Mpr10014
A6	6	26	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	-	II	2	Malignant	Mpr00006
A7	7	72	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	1	I	1	Malignant	Mpr04048
A8	8	76	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	2	II	2	Malignant	Mpr00106
A9	9	71	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	1	II	2	Malignant	Mpr07077
A10	10	71	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	2	II	2	Malignant	Mpr00033
B1	11	71	M	Prostate	Adenocarcinoma	0	0	0	0	0	0	T1NM0	2	I	1	Malignant	Mpr00063
B2	12	66	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	2	II	2	Malignant	Mpr00031
B3	13	75	M	Prostate	Adenocarcinoma	1	1	1	4	1	4	T3N1M1	1	IV	4	Malignant	Mpr00042
B4	14	60	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	2	II	2	Malignant	Mpr02011
B5	15	67	M	Prostate	Adenocarcinoma	0	1	0	4	2	8	T2NM1	2	IV	4	Malignant	Mpr00020
B6	16	60	M	Prostate	Adenocarcinoma	1	0	1	4	1	4	T3NM0	2	IV	4	Malignant	Mpr00011
B7	17	71	M	Prostate	Adenocarcinoma	0	0	0	0	0	0	T2NM0	2	IIA	2	Malignant	Mpr10007
B8	18	75	M	Prostate	Adenocarcinoma	1	1	1	4	3	12	T4N1M1	2	IV	4	Malignant	Mpr03007
B9	19	71	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	-	I	1	Malignant	Mpr10042
B10	20	66	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	2	IIA	2	Malignant	Mpr10012
C1	21	64	M	Prostate	Adenocarcinoma	0	0	0	4	2	8	T2NM1	2	IV	4	Malignant	Mpr00059
C2	22	71	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	2	II	2	Malignant	Mpr00123
C3	23	64	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr10054
C4	24	73	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr00053
C5	25	56	M	Prostate	Adenocarcinoma	0	0	0	0	0	0	T2NM0	2	II	2	Malignant	Mpr04026
C7	27	70	M	Prostate	Adenocarcinoma	1	1	0	4	1	4	T3N1M1	2	IV	4	Malignant	Mpr00345
C8	28	82	M	Prostate	Adenocarcinoma	1	0	1	4	3	12	T3N1M1	3	IV	4	Malignant	Mpr10019
C9	29	64	M	Prostate	Adenocarcinoma	0	0	0	0	0	0	T2NM0	3	IB	1	Malignant	Mpr07166
C10	30	61	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	2-3	II	2	Malignant	Mpr07019
D1	31	69	M	Prostate	Adenocarcinoma	0	0	1	4	3	12	T2NM0	2-3	III	3	Malignant	Mpr00166
D2	32	73	M	Prostate	Adenocarcinoma	1	1	1	4	2	8	T3N1M1	3	IV	4	Malignant	Mpr00374
D3	33	60	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr00024
D4	34	74	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	-	IIA	2	Malignant	Mpr10029
D5	35	20	M	Prostate	Adenocarcinoma	0	0	1	4	2	8	T3NM0	3	III	3	Malignant	Mpr06071
D6	36	70	M	Prostate	Adenocarcinoma	0	0	0	0	0	0	T2NM0	3	-	-	Malignant	Mpr06100
D7	37	73	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr00122
D8	38	73	M	Prostate	Adenocarcinoma	1	0	1	4	1	4	T2NM0	3	IV	4	Malignant	Mpr00433
D9	39	72	M	Prostate	Adenocarcinoma	0	0	1	4	1	4	T2NM0	3	III	3	Malignant	Mpr00093
D10	40	64	M	Prostate	Adenocarcinoma	0	0	1	4	2	8	T2NM0	-	2-3	3	Malignant	Mpr00003
E1	41	74	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr04041
E2	42	62	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr00147
