

Supplementary Table S3. Results of comparative analyses

ID	Metabolite	PubChem CID	HMDB ID	Concentration (nmol/g)										Comparative Analysis	
				Group I			Group C			Group I		Group C		Group I vs Group C	
				I1	I2	I3	C5	C6	C7	Mean	S.D.	Mean	S.D.	Ratio <sup>†</sup>	p-value <sup>‡</sup>
A_0007	2-Hydroxybutyric acid	440864	HMDB00000008	23	N.D.	42	68	74	27	32	14	56	26	0.6	0.267
A_0021	2-Oxoglutaric acid	51	HMDB00000028	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0009	2-Oxosuccinic acid	49	HMDB00000019	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0041	2-Phosphoglyceric acid	439278	HMDB00003391	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0006	3-Hydroxybutyric acid	441	HMDB00000011, HMDB00000357, HMDB00000442	240	322	413	727	1,008	499	325	87	744	255	0.4	0.092
A_0040	3-Phosphoglyceric acid	439183	HMDB00000807	N.D.	N.D.	28	17	28	28	28	N.A.	25	6.3	1.1	N.A.
A_0077	6-Phosphogluconic acid	91493	HMDB00013116	110	99	81	37	48	44	97	15	43	5.6	2.2	0.015
A_0104	Acetyl CoA_divalent	444493		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
C_0071	Adenine	190	HMDB00000034	8.1	7.1	6.9	7.2	6.8	11	7.4	0.8	8.3	2.2	0.9	0.537
C_0169	Adenosine	60961	HMDB00000050	69	49	47	63	83	73	55	12	73	10	0.8	0.123
A_0109	ADP	6022	HMDB0001341	106	99	115	141	146	99	107	7.9	129	26	0.8	0.278
C_0012	Ala	602	HMDB00000161, HMDB0001310	2,722	2,240	2,372	1,435	1,167	1,651	2,445	249	1,418	243	1.7	0.007
A_0093	AMP	6083	HMDB00000045	788	748	889	894	791	331	808	72	672	299	1.2	0.516
C_0075	Anthranilic acid	227	HMDB00011123	N.D.	N.D.	0.4	0.3	0.3	0.4	0.4	N.A.	0.3	0.07	1.2	N.A.
C_0112	Arg	6322	HMDB00000517, HMDB00003416	8.7	7.6	5.8	3.5	2.8	2.9	7.4	1.4	3.1	0.4	2.4	0.030
C_0066	Asn	236	HMDB00000168, HMDB00033780	230	215	246	200	168	142	230	16	170	29	1.4	0.050
C_0070	Asp	424	HMDB00000191, HMDB0006483	576	592	519	366	473	413	562	38	417	54	1.3	0.023
A_0119	ATP	5967	HMDB00000538	15	18	16	28	37	40	16	1.6	35	6.5	0.5	0.031
C_0037	Betaine	247	HMDB00000043	1,077	948	1,092	1,155	1,520	1,624	1,039	79	1,433	247	0.7	0.098
C_0044	Betaine aldehyde_+H2O	249		52	53	64	64	99	84	56	7.1	82	17	0.7	0.107
A_0088	cAMP	6076	HMDB00000058	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
C_0144	Carnosine	439224	HMDB00000033	0.4	0.8	0.6	0.8	0.5	1.0	0.6	0.2	0.8	0.3	0.8	0.451
A_0102	CDP	6132	HMDB0001546	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0092	cGMP	24316	HMDB00013114	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
C_0024	Choline	305	HMDB00000097	398	417	488	581	857	552	434	47	664	168	0.7	0.134
A_0034	cis -Aconitic acid	643757	HMDB00000072	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0049	Citric acid	311	HMDB00000094	187	225	182	137	148	187	198	24	157	26	1.3	0.118
C_0114	Citrulline	9750	HMDB00009094	33	30	34	36	40	41	32	1.8	39	2.7	0.8	0.028
A_0085	CMP	6131	HMDB00000095	78	60	64	70	78	69	68	9.4	73	4.8	0.9	0.474
A_0098	CoA_divalent	87642		105	98	130	142	143	117	111	17	134	15	0.8	0.147
C_0063	Creatine	586	HMDB00000064	193	165	244	211	152	230	201	40	198	41	1.0	0.931
C_0032	Creatinine	588	HMDB00000562	4.4	4.3	5.5	5.4	4.3	5.9	4.7	0.7	5.2	0.8	0.9	0.471
A_0115	CTP	6176	HMDB00000082	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
C_0046	Cys	594	HMDB00000574, HMDB0003417	8.3	7.8	7.5	3.8	2.6	1.4	7.9	0.4	2.6	1.2	3.0	0.011
C_0152	Cytidine	6175	HMDB00000089	6.8	4.4	4.9	6.6	8.2	11	5.4	1.2	8.8	2.5	0.6	0.125
C_0029	Cytosine	597	HMDB00000630	0.6	0.5	0.5	N.D.	N.D.	N.D.	0.5	0.08	N.A.	N.A.	1<	N.A.
