

Supplementary Table I – Metabolomics report (values for each metabolite are reported as peak areas – arbitrary units)

N	compound	Compound	Pathway	parent	molRS	Lymph										Polarity	Plasma					p-value
						Patron 1	Patron 2	Patron 3	Patron 4	Patron 5	Patron 6	Patron 7	Patron 8	Patron 9	Patron 10		Patron 11	Patron 12	Patron 13	Patron 14	Patron 15	
1	Alanine	C00041	Amino acids	90.05566	1.174215	1.67E-07	1.27E-07	1.03E-07	1.36E-07	6924436	2.13E-07	1.25E-07	1.24E-07	1.59E-07	8993585	+	7.82E-01	1.02E-00	8.29E-01	8.66E-01	7.70E-01	0.05
2	Arginine	C00062	Amino acids	175.1191	1.135574	1439308	4487429	2965745	6632798	1065597	4852439	2144264	2432830	7589962	54205.7	+	2.97E-01	2.09E-01	1.22E-01	8.75E-01	1.96E-01	0.27
3	Asparagine	C00052	Amino acids	133.001	1.181709	4991.61.3	304873.1	584691.3	927393.8	33401	648040.2	610477.1	728990.2	1482362	383034.2	+	7.61E-01	4.99E-01	8.03E-01	6.26E-01	8.74E-01	0.05
4	Aspartate	C00049	Amino acids	134.0449	1.380647	871212.8	4655227	636245.9	2500554	1293725	388804	941600	5519255	237802.2	+	2.15E-01	4.93E-01	2.01E-01	4.44E-01	5.44E-01	0.07	
5	Cysteine	C00097	Amino acids	122.0274	1.194338	85432.75	108290.2	111106.8	277286.4	89563.29	146794.7	109475.9	185782.4	175408.8	130713.7	+	5.62E-01	9.89E-01	5.99E-01	7.39E-01	6.85E-01	0.03
6	Glutamate	C00025	Amino acids	148.0005	1.185457	706234.6	1180147	511840.0	1709957	365097.8	1026442	1635088	1501414	816703.5	256278.1	+	6.88E-01	7.22E-01	3.41E-01	8.71E-01	6.57E-01	0.06
7	Glutamine	C00064	Amino acids	147.0765	1.181116	118E-07	8647220	1.05E-07	1.43E-07	1.01E-07	1.30E-07	1.05E-07	1.18E-07	1.90E-07	1.27E-07	+	6.53E-01	8.27E-01	8.93E-01	7.55E-01	7.91E-01	0.02
8	Glycine	C00039	Amino acids	76.04021	1.17444	1.01E-07	3085.761	1.01E-07	9374916	9297892	1.07E-07	1.06E-07	8866552	1.11E-07	9820547	+	9.46E-01	2.92E-01	1.14E-01	8.44E-01	9.66E-01	0.31
9	Histidine	C00135	Amino acids	156.077	1.154125	3000593	1765991	2157750	3240890	2679106	2620183	2341403	2408225	3119433	+	1.12E-01	5.43E-01	8.23E-01	8.96E-01	1.04E-01	0.38	
10	Isotriiodocysteine	C00407	Amino acids	132.102	1.214039	4.34E-07	4.92E-07	5.65E-07	7.16E-07	2.30E-07	5.16E-07	4.96E-07	4.04E-07	2.21E-07	+	8.41E-01	1.12E-01	1.26E-01	1.77E-01	1.04E-01	0.28	
11	Isoleucine	C00047	Amino acids	147.1128	1.001849	5796530	6379192	6345352	1.62E-07	2846016	6032066	1.07E-07	6943244	1.69E-07	2666199	+	9.61E-01	5.97E-01	9.14E-01	1.01E-01	1.07E-01	0.32
12	Methionine	C00073	Amino acids	150.0585	1.214039	2045257	3804873	4283982	1.13E-07	9718915	2239859	2152992	2874340	8257055	727291.3	+	9.13E-01	1.77E-01	1.50E-01	1.32E-01	1.26E-01	0.09
