

Urinary metabolites are predictive of radiation induced cardiac dysfunction in mice

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CE205	0.025904	0.53437	0.62916	0.669	0.038271	0.52469	1.6774	0.7462	0.65328	0.90438	0.3005	-1.735	0.22127	0.99441	1.3039	0.3828	0.78678	0.95228	0.97992	-0.029
O-ACETYL SERINE_pos_3	0.18715	0.72412	2.0492	1.0351	0.048402	0.59454	0.73532	-0.444	0.40671	0.77512	0.72612	-0.462	0.82674	0.99441	1.0636	0.0889	0.90894	0.96019	1.0129	0.0185
TAG544-FA183	0.20675	0.72412	0.76318	-0.39	0.30285	0.89138	1.5735	0.654	0.48649	0.8154	0.59663	-0.745	0.54046	0.99441	1.1352	0.1829	0.041117	0.54839	1.5314	0.6148
TAG502-FA182	0.001212	0.14065	1.3434	0.4259	0.53752	0.89587	0.99988	-2E-04	0.24289	0.64952	0.69552	-0.524	0.69353	0.99441	0.98149	-0.027	0.41899	0.81279	0.9415	-0.087
TAG524-FA161	0.025975	0.53437	1.3428	0.4252	0.37498	0.89138	0.93278	-0.1	0.16365	0.59496	0.40092	-1.319	0.64863	0.99441	0.92973	-0.105	0.46289	0.8197	0.89102	-0.166
TAG502-FA140	0.53182	0.88822	1.0953	0.1313	0.86496	0.986	0.98865	-0.016	0.8158	0.94216	0.81193	-0.301	0.70852	0.99441	0.9675	-0.048	0.046	0.54839	0.86154	-0.215
TAG461-FA180	0.28656	0.78188	0.84951	-0.235	0.5835	0.89995	1.1023	0.1405	0.008251	0.25047	1.4686	0.5545	0.20628	0.99441	0.88423	-0.178	0.25887	0.67735	0.8758	-0.191
MYOINOSITOL_neg_3	0.69403	0.9716	0.55353	-0.853	0.50361	0.89138	0.84704	-0.239	0.012975	0.31736	0.58412	-0.776	0.49663	0.99441	0.62893	-0.669	0.69708	0.91156	0.67767	-0.561
ASPARTATE_pos_3	0.25997	0.77754	1.2131	0.2787	0.58481	0.89995	0.9979	-0.003	0.030484	0.38105	1.4773	0.563	0.15291	0.99441	1.5975	0.6758	0.060721	0.54839	1.4918	0.577
TAG472-FA182	0.19253	0.72412	0.85769	-0.221	0.92084	0.99	0.96578	-0.05	0.41407	0.78213	1.0062	0.009	0.56608	0.99441	1.1004	0.1381	0.007358	0.34678	0.84219	-0.248
TAG568-FA204	0.50722	0.87452	0.91645	-0.126	0.27862	0.89138	1.0917	0.1265	0.043545	0.42979	1.2326	0.3017	0.72618	0.99441	1.0258	0.0367	0.55676	0.85329	1.9027	0.928
SM240	0.19681	0.72412	0.90956	-0.137	0.003548	0.25129	2.4871	1.3145	0.125	0.52084	1.338	0.42	0.80761	0.99441	0.96977	-0.044	0.68687	0.90885	1.115	0.1571

Supplementary Table S4. List of metabolites showing co-relation with heart dysfunction following 9.5 Gy of Gamma-radiation at 1 week and 1 month post-irradiation.

Name	1 Week				1 Month			
	p-value	FDR	Fold Change	Log2(FC)	p-value	FDR	Fold Change	Log2(FC)
TAG544-FA160	0.014408	0.31041	1.4308 ↑	0.51678	0.00076955	0.32706	2.0944 ↑	1.0665
TAG524-FA204	0.20853	0.60702	1.2322 ↑	0.30129	0.0020708	0.44004	1.7497 ↑	0.80709
SPERMIDINE_pos_4	0.15569	0.56567	0.72461 ↓	-0.46473	0.0070866	0.51123	0.66972 ↓	-0.57837
FFA161	0.00031319	0.066554	0.49327 ↓	-0.195	0.0081376	0.51123	0.64731 ↓	-0.62748
CE226	0.029381	0.31041	1.4628 ↑	0.54874	0.0092877	0.51123	2.9805 ↑	1.5755
INDOLE-3-CARBOXYLIC ACID_neg_1	0.11573	0.53256	0.63227 ↓	-0.66139	0.014323	0.51123	1.5816 ↑	0.66141
TAG522-FA161	0.057556	0.43372	0.79515 ↓	-0.3307	0.01441	0.51123	1.5213 ↑	0.60533
TAG545-FA160	0.020139	0.31041	1.9306 ↑	0.94906	0.016435	0.51123	2.2189 ↑	1.1499
TAG543-FA160	0.065619	0.44981	1.4114 ↑	0.49708	0.019341	0.51123	1.8954 ↑	0.92251
TAG472-FA181	0.86526	0.97815	1.004 ↑	0.0058141	0.022537	0.51123	0.80089 ↓	-0.32033
TAG564-FA204	0.81591	0.95527	1.117 ↑	0.15963	0.024565	0.51123	1.487 ↑	0.57239
SM160	0.060555	0.4362	1.2766 ↑	0.35233	0.024722	0.51123	1.4404 ↑	0.52643
TAG542-FA182	0.69838	0.91456	1.1352 ↑	0.18288	0.025882	0.51123	1.434 ↑	0.52007
CER220	0.9792	0.98616	1.1138 ↑	0.15553	0.028253	0.51123	2.1789 ↑	1.1236
TAG523-FA203	0.98783	0.99072	0.97949 ↓	-0.029896	0.029307	0.51123	1.4785 ↑	0.56412
TAG471-FA181	0.6076	0.88738	0.96988 ↓	-0.044125	0.030319	0.51123	0.83447 ↓	-0.26107
TAG451-FA181	0.60343	0.88434	0.98783 ↓	-0.017671	0.030518	0.51123	0.82418 ↓	-0.27896
TAG523-FA161	0.49301	0.83477	1.0035 ↑	0.0050856	0.03167	0.51123	1.8816 ↑	0.91196
TAG521-FA160	0.12591	0.54053	1.3115 ↑	0.39118	0.033322	0.51123	1.8712 ↑	0.90398
ANTHRANILIC ACID_pos_4	0.010778	0.30971	1.7307 ↑	0.79138	0.035273	0.51123	0.65952 ↓	-0.60052
TAG543-FA161	0.055942	0.43372	0.58385 ↓	-0.77634	0.035527	0.51123	1.465 ↑	0.55091
TAG534-FA160	0.86096	0.97815	0.93521 ↓	-0.096642	0.036364	0.51123	1.4131 ↑	0.49882
HOMOCYSTEINE_pos_2	0.00083077	0.080514	0.37503 ↓	-1.4149	0.040291	0.51123	0.58392 ↓	-0.77615
TAG470-FA170	0.11026	0.53251	0.87683 ↓	-0.18963	0.040591	0.51123	0.80787 ↓	-0.3078
TAG541-FA160	0.19849	0.60053	0.88692 ↓	-0.17312	0.041645	0.51123	1.4168 ↑	0.50268
TAG500-FA140	0.068285	0.46065	0.8511 ↓	-0.2326	0.042557	0.51123	0.82893 ↓	-0.27068