A_0118	dATP	15993	HMDB0001532	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0113	dCTP	65091	HMDB00009098	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0029	Dihydroxyacetone phosphate	668	HMDB0001473	698	522	436	134	189	150	552	133	158	28	3.5	0.032
A_0101	dTDP	164628	HMDB0001274	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0084	dTMP	9700	HMDB0001227	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0114	dTTP	64968	HMDB0001342	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0056	Erythrose 4-phosphate	122357	HMDB0001321	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0091	Fructose 1,6-diphosphate	172313	HMDB0001058	412	313	257	30	20	42	327	78	31	11	11	0.021
A_0074	Fructose 6-phosphate	603	HMDB00000124	419	95	59	80	98	116	191	198	98	18	1.9	0.503
A_0008	Fumaric acid	444972	HMDB00000134	860	792	835	261	331	332	829	34	308	41	2.7	8.9E-05 ***
C_0020	GABA	119	HMDB00000112	38	41	49	24	27	18	43	5.5	23	4.5	1.9	0.009
A_0110	GDP	8977	HMDB0001201	21	21	26	24	25	20	23	2.8	23	2.3	1.0	0.875
C_0086	Gln	738	HMDB00000641, HMDB0003423	2,245	2,531	2,173	1,737	1,667	1,272	2,316	189	1,559	251	1.5	0.016
C_0089	Glu	611	HMDB00000148, HMDB0003339	1,662	1,528	1,422	1,735	2,099	1,743	1,537	120	1,859	208	0.8	0.098
A_0055	Gluconic acid	10690	HMDB00000625	629	483	602	1,014	1,045	734	571	78	931	172	0.6	0.051
A_0073	Glucose 1-phosphate	65533	HMDB0001586	222	106	72	25	20	25	133	79	23	3.2	5.7	0.136
A_0071	Glucose 6-phosphate	5958	HMDB0001401	1,726	234	126	149	163	155	695	894	156	6.9	4.5	0.405
C_0183	Glutathione (GSH)	124886	HMDB00000125	4,479	3,705	3,391	2,212	2,224	2,287	3,858	560	2,241	40	1.7	0.037
C_0182	Glutathione (GSSG)_divalent	65359		671	563	540	540	571	574	591	70	561	19	1.1	0.543
C_0060	Gly	759	HMDB00000123	1,980	1,679	1,781	1,396	1,404	1,388	1,814	153	1,396	7.7	1.3	0.042
A_0030	Glycerinaldehyde 3-phosphate	729	HMDB0001112	36	N.D.	N.D.	N.D.	N.D.	N.D.	36	N.A.	N.A.	N.A.	1<	N.A.
A_0031	Glycerol 3-phosphate	439162	HMDB0000126	2,125	2,306	2,255	1,994	2,526	1,990	2,229	93	2,170	308	1.0	0.778
A_0002	Glycolic acid	757	HMDB00000115	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0001	Glyoxylic acid	790	HMDB00000119	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0096	GMP	6894	HMDB0001397	245	230	300	281	276	116	259	37	225	94	1.2	0.806
A_0121	GTP	6830	HMDB0001273	N.D.	N.D.	N.D.	7.1	12	14	N.A.	N.A.	11	3.8	<1	N.A.
C_0092	Guanine	764	HMDB00000132	2.9	2.7	3.3	3.3	5.3	5.6	3.0	0.3	4.7	1.2	0.6	0.130
C_0175	Guanosine	6802	HMDB00000133	57	47	46	51	66	82	50	6.3	66	16	0.8	0.199
C_0096	His	773	HMDB00000177	693	644	618	571	556	535	652	38	554	18	1.2	0.031
C_0042	Homoserine	12847	HMDB00000719	2.1	1.8	2.2	0.8	1.0	1.4	2.0	0.2	1.1	0.3	1.9	0.014
C_0061	Hydroxyproline	5810	HMDB00000725	22	19	24	9.6	10	16	22	2.3	12	3.3	1.8	0.017
C_0072	Hypoxanthine	790	HMDB00000157	821	721	792	821	972	1,175	778	52	989	178	0.8	0.168
C_0064	Ile	791	HMDB00000172	280	283	317	317	319	239	293	20	292	46	1.0	0.956
A_0095	IMP	8582	HMDB00000175	217	207	216	262	252	61	214	5.8	191	113	1.1	0.767
C_0170	Inosine	6021	HMDB00000195	2,078	1,789	1,834	1,708	1,856	2,241	1,901	155	1,935	275	1.0	0.862
A_0047	Isoelectric acid	1198	HMDB00000193	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.	N.A.	N.A.
A_0005	Lactic acid														