13	Phenylalanine	C00079	Amino acids	166.0805	1.210995	2144868	4201.413	2277500	2796684	1241681	1500599	2072548	2196579	2526657	1664685	+	1.43E-01	2.03E-01	1.04E-01	1.11E-01	7.49E-01	0.28
14	Proline	C00148	Amino acids	116.071	1.199462	5.76E-07	4.68E-07	3.14E-07	7.60E-07	2.04E-07	5.33E-07	2.74E-07	2.45E-07	5.07E-07	1.85E-07	+	1.09E-01	1.71E-01	1.28E-01	1.50E-01	1.31E-01	0.05
15	Serine	C00065	Amino acids	106.0504	1.179736	32719.8	281160.7	480118.2	73292.1	165123.7	425273.1	576715	596349.3	1278051	491712.5	+	7.70E-01	4.88E-01	8.05E-01	5.73E-01	8.61E-01	0.08
16	Threonine	C00188	Amino acids	120.0699	1.1823	1790000	3011191	2116378	6276048	632873.4	2489999	3892522	2378773	7684470	719041.2	+	7.19E-01	8.36E-01	8.93E-01	8.17E-01	8.80E-01	0.06
17	Tryptophan	C00078C0025C0086	Amino acids	208.0973	1.216601	158711.6	1215978	915324.8	1382621	33421.05	0	672382.8	948476.5	1407000	+	4.75E-01	8D9V0	1.08E-01	9.65E-01	8.93E-01	0.32	
18	Tyrosine	C00082	Amino acids	182.0813	1.213843	8298726	6881450	1.18E-07	9758917	489428	7818154	5748086	6197974	9034245	4896336	+	1.06E-01	1.20E-01	1.23E-01	1.08E-01	1.00E-01	0.07
19	Valine	C00183	Amino acids	118.0806	1.204386	5.11E-07	6.91E-07	6.95E-07	1.04E-07	4.79E-07	5.98E-07	8.08E-07	4.90E-07	6.78E-07	3.47E-07	+	8.57E-01	1.34E-01	1.42E-01	1.54E-01	1.38E-01	0.09
20	Cysteine	C00491	Amino acids	241.0312	1.184475	155177.8	7814324	5259939.4	542476	45385.81	70180.52	8601.863	4702866	1011080	24959.13	+	2.19E-01	2.19E-01	1.12E-01	5.26E-01	1.82E-01	0.34
21	Hypoxanthine	C00302	Nucleotides	135.029	1.234113	2047975	1556036	1556938	778279.8	3015407	2173709	1913492	2217339	1020967	3271338	-	9.42E-01	8.13E-01	7.02E-01	7.62E-01	9.21E-01	0.02
22	Xanthine	C00385	Nucleotides	155.0392	1.088866	117698	91872.32	809900.4	158853.5	184900.5	105084.8	125457.3	181563.8	495857.2	85306.29	+	1.12E-01	7.32E-01	2.10E-01	3.20E-01	2.17E-01	0.90
23	Guanine	C00242	Nucleotides	152.0545	1.231964	101275.2	148906.1	379077.1	448556.6	8932.55	85997.3	71787.1	141667.9	401274	12630.13	+	1.18E-01	2.06E-01	2.68E-01	1.12E-01	7.07E-01	0.85
24	Allantoin	C00499	Nucleotides	177.0609	1.14664	107723.6	203890.05	9873994	133634.8	17541.15	372013.9	528419.6	412231.1	387748.2	73827.34	+	2.89E-01	8.33E-02	2.40E-01	2.58E-01	2.38E-01	0.02
25	5-(γ-Allyl) -Adenon	C00250	Nucleotides	159.0435	1.063995	1243481	41395469	2051631	5961871	180561	8194048	6283183	3801338	56195.75	45330.19	+	1.74E-01	6.54E-01	6.64E-01	1.07E-01	3.98E-01	0.21
