

Supplementary Table S5. Differentially abundant metabolites in enriched pathways for correlation analysis.

Pathway	Peak	Con1	Con2	Con3	Con4	Con5	Con6	Dis1	Dis2	Dis3	Dis4	Dis5	Dis6
Alanine,	oxalacetic acid	0.00069376	0.000775381	0.00111535	0.00101158	0.000985463	0.00078927	0.001663509	0.000925736	0.001222204	0.001200864	0.00151636	0.001318499
aspartate and aspartic acid		1.245602617	1.115647598	1.169873277	1.344638615	1.315988664	1.194687867	0.997435413	1.207555147	0.894560244	1.174310246	1.041881507	0.969536812
glutamate	glutamine	0.006504834	0.004754972	0.002107914	0.002702488	0.003454423	0.002677228	0.010017281	0.009867015	0.011405403	0.007461883	0.006345433	0.007745412
metabolism													
Valine,	alpha-ketoisocaproic	2.32584E-08	2.43822E-08	2.46245E-08	2.68561E-08	2.81891E-08	3.30552E-08	0.001808934	0.002014879	2.86198E-08	0.002908737	2.75615E-08	0.002552014
leucine and	acid												
isoleucine	valine	1.347067655	0.95798684	1.100705123	1.328439253	1.319294501	1.009303362	1.969645684	1.828905948	1.73089642	1.703842288	1.646863532	1.784712606
biosynthesis	Isoleucine	0.756467046	0.51328024	0.615290369	0.7644325	0.745037067	0.527943092	1.163672517	0.997390744	0.950799299	1.004283569	0.939901522	0.998628549
	threonine	0.639825259	0.477412263	0.511098378	0.57224298	0.607332733	0.482803525	0.895383097	1.064144738	0.726852101	0.871724753	0.73855603	0.845096511
Arginine and sarcosine													
proline													
metabolism													
		0.026200365	0.021030481	0.015067966	0.020069122	0.026695531	0.025839572	0.027126155	0.031256197	0.039481909	0.032399634	0.023963886	0.026426527
	proline	1.809536368	1.380092931	1.414305467	1.614864375	1.732238802	1.294432694	2.129820516	2.078096425	1.869587314	1.946557224	2.13341911	2.038305959
4-Acetamidobutyric													
acid		0.443652301	0.368966921	0.322735892	0.444951852	0.468452029	0.298157594	0.600173983	0.522831342	0.445218888	0.608786123	0.595380281	0.538194332
trans-4-hydroxy-L-													
proline		0.003554071	0.003723472	0.003975702	0.003903037	0.005710748	0.004124704	0.001106948	0.001452241	0.002328569	0.002758136	0.003406049	0.002000451
creatine		0.652634916	0.639044267	0.533070728	0.601087609	0.660223668	0.491189179	0.53004083	0.449339273	0.491131763	0.403062037	0.456401113	0.442155112
1,3-diaminopropane		0.022866514	0.01161995	0.01995071	0.016753506	0.010162768	0.00955513	0.089788665	0.077093926	0.093719784	0.080220754	0.060162905	0.082256289
Taurine and	alpha-ketoglutaric	2.32584E-08	2.43822E-08	2.46245E-08	2.68561E-08	2.81891E-08	3.30552E-08	0.002276523	0.003163532	2.86198E-08	2.39197E-08	0.002864803	0.004999436
hypotaurine	acid												
metabolism	taurine	0.264335014	0.151974736	0.161436719	0.166132743	0.208823474	0.288137022	0.394439899	0.573998774	0.776059348	0.309253305	0.487448998	0.691151523
Glutathione	oxoproline	0.978397115	1.133065815	0.957530716	1.163982759	1.134511874	1.14671496	0.839841805	0.935837837	0.814526421	0.964857603	0.810364122	0.838911237
metabolism	glutathione	0.049523975	0.071254053	0.027050411	0.048412323	0.034008427	0.012808341	0.006364589	0.008683468	0.003772334	0.009364897	0.008492777	0.006441679
others	phenylalanine	0.643322328	0.399856889	0.426208142	0.555333741	0.572795858	0.358442253	0.772510391	0.72916533	0.613069789	0.789921659	0.668087546	0.681186762
	beta-												
Mannosylglycerate		0.04469574	0.054241862	0.023946093	0.036955535	0.037968563	0.02897247	0.068155819	0.073446344	0.040582493	0.078567108	0.071773785	0.088513879
uric acid		0.318763088	0.16704227	0.192946018	0.288602988	0.434143096	0.208486175	1.188426024	1.27935287	1.237294221	0.783340446	1.135820205	1.244276545
guanine		0.02759396	0.036703792	0.022421724	0.026228451	0.034371404	0.026652261	0.014538958	0.026263732	0.016747178	0.015715016	0.014682808	0.013255997
2-hydroxybutanoic													
acid		0.019864606	0.018336624	0.017340744	0.020016743	0.022931839	0.024881757	0.050434261	0.049984603	0.04938632	0.048128579	0.040065003	0.045396672
thymine		0.001308585	0.001536876	0.001792925	0.001300083	0.001706634	0.001057195	0.005353691	0.004166249	0.004930615	0.004783609	0.005803243	0.007113627
2-Methylglutaric Acid		0.001831177	0.002012992	0.00178918	0.00207314	0.002310606	0.001925229	0.005943169	0.005153906	0.005031716	0.004946772	0.005161338	0.006102723
malonamide		0.017655895	0.012234328	0.012825913	0.012497339	0.009715402	0.01040834	0.052679766	0.056004286	0.056889343	0.056900387	0.041812956	0.054350923
5,6-dihydrouracil		0.027501838	0.017922347	0.022768039	0.022963891	0.022315751	0.020268934	0.111049907	0.098244591	0.107836882	0.068634962	0.083435387	0.126321175

N-Acetyl-L-leucine	2.32584E-08	2.43822E-08	2.46245E-08	2.68561E-08	0.001131378	3.30552E-08	0.001634826	0.001857144	0.001167163	0.001911199	0.001259605	0.001308118
3-Phenyllactic acid	2.32584E-08	2.43822E-08	2.46245E-08	2.68561E-08	2.81891E-08	3.30552E-08	0.009178447	0.002247432	0.009872479	0.00399107	0.006074694	0.00474583
2,4-diaminobutyric acid	0.022603107	0.015262196	0.011330833	0.016540789	0.018036951	0.01654055	0.066925656	0.07017107	0.067588549	0.072944019	0.074913143	0.060498922
4- hydroxyphenylacetic acid	2.32584E-08	2.43822E-08	2.46245E-08	2.68561E-08	2.81891E-08	3.30552E-08	0.00163529	0.00269735	0.001217355	0.001694655	0.002160488	0.001116437
N-formyl-L- methionine	2.32584E-08	2.43822E-08	2.46245E-08	2.68561E-08	2.81891E-08	3.30552E-08	0.001592506	0.001630243	0.001072844	0.001680693	0.001405279	0.001103393
3,6-Anhydro-D- galactose	0.096815713	0.092099465	0.065536342	0.084598038	0.092098967	0.071028205	0.007144997	0.005744668	0.00837207	0.006746821	0.010048667	0.007332523
canavanine	2.32584E-08	2.43822E-08	2.46245E-08	2.68561E-08	2.81891E-08	3.30552E-08	0.020799683	0.01303014	0.009838741	0.015776946	0.016584108	0.009319571
noradrenaline	0.000555252	2.43822E-08	2.46245E-08	2.68561E-08	2.81891E-08	3.30552E-08	2.72188E-08	0.005267914	0.002794963	0.00336318	0.003401643	0.002235354
