

Supplementary Table 1 Absolute concentrations of cellular metabolites for NSC11, U251, and U87 cell lines

Line	ID	※The background color of cells are same as HeatMap in newer version of MS-Excel 2007.																														
		Compound name		KEGG ID		HMDB ID		Standardized Retention Area [§]						IR																		
								NSC11	NSC11	NSC11	U87 1	U87 2	U87 3	U251 1	U251 2	U251 3	IR1	IR2	IR3													
1	A_0033	Dihydroxyacetone phosphate	C00111	HMDB01473	-0.642	-0.642	-0.642	2.127	2.389	1.606	-0.642	-0.547	-0.234	-0.642	-0.187	-0.642	-0.225	0.085	0.527	-0.642	-0.404	-0.642	-0.642	-0.642	-0.642	-0.642	-0.642	-0.642				
2	A_0010	NADP ⁺	C00006	HMDB00217	-1.05	-1.137	-1.262	0.328	1.719	0.851	-0.591	-0.85	-0.740	-0.551	-0.935	-1.259	-0.410	1.299	0.184	0.601	1.476	1.026										
3	A_0043	GMP ⁺	C00144	HMDB01397	-1.292	-1.178	-1.203	0.024	0.292	-0.130	-0.879	-0.905	-0.711	-0.797	-0.290	-0.718	1.151	1.300	1.458	1.299	0.184	0.601	1.476	1.026								
4	A_0014	Fructose-6-phosphate	C05345_C00095	HMDB0124	-1.147	-1.042	-1.048	1.086	0.685	0.446	-0.785	0.598	-0.581	-0.819	-0.687	-1.116	0.720	1.860	1.703	0.627	1.142	0.744										
5	A_0001	NAD ⁺	C00003	HMDB00802	-1.117	-1.090	-1.194	0.322	1.112	0.623	0.605	0.553	0.565	0.701	-0.663	-1.226	1.329	1.591	1.569	0.419	0.908	0.369										
6	A_0055	N-Acetylglutamic acid	C00624	HMDB01138	-1.276	-1.063	-1.074	1.774	1.422	1.167	0.777	0.703	0.633	0.661	0.499	-1.441	1.763	1.637	1.014	1.248	0.568	0.498										
7	A_0006	ADP-ribose	C00301	HMDB01178	-0.798	-1.136	-0.650	0.569	1.594	0.972	0.978	-1.182	-0.713	-1.133	0.000	0.648	0.914	1.092	1.655	0.175	1.025	0.711										
8	A_0044	AMP	C00020	HMDB00245	-0.878	0.838	0.834	0.844	0.740	0.408	-1.093	-1.061	-1.168	0.479	-0.084	-0.946	1.638	1.669	1.736	-0.087	0.276	0.157										
9	A_0013	Glucose-6-phosphate	C00668_C01172_C0392	HMDB01401	-0.596	-0.669	-0.728	0.548	1.473	0.727	-1.163	-1.083	-0.993	-0.560	-0.157	-0.830	1.093	1.959	1.696	-0.475	-0.084	0.188										
10	A_0002	cAMP	C00575	HMDB00058	-0.355	0.406	0.428	0.416	1.746	0.642	-1.199	-1.241	-1.219	0.604	-0.492	-0.123	0.626	1.510	1.526	0.951	-0.916	0.924										
11	C_0046	Adenosine	C00212	HMDB00050	-0.674	0.674	0.674	0.515	1.140	1.553	0.590	0.674	-0.553	-0.674	-0.674	-0.674	1.282	1.674	0.570	0.494												
12	A_0012	Sedoheptulose-7-phosphate	C00582	HMDB01068	-0.318	0.318	0.318	0.318	0.318	0.318	0.318	0.318	0.318	0.318	0.318	0.318	0.318	0.308	3.795	0.67	0.318	0.318										
13	C_0048	Guanosine	C00387	HMDB00133	-0.343	0.343	0.343	0.343	-0.343	-0.343	-0.343	0.343	0.343	0.343	0.343	0.343	0.343	0.343	0.343	0.343	0.343	0.343										
14	C_0052	S-Adenosylmethionine	C00019	HMDB01185	-0.431	0.431	0.431	0.431	-0.431	-0.431	-0.431	0.431	0.431	0.431	0.431	0.431	0.431	0.431	0.431	0.431	0.431	0.431										
15	A_0021	Ribose-5-phosphate	C00117	HMDB01548	-0.149	1.515	0.560	0.250	0.220	0.194	0.622	0.404	0.926	-0.768	-0.337	-0.515	0.086	0.091	2.670	0.621	1.294	0.315										
16	A_0032	XMP	C00655	HMDB01554	-1.163	-1.163	-1.163	0.130	0.510	0.308	0.669	0.718	0.991	-1.163	-0.475	-1.163	-0.349	0.059	1.845	1.875	0.487	0.638										
17	A_0038	PRPP	C00119	HMDB00280	-1.027	-1.027	-1.027	0.210	0.397	-0.327	0.636	-0.037	-0.191	-1.027	-1.027	-1.027	0.393	0.697	2.609	1.703	1.409	0.348										
18	A_0063	cis-Aconitic acid	C00417	HMDB00072	-1.162	-1.162	-1.162	0.703	0.895	0.721	0.128	-0.116	-0.208	-1.162	-1.162	-1.162	0.200	0.978	1.188	2.059	0.600	0.078										
19	A_0062	Citric acid	C00158	HMDB00094	-1.223	-0.689	-1.042	0.342	-0.448	-0.098	-0.366	-0.570	-0.423	-1.146	-0.521	-1.276	-0.093	-0.912	0.811	2.353	1.495	0.704										