E3	43	68	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	3	II	2	Malignant	Mpr10039
E4	44	66	M	Prostate	Adenocarcinoma	0	0	1	4	1	4	T3NM0	3	III	3	Malignant	Mpr06047
E5	45	67	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr10032
E6	46	82	M	Prostate	Adenocarcinoma	1	0	1	3	3	9	T3NM0	3	IV	4	Malignant	Mpr10019
E7	47	64	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr10033
E8	48	76	M	Prostate	Adenocarcinoma	0	0	1	4	0	0	T2NM0	3	III	3	Malignant	Mpr02087
E9	49	75	M	Prostate	Adenocarcinoma	1	1	1	4	2	8	T4N1M1	3	IV	4	Malignant	Mpr00029
E10	50	75	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	2	IIA	2	Malignant	Mpr04053
F1	51	62	M	Prostate	Adenocarcinoma	0	0	1	4	1	4	T2NM0	3	III	3	Malignant	Mpr04059
F2	52	70	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	-	II	2	Malignant	Mpr02038
F3	53	70	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	IB	2	Malignant	Mpr00166
F4	54	64	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	3	II	2	Malignant	Mpr04071
F5	55	62	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	3	II	2	Malignant	Mpr040163
F6	56	77	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	3	II	2	Malignant	Mpr04016
F7	57	60	M	Prostate	Adenocarcinoma	1	0	1	4	2	8	T3NM0	3	IV	4	Malignant	Mpr03026
F8	58	56	M	Prostate	Adenocarcinoma	0	0	1	0	0	0	T2NM0	3	III	3	Malignant	Mpr10006
F10	60	67	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr040165
G1	61	67	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr00042
G2	62	81	M	Prostate	Adenocarcinoma	0	0	1	4	1	4	T2NM0	3	III	3	Malignant	Mpr020317
G3	63	73	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	IIA	2	Malignant	Mpr10034
G4	64	69	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	3	II	2	Malignant	Mpr03032
G5	65	62	M	Prostate	Adenocarcinoma	0	0	0	4	0	0	T2NM0	3	II	2	Malignant	Mpr00083
G6	66	64	M	Prostate	Adenocarcinoma	0	0	0	0	0	0	T2NM0	3	II	2	Malignant	Mpr06077
G7	67	82	M	Prostate	Adenocarcinoma	0	0	1	4	1	4	T2NM0	3	III	3	Malignant	Mpr04075
G8	68	80	M	Prostate	Adenocarcinoma	1	1	1	4	2	8	T4N1M1	3	IV	4	Malignant	Mpr00382
G9	69	63	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr03047
G10	70	73	M	Prostate	Adenocarcinoma	0	0	1	4	2	8	T4NM0	3	IV	4	Malignant	Mpr00166
H1	71	60	M	Prostate	Adenocarcinoma	0	0	0	4	1	4	T2NM0	3	II	2	Malignant	Mpr020323
H4	74	27	M	Prostate	Adjacent normal prostate	NAT	NAT	NAT			0	-	-	-	-	NAT	Mpr04012
H5	75	35	M	Prostate	Adjacent normal prostate	NAT	NAT	NAT			0	-	-	-	-	NAT	Mpr07058
H6	76	21	M	Prostate	Adjacent normal prostate	NAT	NAT	NAT			0	-	-	-	-	NAT	Mpr04014
H7	77	45	M	Prostate	Prostate tissue	Normal	Normal	Normal			0	-	-	-	-	Normal	Mpr07030
H8	78	37	M	Prostate	Prostate tissue	Normal	Normal	Normal			0	-	-	-	-	Normal	Mpr07028
H9	79	33	M	Prostate	Prostate tissue	Normal	Normal	Normal			0	-	-	-	-	Normal	Mpr07028
H10	80	43	M	Prostate	Prostate tissue	Normal	Normal	Normal			0	-	-	-	-	Normal	Mpr09019

(5) Supplementary Table 2

