

μmol/mmo	U01	U02	Leu	Val	Ile	3-HIBA	Erythro 2,3	Threo 2,3	I
CTRL01	0.634381	7.499193	9.239957	5.445271	1.034077	18.12564	11.97423	104.7577	
CTRL02	2.679074	3.860739	7.999585	8.371851	2.038517	21.54117	19.84516	38.95042	
CTRL03	3.4872	0.547643	5.689067	4.987828	0.921144	25.1746	19.04982	92.18963	
CTRL04	5.295638	0.930079	6.102479	6.578249	1.348958	18.81439	26.20267	33.92485	
CTRL05	7.91908	22.76864	7.189993	9.303837	1.013977	24.21406	14.87547	51.74935	
CTRL06	3.209934	4.030624	12.78032	7.100484	2.257109	51.36525	22.90411	97.11906	
CTRL07	2.365328	2.860728	10.31406	10.37773	3.105057	28.34826	11.93528	87.52176	
CTRL08	4.418674	5.155479	8.119523	6.413308	1.623087	23.09549	17.06276	67.36322	
CTRL09	3.808513	2.137792	6.691537	4.836889	0.833009	20.82503	16.49137	49.38289	
CTRL10	1.997284	0.713739	6.727272	4.478012	1.404554	16.00738	12.00456	58.62148	
CTRL11	3.533398	4.710815	5.206913	5.215385	0.425323	21.16194	15.16685	45.5283	
CTRL12	3.523315	2.617915	11.63863	13.27786	2.527797	39.08868	23.89322	75.26321	
CTRL13	1.510185	7.890436	7.198624	6.178518	1.150176	35.10649	27.186	59.99925	
Worker01	3.271486	2.135283	5.17871	6.241449	1.776369	15.12277	21.56025	41.58389	
Worker02	5.35156	3.6942	4.303496	4.185083	0.350382	14.50135	17.07034	62.91726	
Worker03	3.512577	51.39131	4.004551	5.133527	0.671349	10.29276	13.20761	24.69993	
Worker04	9.212738	3.090961	5.562122	5.850468	1.325538	25.80588	19.62524	60.97744	
Worker05	5.955491	5.714439	3.671153	4.155787	0.559745	7.833911	10.75323	26.05136	
Worker06	3.301568	3.371992	3.581983	5.673287	1.397096	15.53336	10.42717	44.74959	
Worker07	3.556274	2.176633	6.868205	5.095338	0.987973	14.04775	8.406945	44.88648	
Worker08	4.336624	7.603934	3.060559	3.914622	0.265402	17.01296	15.45891	68.29942	
Worker09	3.216677	3.708046	1.445168	3.703145	0.881866	7.66663	15.24348	22.15789	
Worker10	2.319323	4.359566	6.822508	6.497801	0.768311	16.58362	17.22886	31.24062	
Worker11	2.930885	5.931114	4.854711	5.349145	0.422633	19.92741	23.30125	41.86152	
Worker12	4.408054	2.970248	8.068406	6.894483	0.974406	18.42748	21.31604	42.66416	

3-H-3-MBA	2-HIBA	DMMA	Ala	Adipic acid	Lys	AA	N-AcGln	p-CrS
10.98265	7.972102	2.176451	59.81194	70.53481	29.85953	68.6893	382.0925	101.6367
8.940706	9.063569	1.768007	76.00411	25.28989	31.65523	48.02162	288.6992	114.6391
13.10799	7.395409	2.363937	48.76422	10.60371	28.90295	25.81311	63.64266	12.06424
11.96944	7.085418	1.849819	59.97995	6.510571	25.42453	67.6272	218.448	9.97115
11.26968	6.837113	1.226662	55.57719	17.41816	19.80985	53.56959	122.7476	38.34479
12.51128	12.3584	2.570014	64.85569	7.956192	13.14737	28.90864	227.1692	61.95108
10.28519	9.217689	1.550156	66.90069	9.986233	38.3882	69.06851	197.0319	59.59919
21.99161	10.30753	2.015191	78.12018	23.49404	25.4994	36.22928	140.0936	47.21994
14.9985	10.21302	1.787822	47.35373	14.18611	8.497238	28.63434	126.6863	41.59589
11.12254	10.28637	2.132986	36.75328	26.17898	12.32428	43.21172	220.2517	91.48474
12.04005	9.274705	1.664086	62.55956	16.1992	14.44245	153.7691	135.3355	30.78028
28.98248	11.02805	2.542754	48.67993	8.063272	79.37916	75.28165	143.5457	68.93845
19.06572	7.563999	1.638784	49.63055	6.969811	21.56391	42.6284	92.96	26.02982
11.4122	7.113676	3.951287	65.08706	3.842415	62.40131	17.72855	134.9141	51.01595
5.850487	6.957081	3.174688	34.54485	7.961812	49.35893	28.60725	101.2766	34.95189
7.118657	7.444829	0.771286	37.92795	17.21007	17.35658	13.42444	69.90005	25.7641
8.953638	9.798548	1.395217	47.12602	9.9492	20.66915	16.31752	109.1064	37.09761
5.342901	8.530612	2.60672	25.9313	5.387336	32.81849	16.66132	49.17233	9.394985
5.788993	8.35362	1.942255	60.27731	12.95358	11.07724	20.75622	44.42184	11.97602
8.179368	7.141782	1.465355	56.07401	42.32845	49.70198	12.04704	61.86711	30.09769
9.407366	12.7908	1.150636	29.17803	9.705398	12.69371	23.20508	66.09071	20.69231
5.149509	8.072769	0.848776	20.31043	3.922347	7.244782	53.65649	156.0753	88.06303
9.202534	11.14447	1.679786	45.07196	13.62016	14.83601	17.56888	145.7608	60.79122
12.71203	7.587921	1.282079	65.17745	8.014864	15.2381	18.80293	101.175	64.08567
10.6522	7.424606	3.85016	79.55434	5.646917	34.03079	22.72761	252.6378	82.94051

