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

HCA					※The background color of cells are same as HeatMap in newer version of MS Excel 2007.															
	HMT DB				Standardized Relative Area[1]															
Line	ID	Compound name	KEGG ID	HMDB ID	NSC11 1	NSC11 2	NSC11 3	U87 1	U87 2	U87 3	U251 1	U251 2	U251 3	NSC11 IR 1	NSC11 IR 2	NSC11 IR 3	U87 IR 1	U87 IR 2	U87 IR 3	U251 IR 1	U251 IR 2	U251 IR 3
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
2	A_0010	NADP+	C00006	HMDB00217	-1.105	-1.137	-1.262	0.328	1.719	0.853	-0.591	-0.825	-0.740	-0.551	0.395	-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	0.673	1.435	1.188
4	A_0014	Fructose 6-phosphate	C05345 C00085	HMDB00124	-1.147	-1.042	-1.044	-0.108	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	HMDB00902	-1.117	-1.090	-1.194	0.322	1.132	0.623	-0.603	-0.535	-0.563	-1.071	-0.663	-1.226	1.329	1.591	1.369	0.419	0.908	0.369
6	A_0055	*N*-Acetylglutamic acid	C00624	HMDB01138	-1.276	-1.066	-1.037	0.774	1.422	1.167	-0.777	-0.700	-0.633	-0.661	-0.499	-1.441	0.763	1.637	1.014	0.248	0.568	0.498
7	A_0006	ADP-ribose	C00301	HMDB01178	-0.798	-1.138	-0.650	0.569	1.594	0.927	-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	HMDB00045	-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	HMDB01401	-0.596	-0.669	-0.728	0.548	1.473	0.727	-1.163	-1.083	-0.993	-0.560	-0.157	-0.800	1.093	1.959	1.696	-0.475	-0.084	-0.188
10	A_0002	cAMP	C00575	HMDB00058	-0.355	-0.406	-0.428	0.616	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	0.646	2.492	1.261	-0.674	-0.570	-0.494
12	A_0012	Sedoheptulose 7-phosphate	C05382	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	1.038	3.795	-0.067	-0.318	-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	2.655	2.839	-0.343	-0.343	-0.343
14	C_0052	*S*-Adenosylmethionine	C00019	HMDB01185	-0.431	-0.431	-0.431	-0.431	1.715	-0.431	-0.431	-0.431	-0.431	-0.431	-0.431	-0.431	-0.431	2.260	2.474	-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	1.768	-0.337	-0.515	-0.082	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	2.069	1.700	1.409	0.348
18	A_0063	cis -Aconitic acid	C00417	HMDB00072	-1.162	-1.162	-1.162	0.703	0.495	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 C01905	HMDB00168	-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	2.587	2.900
21	A_0035	Fructose 1,6-diphosphate	C00354	HMDB01058	-0.668	-0.612	-0.657	-0.419	-0.315	-0.352	-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	1.027	2.135	2.625
23	A_0008	UDP-glucose	C00029	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	-0.484	-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	-0.213	-0.463	1.856	2.325	1.777