TAG567-FA204	0.0011399	0.080743	1.8834 ↑	0.91331	0.043629	0.51123	1.7223 ↑	0.78432
TAG542-FA180	0.044691	0.39704	1.5887 ↑	0.66781	0.047086	0.51123	1.9379 ↑	0.95449
TAG531-FA181	0.039109	0.38654	1.2567 ↑	0.32966	0.048942	0.51123	1.2781 ↑	0.35398
TAG542-FA181	0.085124	0.4961	1.4516 ↑	0.53769	0.051191	0.51123	1.8945 ↑	0.92181
TAG470-FA140	0.089932	0.49873	0.87058 ↓	-0.19995	0.051599	0.51123	0.82618 ↓	-0.27547
TAG525-FA161	0.42824	0.79826	1.6649 ↑	0.73547	0.051938	0.51123	2.7036 ↑	1.4349
TAG541-FA180	0.022596	0.31041	1.5353 ↑	0.61852	0.053086	0.51123	1.8916 ↑	0.91963
TAG470-FA150	0.09722	0.50224	0.88393 ↓	-0.178	0.053475	0.51123	0.84262 ↓	-0.24705
ADENOSINE PHOSPHOSULFATE_neg_2	0.61355	0.88757	0.96239 ↓	-0.055305	0.053781	0.51123	2.0219 ↑	1.0157

CE204	0.69009	0.91456	0.98164 ↓	-0.02674	0.054074	0.51123	4.1714 ↑	2.0605
TAG484-FA182	0.3529	0.74991	1.1412 ↑	0.19051	0.05449	0.51123	0.75427 ↓	-0.40684
TAG522-FA160	0.17355	0.57755	1.3789 ↑	0.46356	0.055193	0.51123	2.3272 ↑	1.2186
LACTATE_neg_1	0.3251	0.73885	1.6736 ↑	0.74292	0.055442	0.51123	2.0289 ↑	1.0207
TAG524-FA161	0.26284	0.66099	1.5904 ↑	0.6694	0.056067	0.51123	2.5691 ↑	1.3613
TAG451-FA160	0.37556	0.76877	0.94654 ↓	-0.079266	0.057856	0.51123	0.83964 ↓	-0.25216
DAG120/181	0.42584	0.79727	0.91712 ↓	-0.12482	0.058383	0.51123	0.80524 ↓	-0.31252
CER240	0.20598	0.60554	2.5189 ↑	1.3328	0.058433	0.51123	4.1368 ↑	2.0485
TAG502-FA180	0.33183	0.7434	1.1038 ↑	0.14252	0.062135	0.51123	1.3508 ↑	0.43379
TAG440-FA140	0.22649	0.62122	0.90369 ↓	-0.14611	0.067994	0.51123	0.85128 ↓	-0.23229
DAG160/181	0.63003	0.90045	0.98116 ↓	-0.027444	0.068448	0.51123	0.8351 ↓	-0.25997
TAG522-FA181	0.12582	0.54053	1.325 ↑	0.40599	0.071266	0.51123	2.2336 ↑	1.1594
TAG522-FA180	0.094649	0.49873	1.6707 ↑	0.74046	0.071638	0.51123	2.1273 ↑	1.089
TAG564-FA181	0.095052	0.49873	1.546 ↑	0.6285	0.072057	0.51123	1.8379 ↑	0.87803
TAG562-FA201	0.0346	0.35012	1.3665 ↑	0.45051	0.073396	0.51123	1.4399 ↑	0.526
TAG565-FA181	0.026159	0.31041	2.5025 ↑	1.3234	0.074315	0.51123	2.5195 ↑	1.3331
TAG542-FA160	0.9715	0.98616	1.0646 ↑	0.090286	0.075511	0.51123	1.6527 ↑	0.72483
TAG501-FA160	0.099267	0.50224	1.2361 ↑	0.30577	0.076784	0.51123	1.7452 ↑	0.8034
TAG502-FA182	0.46225	0.8244	1.208 ↑	0.27256	0.076884	0.51123	1.6327 ↑	0.70722
TAG462-FA182	0.89257	0.97842	0.99989 ↓	-0.00015971	0.078626	0.51123	0.85709 ↓	-0.22249
TAG503-FA140	0.11654	0.53256	1.2794 ↑	0.3555	0.078777	0.51123	1.8994 ↑	0.92558
DAG160/161	0.056302	0.43372	0.81457 ↓	-0.29588	0.078895	0.51123	0.81287 ↓	-0.2989
TAG450-FA140	0.12427	0.54053	0.87457 ↓	-0.19335	0.079531	0.51123	0.8363 ↓	-0.2579
TAG543-FA181	0.40341	0.77932	1.2773 ↑	0.35305	0.080118	0.51123	1.6481 ↑	0.72084
TAG561-FA160	0.56273	0.86967	1.1499 ↑	0.20149	0.080686	0.51123	1.7216 ↑	0.78378
TAG440-FA160	0.55261	0.86029	0.95767 ↓	-0.062399	0.081305	0.51123	0.85617 ↓	-0.22404
TAG420-FA120	0.16756	0.57186	0.86518 ↓	-0.20893	0.081621	0.51123	0.81991 ↓	-0.28646
FFA160	0.57724	0.86994	0.96068 ↓	-0.057867	0.086666	0.51123	0.77382 ↓	-0.36994
TAG463-FA141	0.013651	0.31041	0.7454 ↓	-0.42391	0.0876	0.51123	0.80883 ↓	-0.30609
TAG460-FA160	0.32343	0.73885	0.93515 ↓	-0.096726	0.088169	0.51123	0.89055 ↓	-0.16723
TAG563-FA201	0.32289	0.73885	1.2545 ↑	0.32714	0.088652	0.51123	1.5019 ↑	0.58674
TAG567-FA180	0.34018	0.74524	1.0534 ↑	0.075029	0.089157	0.51123	0.80431 ↓	-0.31417
TAG470-FA160	0.17661	0.57755	0.89778 ↓	-0.15557	0.089338	0.51123	0.858 ↓	-0.22094
TAG510-FA160	0.47973	0.82568	1.0556 ↑	0.078045	0.089645	0.51123	0.85264 ↓	-0.22999
TAG471-FA170	0.35119	0.74991	0.90002 ↓	-0.15197	0.093143	0.51123	0.75764 ↓	-0.40042
TAG523-FA160	0.64541	0.90045	1.516 ↑	0.60026	0.093387	0.51123	2.3168 ↑	1.2122
TAG527-FA160	0.53424	0.84948	1.0537 ↑	0.0754	0.093721	0.51123	0.8449 ↓	-0.24314
TAG543-FA180	0.25778	0.65998	1.5472 ↑	0.62965	0.094652	0.51123	1.7762 ↑	0.8288
TAG512-FA150	0.058169	0.43372	1.3139 ↑	0.3939	0.095051	0.51123	1.6226 ↑	0.69833

TAG440-FA120	0.51162	0.84511	0.93894	-0.090897	0.096095	0.51123	0.86704	-0.20584
TAG460-FA140	0.40778	0.78183	0.94462	-0.082199	0.097406	0.51123	0.89054	-0.16725
TAG523-FA181	0.43564	0.8085	1.4977	0.58272	0.097649	0.51123	2.3174	1.2125
OROTATE_neg_1	0.029517	0.31041	0.56329	-0.82805	0.098946	0.51123	0.82506	-0.27743
TAG502-FA160	0.46864	0.82568	1.3603	0.44395	0.099306	0.51123	2.0249	1.0179
METHIONINE_pos_1	0.19551	0.5978	0.67596	-0.56499	0.09947	0.51123	0.87338	-0.19532
TAG521-FA180	0.044416	0.39704	1.4338	0.51981	0.099477	0.51123	1.7988	0.84704