26	5-Hydroxynorvanone	C11821	Nucleotides	185.0322	1.195729	1264753	2662575	1548264	3504855	1549618	783002.2	680544.1	720024.7	4303571.2	843371.2	+	1.62E-01	3.91E-01	2.15E-01	3.77E-01	1.84E-01	0.03
27	3-Phosphoacyl-N-formylglycinate	C04376	Nucleotides	313.068	1.302738	4.64E-07	2.09E-07	4.44E-07	3.32E-07	4.29E-07	3.30E-07	3.51E-07	3.76E-07	3.61E-07	3.50E-07	+	1.40E-01	5.97E-01	1.19E-01	8.89E-01	1.23E-01	0.70
28	UMP	C00105	Nucleotides	323.0607	1.223435	27684.57	38225.51	3601606	19379.37	26525.02	3829403	43161.7	71481.61	18424.45	150870.4	-	7.23E-01	8.86E-01	5.94E-01	1.05E-01	1.76E-01	0.21
29	Cytidine	C00475	Nucleotides	244.0813	1.199085	839574	67674.69	1008935	231927.9	803747.9	775001.5	952984.8	1563855	175425.5	1759230	+	1.08E-01	1.14E-01	6.84E-01	3.20E-01	4.57E-01	0.04
30	5-6-Dihydrothymine	C00066	Nucleotides	129.0699	1.217231	7647330	528661.2	5317876	9103401	2.04E-07	7090320	3615075	5097120	6891686	1.26E-07	+	1.08E-01	1.44E-01	1.64E-01	1.32E-01	1.62E-01	0.14
31	Thymine	C00178	Nucleotides	125.0344	1.209983	1628916	1999810	1766629	1559129	1684812	1642146	1743664	1728031	1754434	1707941	-	9.92E-01	1.15E-01	1.02E-01	8.89E-01	9.66E-01	0.94
32	1-5-Cyclic IMP	C00943	Nucleotides	329.0365	1.301481	5846988	2.11E-07	1.13E-07	1.35E-07	1.10E-07	212125	4233574	264338	1166018	3095623	+	2.76E-01	5.47E-01	4.29E-01	4.29E-01	3.55E-01	0.02
33	Pyridoxal	C00250	Nucleotides	168.0634	1.157317	141396.9	29385.24	9202798	7377822	97968.16	172724.4	146870	1688204	146481.1	179646.8	+	8.19E-01	2.06E-01	4.93E-01	5.01E-01	5.45E-01	0.00
34	Pyridoxamine phosphate	C00447	Nucleotides	247.0545	1.244654	116852.1	2146511	70398.96	202998.9	1382907	88279.1	2820797	139634.7	104467.7	172458.2	-	1.32E-01	7.61E-01	5.04E-01	1.94E-01	8.02E-01	0.40
35	Nicotinamide	C00153	Nucleotides	123.0526	1.085965	1662857	784842.3	1138564	847815.1	1127221	2384952	1630741	1821423	2094975	1706436	+	6.97E-01	4.81E-01	6.24E-01	4.14E-01	6.61E-01	0.00
36	Adenosine	C00212	Nucleotides	266.0576	1.207538	9177032	44801.99	91778.35	5445404	89960.34	82567.33	89138.59	9801104	78665.02	94489.06	+	1.10E-01	5.08E-01	9.36E-01	7.08E-01	9.43E-01	0.20
37	Guanosine	C00387	Nucleotides	282.0782	1.212839	74935.27	87138.97	37675.5	3949492	581997.2	124748.2	50270.54	48001.88	43138.81	36486.65	-	6.01E-01	7.39E-01	7.83E-01	9.24E-01	1.66E-01	0.39
38	Inosine	C00294	Nucleotides	269.114	1.241479	92398.6	373099.2	44425.05	256736.9	27599.9	179401.5	251813	90971.41	197151.8	213105.3	+	1.07E-01	1.48E-01	4.88E-01	1.50E-01	1.29E-01	0.21
39	Uridyl	C00106	Nucleotides	1133.036	1.088232	56543.5	253648.7	411986.6	231221.3	367418.9	1011599	696457.3	6738227	771751.7	686295.6	+	5.54E-01	3.64E-01	6.11E-01	3.00E-01	5.35E-01	0.00