25	A_0051	ATP	C00002	HMDB00538	-0.807	-0.813	-0.819	-0.693	-0.598	-0.607	0.360	0.313	0.459	-0.550	-0.059	-0.712	-0.619	-0.281	-0.503	1.900	2.253	1.777
26	A_0059	Malic acid	C00149 C00497	HMDB00156 HM	-0.646	-0.565	-0.646	-0.617	-0.646	-0.644	0.429	0.537	0.510	-0.646	-0.370	-0.646	-0.646	-0.646	-0.646	1.880	2.232	1.778
27	A_0061	Fumaric acid	C00122	HMDB00134	-0.628	-0.628	-0.628	-0.628	-0.628	-0.628	0.458	0.548	0.443	-0.628	-0.427	-0.628	-0.628	-0.628	-0.628	1.620	2.247	2.024
28	C_0021	Creatine	C00300	HMDB00064	-0.716	-0.667	-0.735	-0.647	-0.608	-0.636	0.549	0.676	0.522	-0.575	-0.380	-0.693	-0.684	-0.552	-0.631	1.814	1.900	2.062
29	C_0013	Pro	C00148 C07643	HMDB00162 HM	-0.631	-0.631	-0.631	-0.631	-0.631	-0.631	0.547	0.719	0.538	-0.631	-0.631	-0.631	-0.631	-0.631	-0.631	2.009	1.847	1.914
30	C_0012	Creatinine	C00791	HMDB00562	-0.733	-0.717	-0.751	-0.653	-0.583	-0.633	0.617	0.761	0.511	-0.585	-0.456	-0.636	-0.668	-0.540	-0.637	2.095	1.849	1.758
31	C_0049	Argininosuccinic acid	C03406	HMDB00052	-0.626	-0.626	-0.626	-0.626	-0.626	-0.626	0.544	0.614	0.565	-0.626	-0.626	-0.626	-0.626	-0.626	-0.626	2.147	1.991	1.652
32	C_0008	γ-Aminobutyric acid	C00334	HMDB00112	-0.653	-0.653	-0.653	-0.653	-0.631	-0.653	0.732	0.858	0.727	-0.653	-0.653	-0.653	-0.653	-0.653	-0.653	1.973	1.848	1.674
33	A_0037	*N*-Carbamoylaspartic acid	C00438	HMDB00828	-0.697	-0.683	-0.708	-0.548	-0.314	-0.394	0.597	0.773	0.819	-0.833	-0.662	-0.850	-0.826	-0.555	-0.615	1.879	1.998	1.620
34	C_0033	Glu	C00025 C00217	HMDB00148 HM	-0.822	-0.790	-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
35	C_0026	Asp	C00049 C00402	HMDB00191 HM	-0.800	-0.800	-0.800	-0.576	-0.522	-0.555	0.583	0.922	0.700	-0.692	-0.570	-0.719	-0.648	-0.524	-0.564	1.401	1.826	2.143
36	C_0005	Ala	C00041 C00133	HMDB00161 HM	-0.741	-0.586	-0.697	-0.711	-0.624	-0.664	0.330	0.588	0.397	-0.474	-0.116	-0.606	-0.783	-0.563	-0.669	2.000	1.890	2.000
37	C_0002	Gly	C00037	HMDB00123	-0.614	-0.480	-0.692	-0.804	-0.727	-0.769	0.427	0.609	0.463	-0.357	0.101	-0.567	-0.906	-0.655	-0.780	2.045	1.763	1.940
38	C_0045	Cystathionine	C00542 C02291	HMDB00099	-0.545	-0.320	-0.372	-0.879	-0.893	-0.902	0.513	0.744	0.482	-0.314	0.110	-0.513	-0.880	-0.885	-0.890	1.974	1.922	1.647
39	A_0015	Fructose 1-phosphate	C01094 C02976	HMDB01076	-0.628	-0.628	-0.628	-0.628	-0.628	-0.628	0.549	0.823	0.758	-0.628	-0.628	-0.628	-0.628	-0.628	-0.628	2.326	2.072	1.007
40	A_0040	2,3-Diphosphoglyceric acid	C01159	HMDB01294	-0.774	-0.745	-0.786	-1.060	0.110	-0.006	0.352	0.523	0.604	-0.812	-0.698	-0.833	-0.285	-1.060	-0.068	1.819	2.019	1.701
41	A_0030	Malonyl CoA	C00083	HMDB01175	-0.825	-0.825	-0.825	-0.130	0.301	-0.400	0.406	0.070	0.422	-0.825	-0.825	-0.825	-0.825	-0.226	-0.449	2.235	1.993	1.552