TAG441-FA161	0.38078	0.76877	0.92376	-0.11441	0.099762	0.51123	0.77616	-0.36558
TAG530-FA160	0.58236	0.86994	1.0153	0.021952	0.099865	0.51123	0.81759	-0.29055
TAG462-FA141	0.16192	0.56567	0.87627	-0.19056	0.10104	0.51123	0.83889	-0.25345
TAG543-FA182	0.27194	0.66919	1.7477	0.80546	0.10855	0.54277	2.1749	1.121
1-METHYLADENOSINE_pos_1	0.95405	0.98616	1.0038	0.0054521	0.11051	0.54488	0.88409	-0.17773
TAG450-FA160	0.07772	0.48415	0.86181	-0.21456	0.11334	0.54488	0.87202	-0.19756
TAG523-FA182	0.58597	0.86994	1.5435	0.62623	0.11461	0.54488	2.3677	1.2435
TAG400-FA120	0.15124	0.56567	0.84478	-0.24335	0.11567	0.54488	0.80705	-0.30928
TAG544-FA181	0.84208	0.97251	1.456	0.542	0.11574	0.54488	1.6461	0.71905
TAG564-FA201	0.025278	0.31041	1.836	0.87659	0.11729	0.54488	1.7229	0.78486
TAG483-FA161	0.44006	0.81316	0.89191	-0.16502	0.11822	0.54488	0.81467	-0.29571
TAG491-FA140	0.23934	0.63872	0.90596	-0.14249	0.12557	0.54488	0.83057	-0.26782
TAG490-FA170	0.14341	0.56567	0.90125	-0.15	0.12574	0.54488	0.88723	-0.17261
TAG566-FA160	0.029945	0.31041	1.1645	0.2197	0.12709	0.54488	1.1784	0.23682
TAG546-FA160	0.15633	0.56567	1.4375	0.52353	0.12894	0.54488	1.3931	0.47829
TAG523-FA180	0.00094722	0.080514	2.0347	1.0248	0.13073	0.54488	1.9901	0.99281
DAG181/181	0.46007	0.8244	0.95417	-0.067689	0.13165	0.54488	0.8853	-0.17576
TAG482-FA182	0.14289	0.56567	1.086	0.11902	0.13295	0.54488	1.2154	0.28149
TAG514-FA182	0.092202	0.49873	1.2687	0.34336	0.13317	0.54488	1.4481	0.53416
TAG512-FA170	0.97757	0.98616	1.0307	0.043598	0.13545	0.54488	1.2838	0.36043
TAG583-FA181	0.17901	0.57997	1.3521	0.43522	0.13651	0.54488	1.7753	0.82806
CE181	0.21546	0.60821	1.1016	0.13958	0.1371	0.54488	3.1239	1.6433
TAG420-FA140	0.2368	0.63696	0.89829	-0.15474	0.1372	0.54488	0.86447	-0.21011
TAG441-FA140	0.39416	0.7769	0.94799	-0.077058	0.13836	0.54488	0.80996	-0.30408
TAG512-FA182	0.05491	0.43372	1.4509	0.53692	0.13866	0.54488	1.6209	0.69681
TAG544-FA182	0.86015	0.97815	1.5725	0.6531	0.13922	0.54488	1.7688	0.82277
TAG524-FA181	0.34835	0.74884	1.3959	0.4812	0.13967	0.54488	1.8136	0.85883
TAG441-FA120	0.69837	0.91456	0.96871	-0.04586	0.13975	0.54488	0.79348	-0.33374
TAG422-FA120	0.027026	0.31041	0.47752	-1.0664	0.14129	0.54589	1.1806	0.2395
TAG421-FA140	0.306	0.71851	0.92833	-0.10729	0.14438	0.54709	0.89936	-0.15303
TAG490-FA160	0.17582	0.57755	0.91039	-0.13544	0.14639	0.54709	0.90099	-0.15041
TAG503-FA182	0.15987	0.56567	1.2267	0.29482	0.14671	0.54709	1.6514	0.72371

TAG400-FA140	0.26281	0.66099	0.86997	-0.20096	0.14685	0.54709	0.8422	-0.24777
TAG462-FA161	0.48582	0.8292	0.92269	-0.11609	0.14827	0.54709	0.79185	-0.3367
TAG567-FA160	0.090767	0.49873	1.0196	0.027989	0.15142	0.54709	0.71542	-0.48314
TAG510-FA170	0.58747	0.86994	0.95229	-0.070533	0.1515	0.54709	0.91159	-0.13354
TAG521-FA181	0.086549	0.49707	1.3155	0.39564	0.153	0.54709	1.681	0.74929
METHYL PHENYLACETATE_neg_3	0.21609	0.60821	0.3492	-1.5179	0.15329	0.54709	1.4383	0.52435
TAG513-FA150	0.66644	0.907	1.5715	0.65217	0.15602	0.54709	2.3248	1.2171
TAG522-FA182	0.094908	0.49873	1.6914	0.75821	0.15675	0.54709	2.0697	1.0494
TAG505-FA160	0.35824	0.75373	1.0472	0.066475	0.15705	0.54709	0.77559	-0.36664
DAG140/181	0.22762	0.62122	0.8602	-0.21726	0.16027	0.55378	0.87106	-0.19916
ASPARTATE_pos_3	0.86058	0.97815	0.80378	-0.31513	0.16633	0.56375	1.1634	0.21831
TAG502-FA161	0.73726	0.92978	0.98841	-0.016814	0.1674	0.56375	1.3533	0.43645
TAG587-FA160	0.79411	0.94763	0.9954	-0.0066447	0.16822	0.56375	0.86991	-0.20106
TAG551-FA160	0.87839	0.97842	0.77047	-0.37619	0.16961	0.56375	1.2429	0.31371
AMINOADIPATE_pos_1	0.40873	0.78183	0.95384	-0.068184	0.16979	0.56375	0.79892	-0.32387
TAG520-FA200	0.63315	0.90045	0.96393	-0.053005	0.17261	0.56869	0.71101	-0.49207
TAG461-FA161	0.53496	0.84948	0.91943	-0.1212	0.18008	0.57493	0.81224	-0.30003
TAG525-FA225	0.19282	0.59695	0.87785	-0.18796	0.18115	0.57493	0.86243	-0.21352
DAG161/181	0.05969	0.4362	0.76049	-0.395	0.18246	0.57493	0.87441	-0.19362
TAG471-FA140	0.2772	0.6714	0.89647	-0.15767	0.1837	0.57493	0.82113	-0.28432
TAG514-FA161	0.64223	0.90045	0.89902	-0.15358	0.18388	0.57493	0.88785	-0.17161
LCER160	0.085212	0.4961	0.81414	-0.29664	0.18463	0.57493	0.8489	-0.23634
FFA181	0.5127	0.84511	0.95224	-0.070602	0.1849	0.57493	0.61241	-0.70742
CYSTEINE_neg_5	0.76056	0.94709	0.97633	-0.034558	0.18533	0.57493	1.6096	0.68671
TAG526-FA181	0.64622	0.90045	1.054	0.075816	0.18929	0.58163	0.81094	-0.30233
DAG160/204	0.94893	0.98616	0.79754	-0.32638	0.19075	0.58163	1.5305	0.61403
TAG460-FA120	0.71697	0.91744	0.97097	-0.042502	0.19159	0.58163	0.91869	-0.12235