40	NAD ⁺	C00003	Nucleotides	664.8801	1.136041	26658.91	179755.6	54911.57	29373.8	63210.49	74148.66	29940.76	46559.22	25745.9	21611.87	+	1.60E-01	6.04E-01	1.18E-01	1.14E-01	2.92E-01	0.40
41	NADH	C00004	Nucleotides	665.9266	1.144549	91363.16	60201.44	7132.955	26736.69	7811.045	31428.9	62849.48	33568.84	152075.2	160297.6	+	2.91E-01	9.58E-01	3.03E-02	1.75E-01	4.87E-02	0.02
42	Uridyl	C15587	Nucleotides	1																		

52	Lactose	C00432	Chitin	850279	144967	4378-07	2368-07	1360-07	1638-07	3448-07	4556-07	4078-07	979181	3598-07		7.88E-01	5.55E-01	5.30E-01	1.04E-01	9.00E-01	0.06	
53	Mannose	C00435	Other sugars	503766	125263	36729	0	0	0	16114.08	322274	266742	306164	10847.7	48902	1.05E+01	0.00E+00	0.00E+00	0.00E+00	1.67E+02	0.03	
54	Mannitol	C00502	Other sugars	1610717	121343	62389.8	379762	360726	556573	498357	101380	108268	91766.78	101733	48158.1	5.99E+01	5.27E-01	5.53E-01	5.48E-01	1.07E+01	0.26	
55	D-Ribose	C00421	Other sugars	1490454	1244584	25064.4	35791.2	28352.5	21994.1	65116.8	36367	66974.6	34259.7	38580.3	1029164	1.46E+01	5.30E-01	8.21E-01	5.67E-01	6.33E-01	0.19	
56	Dulcitol	C00504	Other sugars	1510415	1402559	195438.4	123882.6	165148.7	161026	139891.2	31864.2	31808	219907	24892.1	28148.2	9.15E+01	5.90E-01	7.44E-01	6.72E-01	5.54E-01	0.02	
57	cis-Aconitate	C00347	TCA cycle	1730707	1346107	2639573	126478	2008802	86610.8	2753702	1258309	2296562	106820			9.95E+01	1.06E+01	1.90E+01	3.16E+01	1.55E+01	0.29	
58	Citrate	C00158	TCA cycle	1911093	1245629	5476-07	4250-07	4776-07	1588-07	4726-07	7376-07	8376-07	3326-07	8279808	2.83E+07	7.46E+01	1.51E+01	1.44E+01	1.91E+01	1.66E+01	0.33	
59	2-Oxoglutarate	C00326	TCA cycle	1450146	1235909	1616441	217847	432632.5	339921.2	1346432	2809334	1784660	598204.8	468897.1	984917.7	8.04E+01	1.21E+01	7.23E-01	7.20E-01	1.37E+01	0.95	
60	2-Oxoglutarate	C00940	TCA cycle	1440291	1233965	972329.3	1099568	1131028	1080214	1093564	1204731	1190643	975148.2	1167851	1244993	8.07E+01	8.90E-01	1.16E+01	9.25E-01	8.78E-01	0.25	
61	Succinate	C00342	TCA cycle	1171079	121385	525172.8	503028.2	856904.6	412148.9	686670.2	490127.3	86690.4	704024.9	455800.4	825624.9	1.05E+01	1.03E+01	9.23E-01	9.05E-01	8.32E-01	0.28	
62	Malate	C00352	TCA cycle	1154023	1219147	317931.8	421451.6	290272.7	233867.7	298844.9	288555.8	223906.5	93041.3	220760	367029	1.10E+01	1.88E+01	9.40E-01	1.04E+01	7.90E-01	0.56	
63	Malate	C00568	TCA cycle	1331029	124354	4021371	4239033	1425176	1125588	2987472	3725220	2725303	1842391	1046715	3379144	1.08E+01	8.90E-01	7.74E-01	1.08E+01	8.84E-01	0.57	