pyro-Glu	SA	Gln	CA	DMA	Sar	MG	TMA	Crt
41.08829	4.6125	59.526	189.8649	39.49343	9.111276	10.09303	3.941455	760.2109
47.2677	9.234745	100.6525	434.7553	57.01954	11.51047	14.97127	10.60399	683.717
29.73164	1.421572	41.02171	229.8964	32.26177	7.918069	12.02767	8.48478	683.4974
51.31679	11.41907	68.38706	272.8463	33.76019	19.14008	20.04863	7.248693	624.4106
28.45455	8.605667	86.6557	586.5294	38.51146	9.136899	12.18263	3.480029	710.9598
50.85025	5.090388	61.87339	427.2763	47.25219	12.80003	15.13581	4.329401	675.5438
26.57004	20.67313	98.25293	942.0365	148.9568	13.18038	8.847243	5.465076	678.3097
37.39189	8.78102	88.61806	667.0669	41.0122	10.13376	13.38567	2.694561	613.9629
19.06391	2.975525	63.00276	362.966	38.10823	35.19568	12.79513	2.746964	647.9312
38.52041	11.64931	46.84756	578.8378	42.79316	12.80038	16.57862	8.831835	659.2498
46.65564	8.259231	58.68323	355.2018	78.86685	28.28487	29.1069	6.614176	814.3257
29.05673	21.54724	120.3805	725.3312	37.72537	20.65585	13.8315	4.634372	666.8312
25.59123	3.855218	77.73128	291.6847	35.15874	85.99864	12.20968	8.294798	860.5725
43.57242	10.59507	93.19128	639.8726	32.66648	8.349502	15.4829	10.98229	612.8042
49.83695	6.378888	68.53888	314.1275	37.94072	11.62528	13.6676	3.336883	653.4313
40.1687	6.06159	75.04011	414.3409	34.35702	8.156387	12.46935	7.24664	515.2521
49.13768	4.200544	110.2732	190.9244	64.03742	10.37069	10.75862	2.516497	668.8523
48.28701	9.24508	56.44382	242.9593	35.75444	8.483924	12.33557	2.478113	560.2
32.2729	11.43514	86.85708	450.3732	37.84389	9.963468	16.74105	7.494067	588.542
35.86921	8.07099	113.1954	452.2495	77.10809	7.893685	10.42402	7.23474	577.7469
40.64752	8.532627	65.65404	355.8185	40.12139	6.364671	15.64953	2.607793	590.1022
43.32665	17.47221	44.42695	194.4346	29.2201	5.843219	12.63894	2.312953	646.579
57.82656	4.990418	103.9989	463.5326	36.85181	7.44933	11.85398	8.857994	587.1723
36.79837	12.4417	104.7872	495.8886	30.24951	7.667381	10.51598	3.867381	542.0073
44.43583	6.884136	113.0078	338.0562	32.78197	9.440915	11.62916	3.682592	602.5128