FFA180	0.87314	0.97842	1.0123	0.01769	0.19568	0.58613	0.82324	-0.28062
BIOTIN_pos_4	0.97581	0.98616	0.88633	-0.17408	0.1997	0.58613	1.0757	0.10529
TAG463-FA161	0.27635	0.6714	0.7953	-0.33043	0.20027	0.58613	0.91553	-0.12732
TAG501-FA180	0.051117	0.42597	1.215	0.28091	0.20124	0.58613	1.2853	0.36216
MALONYL-COA_pos_1	0.044842	0.39704	1.4725	0.55825	0.20403	0.58613	1.3494	0.43234
TAG480-FA160	0.40129	0.77932	0.95457	-0.067072	0.20445	0.58613	0.87931	-0.18556
TAG503-FA181	0.13277	0.55322	1.1018	0.13984	0.20557	0.58613	1.243	0.31386
TAG582-FA181	0.017103	0.31041	1.79	0.83999	0.20702	0.58613	1.8262	0.86886
TAG513-FA182	0.028543	0.31041	1.5139	0.59822	0.20731	0.58613	1.7027	0.76784
TAG442-FA161	0.17666	0.57755	0.84407	-0.24457	0.2078	0.58613	0.81803	-0.28977
TAG512-FA160	0.8887	0.97842	1.0116	0.016688	0.20825	0.58613	0.8541	-0.22753
TAG492-FA150	0.76823	0.94709	1.0374	0.053031	0.21205	0.58648	1.1439	0.19391

TAG502-FA181	0.1304	0.5487	1.1464	0.1971	0.21214	0.58648	1.4728	0.55858
TAG511-FA150	0.86535	0.97815	1.0279	0.039652	0.21327	0.58648	1.2792	0.3552
TAG461-FA141	0.01166	0.30971	0.78077	-0.35702	0.21516	0.58648	0.9084	-0.1386
CER160	0.78055	0.94763	1.2038	0.26765	0.21527	0.58648	2.5575	1.3547
MESACONIC ACID_pos_1	0.31038	0.72361	0.72214	-0.46964	0.22154	0.59451	1.3918	0.4769
TAG524-FA160	0.71225	0.91456	1.4319	0.51795	0.22167	0.59451	1.4725	0.55825
TAG532-FA170	0.57453	0.86994	0.95192	-0.071082	0.22242	0.59451	1.2001	0.2631
DAG160/160	0.95751	0.98616	1.0093	0.01331	0.2249	0.59501	0.78332	-0.35233
TAG511-FA160	0.15713	0.56567	0.92962	-0.10528	0.22746	0.59501	1.1191	0.16229
TAG504-FA182	0.3792	0.76877	1.1634	0.21832	0.228	0.59501	1.3775	0.46202
TAG544-FA183	0.39667	0.7769	1.4385	0.52456	0.22821	0.59501	1.2807	0.35699
TAG525-FA182	0.95324	0.98616	1.4457	0.53178	0.23058	0.59754	1.5659	0.64702
TAG568-FA204	0.53429	0.84948	1.0658	0.091934	0.23564	0.59786	0.8249	-0.27771
TAG521-FA201	0.71884	0.91744	0.90928	-0.13721	0.23596	0.59786	1.1305	0.17697
TAG480-FA180	0.86538	0.97815	0.98431	-0.022812	0.23597	0.59786	0.93403	-0.098464
TAG533-FA182	0.21503	0.60821	1.2881	0.36524	0.2367	0.59786	1.4112	0.49689
DAG140/182	0.47573	0.82568	0.79373	-0.33328	0.23774	0.59786	0.84782	-0.23817
TAG563-FA202	0.89566	0.97842	1.0403	0.056987	0.24028	0.60071	0.82273	-0.2815
SM240	0.00055593	0.078757	2.3847	1.2538	0.24343	0.60339	0.76802	-0.38078
TAG534-FA182	0.51082	0.84511	1.0597	0.083591	0.24612	0.60339	0.84057	-0.25056
TAG524-FA183	0.92736	0.98532	1.3083	0.38774	0.24638	0.60339	1.563	0.64428
TAG555-FA181	0.56027	0.86903	1.0526	0.07391	0.2505	0.60339	0.84011	-0.25135
TAG471-FA160	0.34368	0.74884	0.89113	-0.1663	0.2512	0.60339	0.85433	-0.22713
TAG503-FA160	0.2125	0.60821	1.4502	0.53626	0.25124	0.60339	1.9573	0.96888
TAG451-FA150	0.33584	0.7434	0.91097	-0.13453	0.25515	0.60339	0.81104	-0.30215
TAG462-FA140	0.70104	0.91456	0.93964	-0.089813	0.25521	0.60339	0.86196	-0.2143
TAG540-FA160	0.22598	0.62122	1.0593	0.08313	0.25547	0.60339	0.73096	-0.45213
ATROLACTIC ACID_neg_2	0.1239	0.54053	0.57065	-0.80932	0.25739	0.60339	1.354	0.43722
PYRIDOXAMINE_pos_1	0.0088346	0.30971	1.5529	0.63499	0.25805	0.60339	0.67669	-0.56344
ALLANTOIN_neg_2	0.70842	0.91456	1.0274	0.038955	0.25839	0.60339	0.95917	-0.060144
DAG180/182	0.18248	0.58265	0.86007	-0.21747	0.26083	0.60501	1.2403	0.31074
ARGININOSUCCINIC ACID_neg_2	0.018969	0.31041	0.56015	-0.83611	0.26194	0.60501	1.0459	0.064713
TAG524-FA182	0.7901	0.94763	1.4869	0.57232	0.26677	0.61285	1.6211	0.69698
TAG565-FA225	0.93936	0.98616	0.96339	-0.053806	0.27037	0.61349	0.8715	-0.19842
N-ACETYLORNITHINE_neg_3	0.1401	0.56567	0.8215	-0.28367	0.2725	0.61349	1.2297	0.29826
TAG490-FA150	0.19021	0.59441	0.92362	-0.11462	0.27256	0.61349	0.92851	-0.10702
TAG567-FA226	0.0022488	0.13654	1.751	0.80821	0.27533	0.61349	1.5023	0.58719
TAG482-FA141	0.20206	0.60053	0.88418	-0.17759	0.27826	0.61349	1.0857	0.11861
PHENYLPROPIOLIC ACID_neg_1	0.0072568	0.30971	1.515	0.59929	0.28064	0.61349	0.80911	-0.3056

TAG543-FA202	0.84866	0.97745	1.047	0.066261	0.28312	0.61349	0.82916	-0.27028
TAG512-FA181	0.41023	0.78183	1.059	0.082721	0.2854	0.61349	0.92805	-0.10773
TAG491-FA161	0.54609	0.85327	0.9111	-0.13431	0.28683	0.61349	0.82722	-0.27365
TAG510-FA180	0.48195	0.82593	1.0455	0.064151	0.28777	0.61349	0.95243	-0.070311
TAG491-FA181	0.90756	0.98112	0.99645	-0.0051269	0.28787	0.61349	1.0554	0.07783
GLUCOSE 1-PHOSPHATE_pos_2	0.24806	0.65077	0.64373	-0.63547	0.28814	0.61349	0.87181	-0.19791