64	Oxaloacetate	C00336	TCA cycle	1310001	1206466	1481656	1634643	1782871	1543490	1747285	1746462	1873337	1708952	1714211	1598771	8.51E+01	8.72E-01	1.03E+01	9.00E-01	1.10E+01	0.32	
65	2-Hydroxyglutarate	C00240	Aberrant Catabolic cycle	1440291	1246079	1430670	930060.8	487045.7	329773.6	697046.6	7709229	468140	230849	1453772		1.45E+01	1.21E+01	1.04E+01	1.43E+01	8.06E-01	0.49	
66	6-Phospho-D-ribosone	C00345	Pentose Phosphate Pathway	2751082	1220318	899256	1736895	2757512	11911.9	44185.39	1413816	46032.38	26536.64	38082.62	129837.1	5.61E+01	4.38E-01	1.03E+01	3.88E+01	1.66E+01	0.07	
67	D-Glucose 1-6 lactone 6-phosphate	C00236	Pentose Phosphate Pathway	3691154	1099924	20086.69	23780.91	20086.69	23780.91	20086.69	23780.91	23780.91	20086.69	23780.91	23780.91	9.87E+01	7.94E-01	5.33E-01	8.39E-01	9.76E-01	0.11	
68	D-Erythrose 4-phosphate	C00279	Pentose Phosphate Pathway	1983974	1108733	127781.6	57439.84	106121.9	10639.8	10639.8	128545.1	12900.7	12357.6	116179.9	12584.1	9.94E+01	4.66E-01	8.60E-01	8.68E-01	8.62E-01	0.11	
69	alpha-D-Ribose 4-phosphate	C00620	Pentose Phosphate Pathway	2291007	1203389	37117.4	136665.5	46502.6	20863.9	460037.1	263603.5	2208.31	86647.5	223779.9	65308.1	1.28E+01	7.19E-01	9.39E-01	9.32E-01	7.04E-01	0.37	
70	5-Phospho-alpha-D-ribose 1-diphosphate	C00119	Pentose Phosphate Pathway	476942.8	1277131	9088105	977233.8	562491.9	2170917.3	314491.3	219262.3	257343.6	267030.5			2.20E+01	9.32E+01	2.53E+01	1.64E+01	2.11E+01	0.21	
71	Gluconate	C00391	GSH biosynthesis	3060788	1232992	466125	370143.9	0	0	8297148	4742450	42822.81	0	23839.1		5.62E+01	8.09E-01	0.00E+00	#DIV/0!	0.00E+00	0.26	
72	5-Oxoproline	C00379	GSH biosynthesis	128014	1244585	1425591	1901302	1273458	890199.1	1109956	2518149	472566	2258167	1501914	1975566	5.66E+01	4.56E-01	5.64E-01	5.96E-01	5.61E-01	0.02	
73	S-Glutathionyl-L-cystine	C00526	GSH biosynthesis	4270943	1209866	2126265	0	28353.1	9302660	1876361	6836414	608479	784192	6498168	3122616	3.11E+01	0.00E+00	3.00E+01	1.43E+01	5.89E-01	0.22	
74	Acetone	C00372	GSH biosynthesis	1750243	1212841	1183304	683393.5	1647487	802665.5	1538382	936664.5	777327	2802777	6012619	3474922	1.31E+01	8.80E-01	5.70E-01	1.20E+01	4.43E-01	0.26	
75	Dihydroxyacetone	C00322	GSH biosynthesis	1731003	124878	2688873	1348107	2688873	860113.3	104356	2218102	1250309	1069662	247488.8	1056920	9.95E+01	1.06E+01	1.99E+01	3.34E+01	1.55E+01	0.29	