Chn	TMAO	Tau	Gly	Gluconic A	Furoylglyci	catechol	4-HPAA	Tyr
10.14245	193.9559	58.65952	110.8742	55.75936	13.48433	14.29984	71.17005	19.48792
23.21372	237.7761	74.3024	239.5549	58.46226	13.75837	10.06371	41.82754	20.94865
13.01287	84.92998	70.33906	74.75699	41.38037	8.934484	8.092956	26.66663	13.7107
23.53606	93.11358	66.94468	113.3248	28.14617	10.49315	2.660321	109.2649	28.19888
10.27954	78.05301	119.2757	124.6342	11.492	11.50231	13.18079	26.61231	27.2531
14.27143	166.0866	34.74662	69.71334	28.06583	9.926345	4.100969	32.37267	37.39801
22.6404	2213.038	267.8126	176.4595	47.08573	5.146491	4.588554	20.67389	19.88253
8.396091	164.3242	164.2197	193.5169	28.54877	37.47717	16.20234	30.51467	29.16002
15.00456	109.6244	54.78401	90.1294	52.63987	12.38564	12.97559	21.26037	15.08816
4.86397	72.66811	44.24868	61.13607	30.51784	4.246549	13.82447	29.32048	18.60587
9.619341	868.2604	224.571	131.2905	9.626924	11.02251	27.67237	23.66383	10.41831
23.6692	102.6104	65.02635	236.1111	27.30111	1.424569	3.362206	20.575	21.48105
28.0763	160.6133	37.7715	141.3945	31.28641	5.578309	7.014881	37.27923	21.82186
19.44323	77.20177	203.7463	111.3429	61.57773	52.94929	20.95618	22.29987	17.74314
2.841956	177.6528	59.10704	86.09263	40.2117	57.49132	28.22629	25.76277	12.0183
5.809165	20.4194	138.1055	324.1642	48.98224	26.29587	8.51827	21.50659	11.31492
59.44458	380.6379	115.7515	136.1927	32.33661	46.73338	3.983715	37.37892	24.31882
1.219943	64.68311	73.48276	103.6432	46.49858	53.30892	4.70926	15.17727	10.84088
16.11489	79.98371	105.927	186.711	48.34022	6.734894	10.42073	14.66341	8.524329
24.36134	456.8236	117.8171	210.8093	25.5521	14.16611	12.76097	19.56708	18.0791
19.54677	118.3529	114.6956	117.0342	31.20758	41.49797	17.06833	17.29273	9.050122
5.41435	80.65142	44.75748	87.54025	42.53612	53.91607	4.450924	13.27655	5.157975
25.00447	84.79319	132.5142	114.9934	43.18108	40.55477	5.399986	20.09238	11.00725
24.88944	130.3257	109.48	278.8321	37.04999	99.53439	47.84269	23.88733	22.63793
27.66884	137.8844	91.19415	127.7855	35.34848	41.70891	7.517713	44.20861	24.56336

PAG	Trp	Hipp	PSI	4-HbzA	Hyp	2-PY	Formiate	U03
387.1194	75.02122	434.574	45.16715	23.07647	4.944021	12.48858	79.95681	8.946929
340.3886	79.05566	610.2554	68.45722	12.86912	7.559366	19.732	49.31609	20.2042
64.12559	12.54655	185.7232	44.43378	6.915121	1.838719	25.84858	22.77744	7.276464
216.7299	8.988454	89.2996	59.69322	14.52669	4.831323	14.41559	37.09079	1.584803
152.5831	27.14249	1235.47	56.0034	14.90543	9.622156	14.77182	41.96901	12.40516
164.0977	40.11598	165.3371	56.93235	17.73968	3.282398	18.06601	19.27447	4.5069
191.8199	35.3538	915.0781	49.76952	6.151822	2.477023	20.61431	63.95924	11.58685
142.7546	38.3898	354.2335	49.83055	15.38571	4.731565	8.980273	59.60387	38.36429
110.5869	26.23052	328.061	47.24232	16.75425	8.154032	22.62356	38.00712	6.553789
232.9916	55.2771	685.2525	55.22541	11.4065	6.05393	17.62437	53.47607	15.2862
156.3997	44.53325	1341.02	55.42742	14.05207	7.550541	18.41228	126.6527	20.54389
122.2852	65.47391	419.2005	57.5409	14.94971	13.73304	38.73655	77.01231	9.352681
103.1933	36.19559	189.3385	38.10727	10.55373	2.521114	29.06703	41.35449	7.439716
156.6019	41.68155	419.8241	49.6612	20.15149	7.309589	20.65018	41.49398	85.31621
128.4792	13.24041	736.8395	52.92751	15.63011	8.308207	13.13979	52.26856	45.32191
80.58732	27.52747	627.0752	43.40626	10.70741	6.757578	18.11368	31.78198	48.87206
103.2248	39.50042	145.4597	44.79851	6.223917	11.36476	27.67393	28.74365	42.19011
38.60634	10.83734	303.0987	36.96339	9.06272	15.63082	11.73488	29.26182	87.46006
46.26395	12.66904	73.67	70.2326	14.81781	5.192668	16.91837	44.14063	16.99277
59.82263	15.69399	414.2195	34.49699	6.312351	3.116211	14.13136	45.13312	27.47152
91.39246	24.60719	620.2304	41.65823	6.329765	3.369908	13.38217	49.53223	62.73171
171.011	22.74819	170.5231	55.21586	4.001237	5.106219	24.35395	65.60648	57.84598
130.0368	19.56575	173.5168	39.43929	5.346222	4.136803	13.12471	25.87019	55.4442
162.3058	15.52337	557.6882	44.22805	8.218367	8.547464	14.98844	43.49853	112.1072
280.5564	79.90619	442.9962	44.25385	11.70439	4.475173	23.06696	55.30864	28.35741

Trig	1-MNA
34.38163	1.321182
74.31794	5.041777
40.77283	7.821488
38.85859	3.368196
50.74469	9.97397
20.75816	6.692603
40.43785	4.394655
94.60236	2.08607
69.94575	6.252566
112.6023	5.918657
83.50648	7.630346
41.04394	8.8183
26.98838	9.159491
92.51429	3.300707
124.6264	3.312208
72.4285	4.087903
62.92753	9.357624
79.05774	3.156015
42.45494	2.788558
58.69223	2.370011
91.9936	6.513756
62.54875	1.48274
57.78849	1.792383
111.191	7.180274
84.10403	3.481479