DU145- ID	MS2 name	MS2 score	type	mz	rt	MEAN NC	MEAN SH	VIP	P-VALUE	Q-VALUE	FOLD CHANGE	LOG_FOLDCHANGE
5241	1-Myristoyl-sn-glycero-3-phosphocholine	0.9491	MS2 forward	468.300783	181.641	0.08868236	0.113517602	1.54210749	1.14089E-06	4.67872E-06	1.645840347	0.71891205
296	Creatinine	0.9972	MS2 forward	114.066953	160.505	0.025430593	0.045546402	1.432148478	4.11946E-05	6.46202E-05	1.723245581	0.785128316
516	Methyl acetacetate	0.9958	MS2 reverse	134.0817286	329.328	0.01158646	0.018453727	1.45324927	1.92524E-05	3.57749E-05	1.592897637	0.671472407
880	L-Carnitine	0.9481	MS2 forward	162.1135707	357.413	0.252475197	0.36006097	1.215944268	0.004808181	0.003110716	1.428124132	0.512095661
1946	Lys-Val	0.9925	MS2 reverse	246.1821592	525.181	0.016809016	0.024942622	1.320800658	0.000681673	0.000634276	1.483883473	0.56837804
315	L-Proline	0.9959	MS2 forward	116.0716176	294.863	0.351689836	0.718613607	1.532948235	3.32498E-06	1.01032E-05	2.043032052	1.030711838
5906	1-O-Octadecyl-sn-glycero-3-phosphocholine	0.9851	MS2 forward	510.3009364	177.954	0.040523963	0.029504673	1.046237882	0.021178904	0.010144726	0.728079124	-0.45783285
428	Taurine	0.9964	MS2 forward	128.0225643	277.711	0.18688882	0.413370794	1.51582918	2.32426E-06	7.75886E-06	2.216201812	1.14608262
287	Uracil	0.9464	MS2 forward	113.035166	89.4825	0.016498488	0.021035203	1.090009936	0.028845176	0.012363597	1.27497647	0.350471954
3002	Tyr-Met	0.9703	MS2 forward	312.1118534	163.65	0.030122583	0.022748909	1.453447627	0.000680762	0.000633655	0.755144709	-0.405174558
5423	1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	0.6549	MS2 forward	482.3274229	179.784	0.101271127	0.153188719	1.482783748	8.2559E-06	1.98119E-05	1.512659364	0.597607143
2035	Deoxyadenosine	0.9967	MS2 forward	252.1103974	137.571	0.047359591	0.080148641	1.414449248	5.79021E-05	8.43451E-05	1.679012234	0.747612743
845	Cyclohexamine	0.736	MS2 forward	160.1340962	366.77	0.13458957	0.248882508	1.476320113	1.68106E-05	3.26009E-05	1.849483487	0.88712242
552	Hypoxanthine	0.9851	MS2 forward	137.0468347	161.13	0.856308413	0.305811013	1.573326599	2.98852E-08	2.5103E-07	0.357127185	-1.485450135
1532	N-Acetylsarotonin	0.9363	MS2 forward	219.1138801	42.048	0.052150172	0.080338575	1.144200633	0.00698838	0.004055303	1.545232678	0.62342857
5053	1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	0.9854	MS2 forward	454.2934799	183.947	0.04384008	0.059804718	1.422475559	7.24642E-05	0.000101115	1.389566398	0.471932836
1543	Parathionate	0.8664	MS2 forward	220.1192291	253.75	0.010150136	0.007396832	1.325302862	0.00093021	0.000820568	0.728082122	-0.461795365
669	(3-Carboxypropyl)trimethylammonium cation	0.9407	MS2 forward	146.1187644	358.746	0.247834251	0.473767062	1.502070857	1.26983E-05	2.89911E-05	1.911628683	0.93482232
229	Picolinic acid	0.6392	MS2 forward	106.0293815	61.8615	0.05222723	0.004689963	1.581571957	3.4240E-05	5.6471E-05	0.093315181	-3.421744378