76	gamma-Glutamyl-L-serine methylethionine	C00605	Gamma-glutamyl	3110353	1152704	8801156	0	33815.87	2120674	0	185092.4	2301628	17871.7	181724	2838592	3.13E+01	0.00E+00	1.97E-01	1.17E-01	0.00E+00	0.01	
77	gamma-L-Glutamyl-D-alanine	C00738	Gamma-glutamyl	2194973	1237314	305408.9	1831172	214550.2	540957.6	87121	195108	185764.5	143840.2	1232401	159885.2	1.57E+01	9.66E+01	1.49E+01	4.36E+01	2.57E+01	0.17	
78	Bis-gamma-glutamyl-L-cysteine	C00446	Gamma-glutamyl	4974674	1248631	176768.9	134212.7	79547.63	2517712	122887.6	42944.79	122967	2435417	8489407	1013701	4.12E+01	1.07E+01	3.27E+01	2.97E-01	1.21E+01	0.37	
79	(S)-Gamma-L-glutamine	C00283	Gamma-glutamyl	276118	1223629	210557.4	209587	249541.2	249541.2	398387.5	287941.6	906307	249914.4	3711107		5.29E+01	7.28E-01	9.96E-01	9.63E-01	7.07E-01	0.09	
80	S-L-Glutamyl-uracine	C00844	Gamma-glutamyl	2533573	1210748	162292.9	201385.2	161166.3	185904	208954.8	210158.6	175164.6	198972.9	177461.1	167990.9	7.72E+01	1.15E+01	8.10E-01	1.04E+01	1.24E+01	0.91	
81	gamma-L-Glutamyl-[acp]	C18006	Gamma-glutamyl	1611015	1227993	1396445	1531245	1296971	1538923	1576762	1699282	1624656	1497544	1645414	1571508	8.21E+01	9.41E-01	8.14E-01	9.30E-01	1.00E+01	0.06	
82	L-Homocysteine	C00155	Serine biosynthesis and one-carbon metabolism	1361047	1241479	9221605	2950115	50922	6621309	913462	9936974	1268155	895533	3285591	101124.2	9.28E+01	9.22E-01	1.02E+01	7.41E-01	9.02E-01	0.12	
83	Cysteine	C00342	Serine biosynthesis and one-carbon metabolism	3678974	1161621	6738974	7724969	5936725	5837761	4579015	136849	178027	3268534	6446257		2.09E+01	4.34E+01	3.50E+01	1.80E+01	7.10E+01	0.00	
84	N,N-Dimethylglycine	C00206	Serine biosynthesis and one-carbon metabolism	104071	1228899	184898	333392	2790037	3081004	1292275	1766126	2406485	2911738	2173073	1154475	1.06E+01	1.34E+01	1.07E+01	1.42E+01	1.12E+01	0.08	
85	D-3-Phosphoglycerate	C00252	Serine biosynthesis and one-carbon metabolism	1801084	1089074	448008	830991.9	378987.4	2514027	321944.8	633480.2	438977.8	53225.1	498098.6	831117.2	7.01E+01	7.03E-01	7.08E-01	5.12E-01	6.10E-01	0.00	
86	L-Phosphoenolpyruvate	C00252	Serine biosynthesis and one-carbon metabolism	1829767	1159994	9152132	2370392	64398.34	5187282	7413519	9488085	875961	6371103	8191245	7666013	9.65E+01	2.71E-01	9.85E-01	6.33E-01	9.67E-01	0.17	
87	S-Adenosyl-L-homocysteine	C00021	Serine biosynthesis and one-carbon metabolism	3851282	1200717	176559.4	0	59011	0	89328.52	293661.8	36089.49	99961.22	41109.07	14748.3	6.01E+01	0.00E+00	6.15E-01	0.00E+00	6.30E-01	0.03	