42	C_0020	Hydroxyproline	C01015 C01157	HMDB00725 HM	-0.935	-0.935	-0.935	-0.279	-0.348	-0.320	0.627	0.882	0.695	-0.935	-0.935	-0.935	-0.532	-0.058	-0.355	1.938	1.706	1.651
43	C_0004	β-Ala	C00099	HMDB00056	-1.098	-0.975	-1.095	-0.198	-0.079	-0.149	0.369	0.552	0.352	-0.989	-0.780	-0.987	-0.317	-0.001	-0.162	2.001	1.779	1.776
44	C_0016	Thr	C00188 C00820	HMDB00167	-1.021	-0.953	-1.062	-0.376	-0.205	-0.336	0.327	0.437	0.273	-0.837	-0.558	-0.984	-0.376	0.050	-0.132	2.135	1.778	1.841
45	C_0010	Ser	C00065 C00716	HMDB00187 HM	-1.057	-0.925	-1.123	-0.418	-0.272	-0.407	0.189	0.325	0.165	-0.656	-0.183	-0.882	-0.467	-0.008	-0.201	2.000	1.918	2.002
46	A_0036	6-Phosphogluconic acid	C00345	HMDB01316	-0.896	-0.884	-0.866	-0.310	-0.167	-0.227	-0.066	0.167	0.426	-0.913	-0.892	-0.929	-0.276	0.134	-0.129	1.503	2.324	2.003
47	A_0041	3-Phosphoglyceric acid	C00197	HMDB00807	-0.889	-0.672	-0.862	-0.524	-0.479	-0.391	-0.202	0.125	0.368	-0.815	-0.481	-0.889	-0.338	0.026	-0.006	1.656	2.360	2.013
48	A_0039	2-Phosphoglyceric acid	C00631	HMDB03391	-0.649	-0.823	-0.818	-0.641	-0.482	-0.401	-0.356	-0.070	-0.035	-0.981	-0.070	-0.648	-0.179	-0.201	0.167	2.021	2.238	1.928
49	A_0022	CoA	C00010	HMDB01423	-0.629	-0.772	-0.940	-0.443	-0.325	-0.399	0.559	-0.635	-0.284	-0.632	-0.473	-0.539	-0.178	-0.139	-0.338	1.900	2.333	1.933
50	A_0031	Phosphocreatine	C02305	HMDB01511	-0.482	-0.482	-0.482	-0.482	-0.482	-0.482	-0.389	0.119	-0.301	-0.482	-0.482	-0.482	-0.482	-0.482	-0.482	2.305	2.499	1.549
51	A_0064	Isocitric acid	C00311	HMDB00193	-0.714	-0.714	-0.714	0.996	-0.290	-0.178	-0.136	0.033	-0.464	-0.714	-0.714	-0.714	-0.714	-0.359	-0.190	2.662	1.468	1.255
52	A_0024	Ribulose 5-phosphate	C00199 C01101	HMDB00618	-0.961	-0.961	-0.961	0.152	0.230	0.700	-0.051	-0.308	0.427	-0.961	-0.961	-0.961	-0.693	-0.595	0.850	1.205	2.256	1.614
53	C_0051	Glutathione (GSH)	C00051	HMDB00125	-1.119	-1.216	-1.216	0.391	0.611	0.474	0.392	-0.912	-0.309	-1.130	-1.039	-1.084	0.477	0.690	0.666	1.258	1.518	1.546
54	C_0034	Met	C00073 C00855	HMDB00696	-1.288	-1.144	-1.397	0.363	0.749	0.496	-0.210	0.072	-0.240	-1.181	-0.849	-1.340	0.305	0.979	0.555	1.496	1.148	1.485
55	C_0032	Lys	C00047 C00739	HMDB00182 HM	-1.374	-0.738	-1.374	-0.046	0.678	0.498	-0.245	-0.041	-0.088	-1.230	-0.627	-1.374	0.007	1.319	0.540	0.836	1.447	1.811
56	A_0005	Xanthine	C00385	HMDB00292	-1.154	-0.626	-1.154	-0.203	0.716	0.714	-0.300	-0.320	-0.002	-1.154	-1.154	-1.154	-0.137	0.855	0.385	1.015	1.935	1.738
57	A_0045	2-Oxoisovaleric acid	C00141	HMDB00019	-1.076	-1.076	-1.076	-0.250	0.424	0.223	-0.118	-0.034	0.103	-1.076	-1.076	-1.076	-0.072	0.986	0.147	1.277	1.845	1.924
58	C_0017	Homoserine	C00263	HMDB00719	-1.160	-1.160	-1.160	-0.018	0.305	0.503	0.264	0.181	0.304	-1.160	-1.160	-1.160	0.014	0.392	0.332	0.860	1.691	2.128