717	Triethanolamine	0.9353	MS2 forward	150.1131989	281.019	0.019621289	0.013134871	1.589134163	1.02155E-06	4.31364E-06	0.669419409	-0.570917715
2211	Creatine	0.9929	MS2 reverse	263.1471411	329.269	0.00327034	0.008574147	1.401040407	4.71717E-05	7.10241E-05	2.621790668	1.390552501
1378	Acetylcarbitol	0.9997	MS2 forward	204.1244643	288.22	0.804654796	2.91169269	1.517057572	0.000190931	0.00021074	3.618561283	1.855416205
365	Tyramine	0.6795	MS2 forward	120.0813508	245.086	0.041628443	0.09250713	1.381416588	0.000343347	0.000350132	1.447340874	0.53408279
9876	N-Docosanoyl-4-sphingyl-1-O-phosphorylcholine	0.9672	MS2 forward	787.6679738	157.806	0.054259661	0.004626597	1.427348229	0.005067079	0.003210103	0.082627871	-3.55185396
385	Nicotinamide	0.9903	MS2 forward	123.056316	61.942	21.57807896	2.535547177	1.639863365	1.64988E-05	3.22102E-05	0.11750382	-3.082527276
5769	Adenosine 5' triphosphate (ATP)	0.9975	MS2 forward	508.0023413	490.582	0.853789825	0.838646732	1.288705943	0.002851534	0.002840259	0.718473302	-0.47681499
2302	Adenosine	1	MS2 forward	268.1062302	162.349	14.28456311	10.63037793	1.179482052	0.013617399	0.007149147	-0.424242987	
537	Adenine	0.9993	MS2 forward	136.0634393	151.338	5.778614743	1.05121514	1.568461243	0.00015769	0.000183008	0.181878956	-2.458955328
2315	Inosine	0.9998	MS2 forward	269.0892839	206.488	0.115777735	0.02862546	1.570286657	3.20036E-05	5.47955E-05	0.258188071	-1.95300016
1944	2-Methylbutylcarbitol	0.9947	MS2 forward	246.1721331	223.692	0.368477747	2.627169661	1.586641894	5.28797E-06	1.39551E-05	7.129759277	2.833860136
2412	1,2,3-Benzene-triol	0.8925	MS2 reverse	275.0539118	384.625	0.007756626	0.002956457	1.528027054	0.000734162	0.000674848	0.382312798	-1.38711746
1915	Uridine	0.9913	MS2 forward	245.077937	154.749	0.010133541	0.006137275	1.318885233	0.000752486	0.00068878	0.605639723	-0.723468263
746	2-Hydroxyadenine	0.868	MS2 forward	152.0574864	214.36	0.14460689	0.054253653	1.530458694	9.18774E-05	0.000121992	0.375178955	-1.414360958
129	L-Alanine	0.9959	MS2 forward	90.05579365	329.328	0.147753573	0.237192951	1.446721546	1.78035E-05	3.3811E-05	1.60323022	0.652868118
4711	Stearoylcarbitol	0.9978	MS2 forward	428.3733889	152.81	0.236475622	1.404815078	1.584236938	4.0803E-11	9.63406E-10	4.30327002	2.10543571
4338	L-Palmitoylcarbitol	0.9624	MS2 forward	400.3440676	156.009	0.76783325	4.03343981	1.588242307	3.68793E-12	2.49803E-10	5.254731115	2.393616943
5706	1-Eicosatrenoyl-sn-glycero-3-phosphoethanolamine	0.954	MS2 reverse	504.306641	179.46	0.033961813	0.039137701	1.305526992	0.001233583	0.001030065	1.152403183	0.204645551
2914	Cytidine 2, 3'-cyclic phosphate	0.9985	MS2 forward	306.0496902	301.109	0.010396838	0.007483363	1.165704631	0.01287244	0.006882329	0.719772585	-0.474386139
916	L-Phenylalanine	0.9599	MS2 forward	166.0668713	245.32	0.025514705	0.035401957	1.308894926	0.0107916	0.000927996	1.387511883	0.472500127

(6) Supplementary Table 3