TAG420-FA160	0.78394	0.94763	0.95459	-0.067047	0.28822	0.61349	0.91282	-0.1316
TAG480-FA140	0.64186	0.90045	0.9675	-0.047673	0.28909	0.61349	0.94683	-0.078817
TAG421-FA120	0.16238	0.56567	0.88133	-0.18225	0.28929	0.61349	0.79785	-0.3258
TAG540-FA180	0.7982	0.94763	0.97978	-0.029467	0.29073	0.61349	0.8407	-0.25033
TAG564-FA202	0.7689	0.94709	1.046	0.064925	0.29159	0.61349	0.83655	-0.25748
TAG511-FA181	0.1139	0.53256	1.1563	0.20952	0.2941	0.61572	1.1548	0.20769
TAG564-FA182	0.28468	0.68283	1.7076	0.77201	0.29827	0.61602	2.031	1.0222
TAG502-FA140	0.52484	0.84948	1.0893	0.12339	0.30014	0.61602	1.4279	0.51393
TAG505-FA205	0.388	0.77418	0.93916	-0.090557	0.30453	0.61602	0.90119	-0.1501
TAG460-FA180	0.80944	0.95031	1.0153	0.02188	0.3052	0.61602	0.93718	-0.093602
TAG566-FA202	0.15339	0.56567	1.123	0.16731	0.30634	0.61602	0.85328	-0.2289
TAG532-FA181	0.72818	0.92381	1.0322	0.045672	0.30722	0.61602	0.88407	-0.17776
TAG501-FA161	0.68259	0.91227	1.0057	0.0082388	0.3074	0.61602	1.1219	0.16594
TAG501-FA181	0.50505	0.84511	1.057	0.079982	0.30893	0.61602	1.2818	0.3582
TAG520-FA160	0.80047	0.94763	0.98749	-0.01816	0.31051	0.61602	0.845	-0.24298
TAG565-FA202	0.66602	0.907	1.0528	0.074216	0.31174	0.61602	0.83237	-0.26471
L-CARNITINE_pos_1	0.050559	0.42597	0.47649	-1.0695	0.31276	0.61602	0.8066	-0.31007
4-AMINOBENZOIC ACID_pos_1	0.45589	0.8244	1.2684	0.34296	0.31555	0.61602	0.84079	-0.25019
TAG562-FA160	0.20659	0.60554	1.2289	0.29739	0.31699	0.61602	1.5384	0.62145
TAG545-FA182	0.7231	0.92012	1.4836	0.56915	0.31743	0.61602	1.2358	0.30544
BUTYRYL-COA_pos_1	0.67701	0.90766	0.62669	-0.67418	0.31865	0.61602	1.5721	0.65272
3-METHYLAMINO-L-ALANINE_pos_2	0.80364	0.9483	0.98248	-0.025498	0.31898	0.61602	0.82363	-0.27993
TAG545-FA225	0.33535	0.7434	0.91146	-0.13374	0.32004	0.61602	0.8618	-0.21458
TAG471-FA150	0.53694	0.84948	0.90172	-0.14926	0.32114	0.61602	0.85871	-0.21975
TAG442-FA120	0.66929	0.907	0.97794	-0.032176	0.32264	0.61602	0.84422	-0.24431
TAG492-FA160	0.91879	0.98112	1.0194	0.027666	0.32323	0.61602	1.1427	0.19249
TAG492-FA161	0.39587	0.7769	0.88192	-0.18127	0.3269	0.61915	0.83008	-0.26868
TAG555-FA182	0.94592	0.98616	1.0753	0.10467	0.32778	0.61915	0.84334	-0.24581
ACETYLPHOSPHATE_pos_1	0.37313	0.76877	1.2038	0.26759	0.33413	0.62833	0.86084	-0.21619
ACETYL-COA_pos_1	0.18371	0.58265	0.96733	-0.047921	0.33706	0.63106	1.2708	0.34569
TAG472-FA140	0.8595	0.97815	0.95327	-0.069049	0.33905	0.63201	0.81929	-0.28756
TAG545-FA181	0.67418	0.907	1.379	0.46367	0.34513	0.63967	1.1566	0.20987
HCER201	0.75127	0.94186	0.66548	-0.58754	0.34617	0.63967	0.69376	-0.52749

TAG481-FA160	0.523	0.84948	1.0314	0.044628	0.35175	0.64717	1.1075	0.14732
TAG542-FA201	0.16234	0.56567	1.1878	0.2483	0.35452	0.64945	1.3979	0.4833
TAG491-FA150	0.87686	0.97842	1.0268	0.038208	0.3573	0.64995	1.1062	0.14557
TAG482-FA161	0.52944	0.84948	0.88934	-0.16919	0.36019	0.64995	0.84707	-0.23945
ADP_pos_1	0.31413	0.72556	0.98866	-0.016453	0.36076	0.64995	1.2042	0.26805
TAG472-FA182	0.69655	0.91456	1.0018	0.0025886	0.36091	0.64995	0.87701	-0.18934
MEVALONOLACTONE_pos_2	0.95592	0.98616	0.84707	-0.23945	0.36916	0.662	1.0743	0.10333
CE182	0.49224	0.83477	0.45996	-1.1204	0.37856	0.676	7.2083	2.8497
GERANYL-PP_-HPO3_neg_2	0.79502	0.94763	0.93578	-0.095761	0.39315	0.69732	1.195	0.25703
N-ACETYLALANINE_pos_2	0.76522	0.94709	1.0597	0.083667	0.39384	0.69732	1.5383	0.62133
BUTYRYL-COA_neg_2	0.54482	0.85327	0.83118	-0.26677	0.39622	0.69732	1.5296	0.61315
TAG554-FA181	0.88967	0.97842	1.0207	0.029494	0.39789	0.69732	0.83313	-0.26339
TAG483-FA181	0.87504	0.97842	0.99613	-0.0055985	0.40106	0.69732	1.1235	0.16798
SYMMETRIC DIMETHYLARGININE_pos_1	0.97782	0.98616	1.0331	0.046969	0.40351	0.69732	1.3991	0.48445
TAG566-FA225	0.11448	0.53256	1.1163	0.15867	0.40409	0.69732	0.92011	-0.12012
TAG492-FA182	0.34887	0.74884	1.1291	0.17523	0.40659	0.69732	1.2276	0.29579
DAG181/182	0.65256	0.90045	0.98527	-0.021403	0.408	0.69732	0.91303	-0.13127
TAG503-FA161	0.95025	0.98616	1.0103	0.014714	0.40959	0.69732	1.236	0.30568
TAG491-FA170	0.61829	0.89076	0.92131	-0.11824	0.40992	0.69732	0.82326	-0.28057
TAG490-FA180	0.9478	0.98616	0.9946	-0.0078077	0.41071	0.69732	0.95922	-0.060069
TAG587-FA225	0.069515	0.46162	1.0147	0.021117	0.41213	0.69732	0.6592	-0.60122
TAG500-FA180	0.90096	0.9793	1.0117	0.016735	0.41677	0.69732	0.87971	-0.1849
TAG461-FA140	0.66747	0.907	0.95063	-0.073038	0.4177	0.69732	0.88641	-0.17395
TAG421-FA161	0.25977	0.66099	0.92173	-0.11759	0.41804	0.69732	0.80219	-0.31798
TAG504-FA160	0.019008	0.31041	1.3096	0.38912	0.42106	0.69732	1.2199	0.28675