88	S-Adenosyl-L-methionine	C00019	Serine biosynthesis and one-carbon metabolism	3990978	1195889	8105308	5754314	218922.3	6834712	229171.1	1330977	53201.5	62391.84	28802.99	86503.05	6.14E+01	1.06E+01	3.51E+01	2.40E+01	2.65E+01	0.12	
89	Folate	C00304	Folate pool (One carbon metabolism)	4421078	125548	6665084	0	0	0	0	32207.38	1761021	4535312	5153310	7716482	2.07E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.17	
90	5,10-Methylenetetrahydrofolate	C00445	Folate pool (One carbon metabolism)	4531341	7415192	0	2204167	6535065	0	0	0	1161918	2031841	0	0	#DIV/0!	1.89E+01	3.21E-01	#DIV/0!	#DIV/0!	0.87	
91	10-Formyltetrahydrofolate	C00204	Folate pool (One carbon metabolism)	4701531	669880	1425984	5599406	2965633	3225109	1142166	2035588	1419433	1716511	3121549	1016178	7.04E+01	3.94E-01	1.09E+01	1.03E+01	1.12E+01	0.31	
92	Tetrahydrofolate	C00101	Folate pool (One carbon metabolism)	4441602	8148584	7539482	1192131	1694401	7481277	83181.45	118048	299984	1271184	5797051	1792428	6.38E+01	6.03E-01	1.33E+01	1.29E+01	6.04E-01	0.35	
93	10-Formyltetrahydrofolate	C00204	Folate pool (One carbon metabolism)	4721603	7420789	0	1416107	3241374	1128.8	0	0	1468107	892158	891280	0	#DIV/0!	1.01E+01	1.64E+01	1.27E+01	#DIV/0!	0.37	
94	Dihydrofolate	C00415	Folate pool (One carbon metabolism)	442144	7078418	1086094	0	1675634	1729733	176092	589746	2726301	2490332	1152136	191693.8	1.85E+01	0.00E+00	6.73E-01	1.50E+01	9.21E-01	0.22	
95	Oxalate	C00602	Urea cycle	1331072	1049387	0	987752.2	1588215	234707	1112952	1590704	1279314	2232899	2421326	1115727	0	0.00E+00	3.62E-01	7.11E-01	9.68E-01	9.98E-01	0.10
96	L-Citrulline	C00327	Urea cycle	1761028	1200112	799552.9	223577.6	521808.2	589526.1	205402.2	715522.4	253495.8	666402.8	604075.1	340368.2	1.12E+01	8.82E-01	7.83E-01	9.75E-01	8.55E-01	0.48	
97	N-L-Argininosuccinate	C00486	Urea cycle	289071	1235157	419111.1	7561230	1626045	5044310	3309282	359607.3	4455869	340878	246631.1	347842.5	1.19E+01	1.70E+01	4.77E+01	2.05E-01	1.33E-01	0.06	
98	Urea	C00366	Urea cycle	1690367	1241479	7000794	1504190	2764293	2238922	4140250	8062056	5561636	4632122	686092	8357886	8.68E+01	2.79E-01	5.97E-01	5.20E-01	4.95E-01	0.01	
99	Cadaverine	C00256	Polyamines	1031234	1409553	5207511	7575218	9507773	5620625	6238613	2188556	11999.2	4855274	8253104		2.38E+01	6.31E+01	4.22E+01	7.34E+01	7.55E+01	0.13	
100	Spermidine	C00315	Polyamines	1461																		

Table with columns for compound name, ID, CAS, and various numerical values. The table lists various amino acids and related compounds such as Arginine, Glycine, Proline, and various fatty acids. Each row contains a unique ID and associated numerical data points.