PC3-ID	MS2 name	MS2 score	type	mz	rt	MEAN NC	MEAN SH	VIP	P-VALUE	Q-VALUE	FOLD CHANGE	LOG_FOLDCHANGE
5494	1-Myristoyl-sn-glycero-3-phosphocholine	0.9325	MS2 forward	468.308391	181.812	0.051046966	0.066798835	1.522114272	0.000397188	0.001443145	0.764189763	-0.387997163
299	Creatinine	0.9987	MS2 forward	114.0648888	160.394	0.056676825	0.056915466	1.205107778	0.01329476	0.021898852	0.768815395	-0.37929087
531	Methyl acetacetate	0.9956	MS2 reverse	134.0794154	49.599	0.017904285	0.028126949	1.094131948	0.028619252	0.036683579	0.685280336	-0.545233804
895	L-Carnitine	0.9813	MS2 forward	162.1114882	336.82	0.378115916	0.622869035	1.521112892	0.000143403	0.000896687	0.602879295	-0.730059911
1959	Lys-Val	0.9925	MS2 reverse	246.1901166	528.129	0.030403031	0.037540245	1.063641598	0.036574589	0.045330083	0.908978316	-0.304222935
320	L-Proline	0.9999	MS2 forward	116.0298894	294.923	0.260733768	0.458145487	1.594047938	7.71951E-05	0.00046021	0.571602234	-0.908916539
6145	1-O-Octadecyl-sn-glycero-3-phosphocholine	0.8576	MS2 forward	510.390612	178.4305	0.048494489	0.015407819	1.496443835	0.001985556	0.00484653	3.147394739	1.654158129
437	Taurine	0.9972	MS2 forward	128.0202209	278.174	0.055192521	0.076162896	1.32047943	0.003554675	0.007403007	0.724030089	-0.46580488
288	Uracil	0.9624	MS2 forward	113.0332083	155.063	0.180321127	0.274338426	1.439412016	0.002177922	0.000673411	0.65729446	-0.60538627
3064	Tyr-Met	0.9712	MS2 forward	312.1100801	162.295	0.061431098	0.080911317	1.369783457	0.02846882	0.006000068	0.792029871	-0.397372338
9687	1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	0.6575	MS2 forward	482.3257604	179.05	0.034055956	0.105035231	1.736079849	1.99857E-08	1.79263E-06	0.324233647	-1.624894284
2050	Deoxyadenosine	0.9995	MS2 forward	252.1082142	137.501	0.062826506	0.211394428	1.594028763	1.82117E-07	5.2892E-06	0.287200641	-1.750490866
879	Cyclohexylamine	0.7289	MS2 forward	160.131509	366.971	0.026902875	0.032241402	1.052495842	0.041941759	0.050180614	0.834413922	-0.261164866
568	Hypoxanthine	0.9909	MS2 forward	137.0446234	160.392	0.342590181	1.156474829	1.737664854	1.91795E-08	1.7589E-06	0.296236609	-1.755178157
1573	N-Acetylsarcosine	0.9481	MS2 forward	219.1118279	40.851	0.053406017	0.080104907	1.442729285	0.001770455	0.004477754	0.686710394	-0.584888333
5287	1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine	0.9926	MS2 forward	454.2925385	183.823	0.041901617	0.053356606	1.570140097	0.000240187	0.000922276	0.785312653	-0.348900563
1988	Pantoic acid	0.9434	MS2 forward	220.1168798	254.138	0.034304455	0.055018902	1.456015161	0.000642474	0.002837463	0.623507623	-0.601020995
690	(3-Carboxypropyl)trimethylammonium cation	0.8707	MS2 forward	146.1162108	359.911	0.045306047	0.052914246	1.089117653	0.02826988	0.038232243	0.857637616	-0.221223515
410	Picolinic acid	0.9972	MS2 reverse	124.0376372	201.562	0.002220327	0.00498091	1.607195178	5.90548E-05	0.000371975	0.6671815	-1.13054464