TAG440-FA180	0.78943	0.94763	1.0235	0.033449	0.42303	0.69732	0.93849	-0.09159
TAG400-FA160	0.97532	0.98616	0.98532	-0.021331	0.42313	0.69732	0.94348	-0.083935
TAG442-FA140	0.014235	0.31041	0.60969	-0.71385	0.42332	0.69732	1.0472	0.066497
SM220	0.000026818	0.011398	2.3142	1.2105	0.43064	0.70664	0.992	-0.011584
TAG520-FA180	0.8194	0.95671	0.99094	-0.013133	0.4377	0.71546	0.86288	-0.21277
TAG462-FA181	0.71012	0.91456	1.0885	0.12234	0.44068	0.71759	0.97103	-0.042407
TAG568-FA205	0.68749	0.91456	0.98449	-0.022552	0.4535	0.73564	0.8021	-0.31815
TAG481-FA161	0.67251	0.907	0.93354	-0.099211	0.46045	0.74257	0.89854	-0.15435
TAG483-FA160	0.78927	0.94763	0.97077	-0.042794	0.46126	0.74257	1.2385	0.30865
TAG472-FA150	0.79417	0.94763	0.90351	-0.14638	0.46469	0.74525	0.86258	-0.21327
O-ACETYL SERINE_pos_3	0.53631	0.84948	0.98292	-0.024858	0.47036	0.75091	1.036	0.051046
L-ACETYL CARNITINE_pos_1	0.97146	0.98616	0.90076	-0.15078	0.47175	0.75091	1.1539	0.20648
TAG544-FA180	0.93677	0.98616	1.3423	0.42472	0.48381	0.76724	1.1989	0.26175
CE205	0.67438	0.907	1.0556	0.078076	0.48784	0.77076	2.468	1.3033

TAG563-FA181	0.24777	0.65077	1.0933	0.12865	0.49253	0.77117	0.89035	-0.16755
TAG441-FA160	0.89701	0.97842	1.0221	0.031565	0.49327	0.77117	0.97455	-0.037189
TAG501-FA140	0.12524	0.54053	1.1976	0.26013	0.49512	0.77117	1.1505	0.20232
TAG461-FA180	0.64197	0.90045	1.0694	0.096841	0.49536	0.77117	0.99071	-0.013471
TAG463-FA181	0.20021	0.60053	1.1664	0.22205	0.5045	0.77678	1.1301	0.17644
TAG482-FA160	0.89564	0.97842	0.98286	-0.024937	0.50595	0.77678	1.0743	0.10335
TAG481-FA180	0.47684	0.82568	1.0509	0.071575	0.50626	0.77678	1.0261	0.037211
PIPECOLATE_pos_3	0.45484	0.8244	0.75461	-0.40619	0.50901	0.77678	1.1401	0.18921
TAG441-FA181	0.52323	0.84948	1.1492	0.20067	0.51007	0.77678	0.98086	-0.027881
TAG568-FA160	0.070961	0.46397	0.74672	-0.42136	0.51041	0.77678	1.1541	0.20675
TAG511-FA180	0.023828	0.31041	1.2331	0.30233	0.51322	0.77678	1.1463	0.19701
TAG587-FA180	0.020808	0.31041	1.1229	0.16717	0.51359	0.77678	0.74815	-0.4186
TAG553-FA181	0.53767	0.84948	0.97485	-0.036742	0.51715	0.77818	0.89034	-0.16758
DAG160/182	0.1716	0.57755	0.91397	-0.12978	0.51817	0.77818	0.92312	-0.11542
TAG541-FA200	0.64339	0.90045	1.0262	0.037378	0.52073	0.77926	1.5291	0.61264
TAG421-FA160	0.70207	0.91456	1.0841	0.11643	0.52698	0.78585	1.0018	0.002578
TAG503-FA141	0.71228	0.91456	0.98898	-0.015987	0.53325	0.79242	1.1742	0.23171
CHOLINE_pos_1	0.075417	0.47839	0.42092	-1.2484	0.53639	0.7943	1.1178	0.16063
CE150	0.33297	0.7434	0.92017	-0.12003	0.54231	0.79859	0.89271	-0.16373
SM180	0.16819	0.57186	1.085	0.11765	0.54372	0.79859	0.87068	-0.19979
TAG481-FA140	0.27224	0.66919	1.0897	0.12389	0.54492	0.79859	1.1252	0.17016
TAG522-FA202	0.14703	0.56567	0.8583	-0.22044	0.5508	0.80195	1.075	0.10438
FFA204	0.13619	0.55653	0.81698	-0.29163	0.55099	0.80195	1.1324	0.17936
TAG513-FA161	0.0099529	0.30971	0.65199	-0.61708	0.56215	0.80548	0.9586	-0.060996
N-ACETYLGLUTAMINE_pos_2	0.28599	0.68283	0.84536	-0.24236	0.56231	0.80548	1.373	0.45735
CE160	0.78254	0.94763	1.0354	0.050257	0.56288	0.80548	1.1637	0.2187
TAG492-FA140	0.76742	0.94709	0.92926	-0.10585	0.56555	0.80548	0.99185	-0.0118
TAG461-FA181	0.59941	0.88149	1.0968	0.13326	0.56588	0.80548	0.98977	-0.01484
TAG492-FA181	0.5905	0.8714	0.91758	-0.12409	0.56661	0.80548	0.89933	-0.15308
TAG545-FA183	0.34659	0.74884	1.2682	0.34279	0.56824	0.80548	1.1347	0.18233
TAG561-FA181	0.23044	0.62381	1.0834	0.11555	0.57103	0.80548	0.95019	-0.073705
TAG562-FA180	0.2541	0.65849	1.2121	0.27746	0.57266	0.80548	1.2405	0.31096
SPERMIDINE_pos_2	0.91556	0.98112	1.0182	0.026063	0.57425	0.80548	0.80689	-0.30956
TAG568-FA161	0.098253	0.50224	1.1499	0.20157	0.57588	0.80548	0.95821	-0.061584
TAG493-FA161	0.64992	0.90045	0.92193	-0.11727	0.57616	0.80548	0.8708	-0.19959
TAG512-FA161	0.0087817	0.30971	0.65627	-0.60763	0.58138	0.80582	0.9634	-0.053794
FFA201	0.22665	0.62122	0.88412	-0.17769	0.5815	0.80582	0.97363	-0.038558
TAG589-FA226	0.084658	0.4961	1.5366	0.61978	0.58279	0.80582	1.1854	0.24543
TAG545-FA205	0.5848	0.86994	0.85511	-0.22581	0.58398	0.80582	0.87671	-0.18983

2-HYDROXY-3-METHYLBUTYRIC ACID_p ^c	0.88193	0.97842	0.90997	-0.13611	0.58959	0.81093	0.98204	-0.026145
TAG461-FA160	0.77327	0.94709	0.97917	-0.03037	0.59546	0.81611	0.93019	-0.10441
TAG526-FA160	0.041052	0.39652	1.3942	0.47939	0.60028	0.81611	1.1312	0.1779
TAG525-FA205	0.91301	0.98112	1.0737	0.10253	0.60055	0.81611	1.1991	0.262
TAG567-FA225	0.078603	0.48415	1.0431	0.060917	0.60104	0.81611	0.64328	-0.63649