59	C_0028	Adenine	C00147	HMDB00034	-1.197	-1.197	-1.197	-0.150	0.332	0.441	0.076	0.833	0.245	-1.197	-1.197	-1.197	-0.108	0.691	0.376	1.406	1.297	1.743
60	C_0036	Ile	C00135 C07568	HMDB00177	-1.322	-1.111	-1.424	0.068	0.453	0.258	0.200	0.323	0.255	-1.286	-0.759	-1.234	-0.061	0.759	0.305	1.702	1.570	1.323
61	C_0023	Leu	C00123 C01570	HMDB00687	-1.235	-0.926	-1.293	-0.051	0.284	0.159	0.053	0.261	0.094	-1.124	-0.821	-1.306	-0.088	0.604	0.296	1.675	1.656	1.762
62	C_0022	Ile	C00407 C06418	HMDB00172	-1.217	-0.955	-1.203	-0.103	0.222	0.095	0.148	0.339	0.169	-1.105	-0.933	-1.248	-0.148	0.558	0.231	1.780	1.533	1.836
63	C_0014	Val	C00183 C06417	HMDB00883	-1.138	-1.138	-1.138	-0.075	0.214	0.134	0.201	0.416	0.238	-1.138	-1.138	-1.138	-0.115	0.544	0.215	1.681	1.609	1.767
64	C_0038	Phe	C00079 C02057	HMDB00159	-1.136	-0.987	-1.206	-0.175	0.081	-0.030	0.151	0.338	0.159	-1.057	-0.861	-1.162	-0.097	0.434	0.182	1.952	1.701	1.713
65	C_0041	Tyr	C00082 C01536	HMDB00158	-1.113	-1.000	-1.171	-0.190	0.184	-0.053	0.157	0.352	0.165	-1.062	-0.855	-1.153	-0.148	0.340	0.131	1.911	1.704	1.801
66	C_0044	Trp	C00078 C05525	HMDB00929	-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	0.168	1.851	1.679	1.998
67	A_0046	GDP	C00035	HMDB01201	-1.324	-0.821	-1.105	-0.316	-0.138	-0.262	-0.283	0.001	-0.375	-0.872	-0.115	-1.218	0.359	0.708	0.358	1.580	1.661	2.161
68	A_0048	ADP	C00008	HMDB01341	-0.965	-0.686	-0.954	-0.612	-0.433	-0.567	-0.266	0.124	-0.591	-0.279	-0.096	-1.324	0.095	0.616	0.294	1.584	1.640	2.420
69	A_0019	Acetyl CoA	C00024	HMDB01206	-1.168	-1.487	-1.151	-0.506	0.451	-0.504	-0.071	0.632	0.630	-0.938	0.562	-0.997	-0.443	0.446	-0.122	0.891	1.715	2.061
70	C_0050	Glutathione (GSSG)	C00127	HMDB03337	-0.765	-0.759	-0.692	-0.353	-0.295	-0.391	-0.220	3.000	1.524	-0.765	-0.765	-0.765	-0.527	-0.023	-0.271	0.931	0.572	0.566
71	A_0009	Uric acid	C00366	HMDB00289	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	4.007	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236
72	A_0023	Ribose 1-phosphate	C00620	HMDB01489	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	4.007	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236	-0.236
73	A_0027	HMG CoA	C00356	HMDB01375	3.299	-0.479	-0.479	-0.479	-0.479	-0.479	0.349	0.515	0.483	-0.479	-0.479	-0.479	-0.479	-0.479	-0.479	1.584	-0.479	-0.479
74	A_0017	Glucose 1-phosphate	C00103	HMDB01586	1.897	-0.057	1.186	-0.649	-0.367	0.214	-0.853	-0.864	-0.832	2.065	-1.032	-1.032	-0.182	0.967	0.683	-1.032	-0.461	0.348
75	A_0011	IMP	C00130	HMDB00175	1.868	1.629	0.977	-0.999	-0.428	-0.912	-1.290	-1.202	-1.102	0.439	1.217	0.542	-0.051	-0.265	0.829	-0.005	-0.446	-0.801