765	Triethanolamine	0.8838	MS2 forward	150.1108306	283.742	0.00369664	0.019071315	1.004523146	0.042112434	0.003333342	0.803739618	-0.267531911
2875	Creatine	0.9948	MS2 reverse	301.1019067	329.773	0.002748839	0.003831197	1.152142837	0.03110452	0.040798099	0.716769286	-0.480419277
1407	Acetylcarlamine	0.9987	MS2 forward	204.1226211	289.263	2.801273519	3.492838604	1.231099978	0.02641813	0.036494909	0.74474541	-0.425180768
369	Tyramine	0.9125	MS2 forward	120.0794312	239.513	0.046279365	0.080574026	1.65401774	1.11222E-05	0.00107925	0.574370758	-0.799945792
11867	N-Docosanoyl-4-sphingeryl-1-O-phosphorylcholine	0.9979	MS2 reverse	801.5572369	113.377	0.016229189	0.021990181	1.367313807	0.001557422	0.004052789	0.7380198	-0.438268572
395	Nicotinamide	0.999	MS2 forward	123.0540603	145.178	0.266795219	0.473401217	1.533981268	0.000537019	0.001821401	0.563486663	-0.82754151
6099	Adenosine 5'-triphosphate (ATP)	0.9942	MS2 forward	508.0028273	459.231	0.093786737	0.046590666	1.543146052	0.000515779	0.00176722	2.012991433	1.009342968
7276	Adenosine	1	MS2 reverse	573.1449532	347.978	0.004798004	0.008632445	1.602802496	1.13819E-05	0.000109495	0.585879974	-0.847154687
549	Adenosine	0.9997	MS2 forward	136.0614794	151.182	3.544003932	8.871405509	1.711573093	6.4089E-08	3.39097E-06	0.399486184	-1.323762486
2356	Inosine	0.9999	MS2 forward	289.0874033	205.927	0.048893303	0.196437822	1.728958139	1.07533E-07	4.37208E-06	0.2493578	-2.003710763
1958	2-Methylbutyryl carnitine	0.9925	MS2 forward	246.1688287	224.866	0.03067749	0.040307622	1.171686713	0.014580001	0.023483722	0.78600226	-0.384079742
2449	1,2,3-Benzoxazole	0.9905	MS2 reverse	275.051415	382.98	0.00344821	0.020381946	1.597811484	0.003104107	0.00676787	1.6554992	0.727290383
1933	Uridine	0.9972	MS2 forward	245.0757948	155.045	0.029190351	0.044552807	1.530019421	0.00122889	0.000591149	0.655188407	-0.810018385
1029	2-Hydroxyadenine	0.9673	MS2 forward	174.0388337	247.3885	0.002073985	0.003033285	1.697230991	0.00388882	0.001413152	0.414538759	-1.270462959
118	L-Alanine	0.996	MS2 forward	90.05411398	329.763	0.229790623	0.253952673	1.125169509	0.035611011	0.044475424	0.906263577	-0.141965593
4887	Stearoyl carnitine	0.995	MS2 forward	428.3731202	153.07	0.35872784	0.240405033	1.628751136	8.41251E-06	8.98291E-05	1.482157125	0.57739846
4444	L-Palmitoyl carnitine	0.993	MS2 forward	400.3428183	156.421	2.207890216	0.703972216	1.745655367	3.24124E-10	8.57477E-08	3.1360412	1.64894455
6042	1-Eicosatienyl-sn-glycero-3-phosphoethanolamine	0.9738	MS2 reverse	504.3066806	179.833	0.02765256	0.035258665	1.56373289	0.000160878	0.000717606	0.781724322	-0.35628917
2568	Cytidine 2',3'-cyclic phosphate	0.9992	MS2 forward	306.0492931	396.48	0.003361139	0.005048633	1.316962706	0.011994412	0.002009069	0.665752314	-0.586942558
939	L-Phenylalanine	0.9964	MS2 forward	166.0848735	239.617	0.027594047	0.040976299	1.620009336	4.83898E-05	0.000329564	0.665831394	-0.587789935