URIDINE 5-DIPHOSPHATE_neg_2	0.0093381	0.30971	0.53983	-0.88943	0.60402	0.81754	1.0139	0.019965
FFA226	0.15121	0.56567	0.82832	-0.27174	0.60733	0.81942	0.93226	-0.1012
TAG500-FA160	0.97529	0.98616	1.0188	0.026836	0.61385	0.82559	0.90041	-0.15134
TAG442-FA182	0.61066	0.88757	1.0872	0.12065	0.61793	0.82846	1.0018	0.0025802
TAG521-FA161	0.029483	0.31041	0.79878	-0.32414	0.6202	0.82889	1.045	0.063456
TAG523-FA183	0.88563	0.97842	1.0674	0.094083	0.62582	0.8331	1.0394	0.055801
OXOGLUTARATE_neg_2	0.011436	0.30971	2.5043	1.3244	0.62728	0.8331	0.8907	-0.16699
TAG441-FA141	0.8703	0.97842	0.98426	-0.022886	0.63374	0.83653	0.88701	-0.17298
TAG532-FA160	0.16459	0.5687	0.76318	-0.3899	0.6338	0.83653	1.0517	0.072792
TAG461-FA120	0.7584	0.94709	1.0712	0.099253	0.63939	0.83739	0.94164	-0.086746
TAG493-FA160	0.52584	0.84948	0.78727	-0.34507	0.64158	0.83739	1.1777	0.23599
TAG491-FA160	0.975	0.98616	0.98836	-0.01689	0.64379	0.83739	1.0108	0.01548
TAG526-FA182	0.24046	0.63872	1.2349	0.30439	0.64426	0.83739	1.0194	0.027778
DAG181/204	0.028678	0.31041	0.67151	-0.57452	0.6443	0.83739	1.1242	0.16886
ASCORBATE_neg_2	0.10931	0.53251	0.73765	-0.439	0.64811	0.83978	0.79561	-0.32987
FFA241	0.56857	0.86994	0.93372	-0.098935	0.65594	0.84199	0.87944	-0.18535
TAG528-FA161	0.92287	0.983	0.90044	-0.15129	0.6581	0.84199	0.88331	-0.179
TAG482-FA140	0.29782	0.70319	1.0455	0.064199	0.65888	0.84199	1.0744	0.10353
DAG180/181	0.22802	0.62122	0.86148	-0.21511	0.66091	0.84199	0.97144	-0.041809
SM261	0.027958	0.31041	1.6345	0.70885	0.66214	0.84199	0.98469	-0.02226
NADPH_pos_1	0.84075	0.97251	0.95863	-0.060953	0.66289	0.84199	0.64243	-0.63839
4-IMIDAZOLEACETATE_pos_1	0.044438	0.39704	0.56138	-0.83296	0.66582	0.84199	1.1826	0.242
2-KETOHEXANOIC ACID_pos_2	0.91434	0.98112	0.8459	-0.24145	0.66653	0.84199	1.0091	0.013065
TAG482-FA181	0.98838	0.99072	0.9904	-0.013913	0.66765	0.84199	0.99014	-0.014298
TAG546-FA226	0.063156	0.44735	1.3306	0.41208	0.6716	0.84447	0.98521	-0.021498
TAG533-FA160	0.65256	0.90045	1.0493	0.069447	0.67793	0.8482	1.0233	0.033253
TAG563-FA182	0.90907	0.98112	1.2047	0.26869	0.67976	0.8482	1.4835	0.56898
UREIDOSUCCINIC ACID_neg_2	0.9715	0.98616	0.90964	-0.13663	0.68065	0.8482	1.3336	0.41533
FFA202	0.27142	0.66919	0.89649	-0.15763	0.68255	0.8482	0.98147	-0.02698
TAG542-FA202	0.51303	0.84511	1.0579	0.081239	0.68684	0.85104	0.95686	-0.063613
TAG531-FA180	0.73611	0.92978	1.0519	0.072976	0.69318	0.8564	1.0032	0.0045745
TAG462-FA120	0.33874	0.74524	1.1214	0.16526	0.70043	0.86285	0.92425	-0.11365
TAG462-FA160	0.050566	0.42597	0.79281	-0.33495	0.70541	0.86647	1.0145	0.02073
CE161	0.37957	0.76877	0.92525	-0.11209	0.71269	0.8704	0.92264	-0.11615

L-2-HYDROXYGLUTARIC ACID_neg_1	0.065294	0.44981	1.8861	0.91543	0.7127	0.8704	1.021	0.029987
TAG511-FA170	0.20138	0.60053	0.9041	-0.14544	0.71601	0.87194	0.96894	-0.04552
DCER260	0.61399	0.88757	0.99247	-0.010898	0.72066	0.87363	0.94206	-0.086111
N-GLYCYL-L-PROLINE_pos_1	0.77212	0.94709	1.0784	0.10892	0.72191	0.87363	1.0508	0.071493
TAG533-FA170	0.57017	0.86994	0.93801	-0.092332	0.72357	0.87363	1.0361	0.051148
PROPIONYL-COA_pos_1	0.10174	0.50868	1.3275	0.40873	0.72625	0.87426	1.1964	0.25874
TAG482-FA120	0.45151	0.8244	1.1034	0.14194	0.72821	0.87426	1.1659	0.22146
TAG552-FA181	0.31158	0.72361	0.83019	-0.26849	0.73222	0.8766	0.95948	-0.05967
BETAINE_pos_2	0.36864	0.76801	0.80015	-0.32166	0.74072	0.88202	0.96494	-0.051484
TAG546-FA182	0.4636	0.8244	1.4502	0.53629	0.74161	0.88202	0.90009	-0.15185
FFA203	0.16024	0.56567	0.84543	-0.24224	0.74297	0.88202	0.92849	-0.10704
L-DIHYDROOROTIC ACID_neg_1	0.33463	0.7434	0.72602	-0.46192	0.7574	0.89665	1.1545	0.20732
HCER160	0.11185	0.53256	0.71283	-0.48837	0.75954	0.89668	0.90171	-0.14926
MYOINOSITOL_neg_3	0.8055	0.9483	1.0603	0.084504	0.77309	0.90242	0.99934	-0.0009508
DAG161/182	0.025004	0.31041	0.59619	-0.74616	0.77343	0.90242	1.1024	0.14062
TAG483-FA120	0.01534	0.31041	1.3103	0.38988	0.77454	0.90242	1.1703	0.22683
TAG541-FA181	0.38284	0.76877	1.0802	0.1113	0.77722	0.90242	0.93592	-0.095539
TAG481-FA181	0.4587	0.8244	1.0729	0.10148	0.77948	0.90242	1.0798	0.11072
MESACONIC ACID_neg_1	0.66417	0.907	1.2123	0.27778	0.7813	0.90242	1.0882	0.12198
FFA205	0.29663	0.70319	0.8646	-0.2099	0.78298	0.90242	1.0814	0.11286
TAG525-FA181	0.21391	0.60821	1.089	0.12297	0.78531	0.90242	0.98068	-0.028144
CE140	0.13475	0.55602	1.1445	0.19471	0.78555	0.90242	0.88331	-0.17901
TAG421-FA181	0.57802	0.86994	1.1272	0.17268	0.78564	0.90242	1.0254	0.036238