20	C_0024	Asn	C00152_C00195_C01648	HMDB0168	-0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.351	0.226	1.587	2.900								
21	A_0035	Fructose-1,6-diphosphate	C00354	HMDB01058	-0.668	0.612	-0.672	0.419	0.315	-0.325	0.215	0.036	0.115	0.605	0.463	-0.650	0.484	0.380	0.458	1.188	2.248	2.690										
22	A_0042	Phosphoenolpyruvic acid	C00074	HMDB00263	-0.566	0.566	-0.566	0.566	-0.566	-0.566	0.107	0.440	0.670	0.566	-0.566	-0.566	0.566	0.566	0.566	0.566	0.566	0.273	1.255	2.625								
23	A_0008	UDPGlucose	C00239	HMDB00286	-0.749	0.676	0.804	0.718	0.463	0.591	0.273	0.171	0.109	0.564	-0.102	-0.770	0.824	-0.484	-0.289	-0.382	1.470	2.566	2.003									
24	A_0049	GTP	C00044	HMDB01273	-0.776	-0.808	-0.854	-0.602	-0.508	-0.493	-0.341	-0.309	-0.428	-0.675	-0.319	-0.824	-0.502	-0.211	-0.463	-1.856	2.325	1.777										
25	A_0051	ATP	C00009	HMDB00538	-0.807	0.813	0.819	0.693	0.598	-0.607	0.360	0.313	0.419	0.550	-0.550	-0.057	0.712	0.619	0.281	0.503	1.908	2.253	1.777									
26	A_0059	Malic acid	C00149_C00497_C00711	HMDB0156_HMDB00744	-0.646	-0.656	-0.646	-0.617	0.646	0.644	0.429	0.537	0.516	-0.646	-0.370	-0.646	-0.646	0.646	1.880	2.232	1.778											
27	A_0061	Fumaric acid	C00122	HMDB01314	-0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628	0.628			
28	C_0021	Creatine	C00300	HMDB00624	-0.716	-0.670	-0.849	-0.466	0.319	-0.386	0.476	0.618	-0.470	-0.740	-0.584	-0.859	-0.665	-0.381	0.495	1.829	1.888	2.076										
29	C_0012	Creatinine	C00307	HMDB01062	-0.733	-0.717	-0.751	0.653	-0.583	-0.653	0.617	0.761	0.511	0.585	-0.456	-0.636	-0.668	-0.540	-0.637	0.205	1.849	1.758										
31	C_0049	Arginosuccinic acid	C00406	HMDB00052	-0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626	0.626			
32	C_0008	γ-Aminobutyric acid	C00205	HMDB01142	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649	-0.649			
33	C_0007	α-Ketoglutarate	C00206	HMDB01147	-0.709	0.709	0.692	0.353	0.291	-0.310	0.220	0.150	0.336	0.264	0.184	-0.160	0.394	0.392	0.391	0.392	0.393	0.394	0.395	0.396	0.397	0.398	0.399	0.398	0.397	0.396		
34	C_0009	Uric acid	C00338	HMDB0289	-0.236	0.236	0.236	0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236			
35	C_0024	β-Alanide	C00205	HMDB0158	-0.113	-0.171	-0.197	0.150	0.332	0.441	0.076	0.834	-0.245	-1.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197	-0.197			
36	C_0014	β-Alanide	C00207	HMDB00618	-0.961	0.961	0.961	0.961	0.152	0.230	0.700	0.051	-0.308	0.471	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961	-0.961			
37	C_0051	Glutathione(GSH)	C00514	HMDB00125	-1.119	-1.216	-1.216	0.991	0.611	0.674	0.474	-0.992	-0.919	-1.130	-1.039	-1.084	-0.477	-0.696	0.666	1.258	1.516	1.546										
38	C_0014	Val	C00183_C00174_C01646	HMDB00883	-1.138	-1.138	-1.138	0.075	0.214	0.134	0.201	0.416	0.238	0.138	-1.138	-1.138	-1.138	0.115	0.544	0.215	1.681	1.697										
40	C_0038	Phe	C00079	HMDB0257	-1.136	-0.987	-1.206	0.175	0.080	-0.151	0.150	0.159	-0.157	-0.861	-1.162	-0.079	0.434	0.182	1.952	1.701	1.713											
41	C_0041	Tyr	C00089	HMDB01540	-1.113	-0.001	-1.171	0.190	0.194	-0.053	0.155	0.315	0.616	-0.062	-0.736	-1.274	2.142	1.048	-0.676	-0.670	-0.650	0.665	0.663									
42	C_0044	Trp	C00789_C00252_C00806	HMDB00299	-0.879	0.582	-1.164	0.209	0.112	-0.081	0.233	0.083	0.142	-1.164	-1.164	-1.164	-0.160	0.320	1.681	1.831	1.67											

ID consists of analysis mode and number. 'C' and 'A' showed cation and anion modes, respectively.

§ Standardized value of relative area in detected peaks. In Calculationg the diatance, the values of N.D. were regarded as $\text{eps}(2^{-52})$.
The order of samples and metabolites in this table corresponded to those of HeatMap.