76	A_0053	Glycolic acid	C00160	HMDB00115	1.382	0.725	0.972	-0.377	-0.175	-0.595	-1.091	0.264	-0.649	0.051	2.393	1.435	-1.091	-0.741	-1.091	-0.457	-0.354	-0.599
77	A_0004	NADH	C00004	HMDB01487	1.332	0.848	0.912	-1.024	-0.611	-0.630	-1.237	-1.442	-1.274	1.144	1.547	1.021	-0.820	-0.430	-0.619	0.184	0.543	0.555
78	A_0034	Adenylosuccinic acid	C03794	HMDB00536	1.506	1.018	1.005	-1.024	-0.787	-1.048	-0.960	-0.923	-0.927	1.312	1.589	1.306	-0.761	-0.589	-0.590	0.037	0.065	-0.230
79	A_0016	Galactose 1-phosphate	C00446	HMDB00759	1.129	1.393	1.049	-0.674	-0.672	-0.682	-0.672	-0.670	-0.672	1.274	2.142	1.048	-0.676	-0.670	-0.677	-0.650	-0.655	-0.663
80	C_0040	Citrulline	C00327	HMDB00904	0.948	1.023	0.579	-0.784	-0.745	-0.761	-0.483	-0.531	-0.551	1.398	2.882	0.315	-0.784	-0.681	-0.784	-0.343	-0.361	-0.295
81	C_0039	Arg	C00062 C00792	HMDB00517 HM	0.557	2.056	0.476	-0.791	-0.318	-0.503	-1.133	-1.047	-1.078	1.148	2.354	0.093	-0.671	0.083	-0.352	-0.517	-0.278	-0.057
82	A_0020	Folic acid	C00504	HMDB00121	0.363	1.891	0.070	-0.627	0.726	0.193	-1.784	-1.339	-1.350	0.421	1.208	-0.416	-0.913	0.656	0.179	-0.891	0.402	1.212
83	C_0031	Gln	C00064 C00303	HMDB00641 HM	-0.287	0.524	-0.581	-0.586	-0.378	-0.540	-1.119	-1.061	-1.361	1.197	2.597	-0.146	-0.460	0.423	0.027	0.367	0.685	0.344
84	C_0003	Putrescine	C00134	HMDB01414	0.176	1.168	0.163	-1.176	-1.176	-1.176	-0.060	0.030	-0.016	1.010	2.146	0.281	-1.176	-1.176	-1.176	0.598	0.721	0.837
85	A_0052	Glycerol 3-phosphate	C00093	HMDB00126	-0.070	0.415	-0.373	-1.123	-1.036	-1.025	-0.546	-0.090	-0.435	1.373	1.385	0.001	-1.085	-0.671	-0.989	1.317	1.087	1.864
86	A_0056	2-Hydroxyglutaric acid	C05630 C01087	HMDB00606 HM	-0.112	0.983	0.054	-1.013	-0.420	-0.870	-0.403	-0.429	-0.208	0.049	0.740	-0.553	-1.263	-0.624	-1.194	1.717	2.063	1.484
87	A_0060	2-Oxoglutaric acid	C00026	HMDB00208	0.772	1.589	0.707	-1.125	-0.936	-1.093	-0.134	-0.405	-0.299	-0.042	0.902	-0.557	-1.242	-1.014	-0.975	1.461	1.449	0.942
88	A_0054	Pyruvic acid	C00022	HMDB00243	1.098	0.468	0.310	-1.346	-0.459	-1.054	-0.664	-1.245	-0.414	0.188	1.653	0.441	-1.245	-0.407	-0.970	0.971	1.186	1.489
89	A_0047	Lactic acid	C01186 C00256	HMDB00190 HM	0.534	0.720	0.231	-1.348	-0.384	-0.660	-1.039	-0.634	-0.676	0.011	1.118	-0.017	-1.496	0.094	-0.957	0.933	1.516	2.054
90	A_0058	Succinic acid	C00042	HMDB00254	0.744	-0.181	-0.024	-1.263	-0.536	-1.074	-1.001	0.440	-0.368	-0.114	0.244	-0.103	-1.206	0.029	-0.952	1.719	1.863	1.782

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

[1] Standardized value of relative area in detected peaks. In Calculating the distances, the values of N.D. were regarded as $\exp(2^{-52})$.

The order of samples and metabolites in this table corresponded to those of HeatMap.