TAG524-FA180	0.27804	0.6714	1.1183	0.16129	0.7949	0.90713	0.98499	-0.021819
TAG442-FA160	0.35597	0.75267	0.9091	-0.1375	0.79515	0.90713	1.0906	0.12517
N-ACETYLALANINE_neg_1	0.10636	0.5256	1.5384	0.62146	0.79614	0.90713	0.79986	-0.32218
TAG503-FA183	0.090845	0.49873	1.1542	0.20692	0.79981	0.90799	0.97278	-0.039807
SM241	0.024886	0.31041	1.4469	0.53298	0.80302	0.90799	0.86877	-0.20295
CE180	0.99508	0.99508	0.99321	-0.0098355	0.8033	0.90799	1.0885	0.12228
TAG543-FA183	0.054902	0.43372	0.80123	-0.31971	0.80832	0.91123	#N/A	#N/A
TAG546-FA181	0.50776	0.84511	1.2896	0.36696	0.81456	0.91215	0.92352	-0.11479
TAG442-FA181	0.39206	0.7769	1.1846	0.24442	0.81474	0.91215	1.052	0.073179
FFA141	0.25745	0.65998	0.86673	-0.20635	0.81691	0.91215	1.1933	0.25502
CE141	0.58211	0.86994	0.92034	-0.11976	0.81772	0.91215	0.858	-0.22096
TAG492-FA170	0.79824	0.94763	0.868	-0.20423	0.82557	0.91762	0.90462	-0.14461
CITRACONIC ACID_neg	0.18013	0.57997	1.3072	0.38653	0.83375	0.91762	0.96854	-0.046109
TAG481-FA141	0.38348	0.76877	0.86498	-0.20926	0.83465	0.91762	1.0145	0.020801
TAG483-FA141	0.26975	0.66919	0.85146	-0.23199	0.83585	0.91762	0.97642	-0.034432
TAG422-FA182	0.40259	0.77932	1.0994	0.13675	0.84062	0.91762	1.1811	0.24014

TAG534-FA170	0.47618	0.82568	0.86791 ↓	-0.20438	0.8409	0.91762	0.93618 ↓	-0.095137	
INDOLEACRYLIC ACID_pos_1	0.42262	0.79475	1.2456 ↑	0.31686	0.84221	0.91762	0.71994 ↓	-0.47405	
TAG545-FA180	0.64909	0.90045	1.3713 ↑	0.45555	0.84252	0.91762	0.8438 ↓	-0.24502	
TAG483-FA140	0.7463	0.9384	1.047 ↑	0.066266	0.84449	0.91762	1.0838 ↑	0.11609	
TAG502-FA141	0.38067	0.76877	1.0322 ↑	0.04573	0.84474	0.91762	1.0553 ↑	0.077621	
TAG483-FA182	0.95053	0.98616	0.98316 ↓	-0.024499	0.84637	0.91762	0.96376 ↓	-0.053255	
N-GLYCYL-L-PROLINE_neg_3	0.45341	0.8244	0.94472 ↓	-0.082041	0.85827	0.92449	0.81145 ↓	-0.30142	
TAG544-FA224	0.12254	0.54053	0.81506 ↓	-0.29503	0.85942	0.92449	0.95867 ↓	-0.060887	
TAG525-FA160	0.82445	0.95998	1.3736 ↑	0.45796	0.85997	0.92449	0.98816 ↓	-0.017177	
RIBOFLAVIN_pos_1	0.41339	0.78434	1.0741 ↑	0.1031	0.86141	0.92449	1.173 ↑	0.23017	
METANEOPHRINE_pos_1	0.017648		0.31041	0.66907 ↓	-0.57978	0.86656	0.92767	1.0786 ↑	0.10913
XANTHURENIC ACID_pos_2	0.15476	0.56567	0.53441 ↓	-0.90397	0.8707	0.92977	0.92844 ↓	-0.10712	
TAG525-FA183	0.46558	0.82447	1.2962 ↑	0.37424	0.88199	0.93946	1.0576 ↑	0.080828	
TAG531-FA170	0.70568	0.91456	0.91366 ↓	-0.13027	0.88772	0.94188	0.97392 ↓	-0.038119	
FFA182	0.49753	0.83908	0.93556 ↓	-0.096096	0.88869	0.94188	0.8759 ↓	-0.19116	
XANTHOSINE_neg_1	0.57485	0.86994	1.1985 ↑	0.26127	0.89488	0.94421	1.2451 ↑	0.31631	
TAG504-FA161	0.42209	0.79475	1.0322 ↑	0.04579	0.89551	0.94421	1.0601 ↑	0.084252	
TAG546-FA183	0.57075	0.86994	1.3872 ↑	0.47219	0.89798	0.94421	0.8979 ↓	-0.15537	
TAG481-FA120	0.47672	0.82568	1.0917 ↑	0.12653	0.89978	0.94421	1.0741 ↑	0.10308	
TAG463-FA182	0.18526	0.58323	1.1217 ↑	0.16569	0.9053	0.94568	1.0156 ↑	0.022275	
N-ACETYLPUTRESCINE_pos_1	0.19383	0.59695	0.69742 ↓	-0.51991	0.90563	0.94568	1.2942 ↑	0.37207	
TAG587-FA182	0.0087084		0.30971	1.5551 ↑	0.63697	0.91122	0.94919	1.0224 ↑	0.031983
CE225	0.69799	0.91456	1.0866 ↑	0.11984	0.91506	0.95086	1.1123 ↑	0.15357	
PYROPHOSPHATE_neg_3	0.022643		0.31041	0.40345 ↓	-1.3095	0.91967	0.95329	1.4951 ↑	0.58025
TAG493-FA182	0.83831	0.97251	0.94598 ↓	-0.080123	0.92189	0.95329	0.95878 ↓	-0.06073	
2-PHOSPHOGLYCERATE_pos_4	0.91663	0.98112	0.94756 ↓	-0.077706	0.92599	0.9552	1.1011 ↑	0.13892	
NORMETANEOPHRINE_pos_1	0.54123	0.85194	1.0721 ↑	0.10042	0.93482	0.96198	1.0322 ↑	0.045779	
FFA225	0.085045	0.4961	0.81424 ↓	-0.29648	0.94235	0.9662	1.0798 ↑	0.11078	
TAG531-FA160	0.16096	0.56567	0.70428 ↓	-0.50577	0.94347	0.9662	0.98068 ↓	-0.028144	
TAG547-FA182	0.36611	0.76648	1.4154 ↑	0.50119	0.94807	0.96858	0.81727 ↓	-0.29111	
DAG181/226	0.15058	0.56567	0.7952 ↓	-0.3306	0.95211	0.97038	1.0357 ↑	0.050639	
TAG547-FA183	0.44299	0.81502	1.4076 ↑	0.49324	0.96791	0.98412	0.84267 ↓	-0.24696	
TAG589-FA181	0.47986	0.82568	1.0365 ↑	0.05174	0.97387	0.98781	0.99269 ↓	-0.010578	
2-HYDROXY-3-METHYLBUTYRIC ACID_n	0.89784	0.97842	0.87792 ↓	-0.18783	0.98733	0.99881	0.86312 ↓	-0.21237	
IMIDAZOLE_pos_1	0.95872	0.98616	0.89246 ↓	-0.16414	0.99114	0.99881	0.76898 ↓	-0.37899	
INDOLE-3-CARBOXYLIC ACID_pos_3	0.64397	0.90045	1.336 ↑	0.41796	0.99571	0.99881	1.4863 ↑	0.57175	
CE170	0.073825	0.47539	0.69734 ↓	-0.52007	0.99689	0.99881	1.0935 ↑	0.12892	
TAG504-FA181	0.25189	0.65676	1.1136 ↑	0.15519	0.99873	0.99881	1.0009 ↑	0.0012678	
L-ORNITHINE_pos_1	0.12934	0.5487	1.7142 ↑	0.77756	0.99881	0.99881	1.0104 ↑	0.014863	