21	2-(5Z, 8Z, 11Z, 14Z-ekosastenoin)-3-octadecanoyl-sn-glycero-1-phosphatidylcholine	LMGP0201019	Phosphoethanolamines	766.5449	12.02365	166909.1	104644.1	104123.6	89957.48	42790.96	23392.53	2797.16	2781.14	2250.66	9891.53	-	-	7.14E+01	3.76E+00	3.74E+00	2.64E+00	4.37E+00	0.02	
21	2-(5Z, 8Z, 11Z, 14Z-ekosastenoin)-3-oxo-1-phenylethyl-sn-glycero-3-phosphoethanolamine	LMGP0201008	Phosphoethanolamines	942.7707	1.154762	26799.8	10720.1	453487.5	510755.6	401937.5	115496	27484	11864.5	82902.01	131102.5	-	-	7.28E+00	3.95E+01	3.44E+00	6.14E+00	3.07E+00	0.12	
21	2-(5Z, 8Z, 11Z, 14Z-ekosastenoin)-3-oxo-1-phenylethyl-sn-glycero-3-phosphoethanolamine	LMGP0201007	Phosphoethanolamines	746.5961	1.188853	69108.62	45899.11	146073.3	676373.5	104664.7	44719.17	89254.1	69557.46	48765.91	-	-	-	6.60E+01	1.71E+00	7.70E+00	2.02E+00	1.39E+00	0.47	
22	1-oxidodecyl-sn-glycero-3-phosphoethanolamine	LMGP0200003	Phosphoethanolamines	466.3088	8.390325	23883.72	14520.2	476087.2	361016.2	32782.2	37432.02	12644.4	516526.6	98329.5	3174.96	-	-	6.38E+00	1.15E+00	9.22E+01	3.47E+00	9.88E+01	0.48	
22	1-oxidodecyl-sn-glycero-3-phosphoethanolamine	LMGP0200002	Phosphoethanolamines	480.39	9.860208	39774.4	58732.1	799590	1586427	214023.1	641624.1	1093561	1442374	150628.4	-	-	-	6.20E+00	5.91E+01	7.60E+01	1.39E+00	1.42E+01	0.63	
22	1-oxidodecyl-sn-glycero-3-phosphoethanolamine	LMGP0200001	Phosphoethanolamines	452.2839	9.845593	4522839	882871.7	739300	1077541	2094663	738481.6	1023222	94073.5	77684.4	2499952	841833.7	-	-	6.68E+01	7.88E+00	1.39E+00	1.09E+00	8.73E+01	0.85
22	1-oxo-2-octadecanoyl-sn-glycero-3-phosphoethanolamine	LMGP0200004	Phosphoethanolamines	478.2945	9.840563	1119297	1054727	1226205	1187160	955418.5	1676621	1329886	1386022	1395531	1305521	-	-	6.68E+01	7.93E+00	8.85E+01	8.51E+01	7.52E+01	0.01	
22	1-(4Z, 8Z, 11Z, 14Z-ekosastenoin)-sn-glycero-3-phosphoethanolamine	LMGP0200009	Phosphoethanolamines	500.2794	9.408232	9951606	5625000	6180990	5698942	4737022	9337683	7342248	7770500	7213776	6165656	-	-	6.44E+01	7.66E+01	7.94E+01	7.88E+01	7.68E+01	0.01	
22	1-(1Z, 12Z-nonadecadienyl)-sn-glycero-3-phosphoethanolamine	LMGP0200001	Phosphoethanolamines	476.2791	9.426203	795423.8	79524.2	1583991	1733948	652638	1232342	1001112	1255274	1625708	81952.4	-	-	6.45E+01	7.94E+01	1.28E+00	1.07E+00	3.97E+01	0.64	
22	3-pentadecanoyl-sn-glycero-1-phosphocholine	LMGP0100017	Phosphocholines	480.3105	10.66415	392734.3	435573.9	795274.2	9754043	403624.9	524576.8	488894	477619.8	800298.1	385289	-	-	7.49E+01	8.91E+01	1.67E+01	1.22E+00	1.05E+01	0.47	
22	2-(8-[3]-lipoic acid)-octanoyl-sn-glycero-3-phosphocholine	LMGP0100026	Phosphocholines	528.3102	9.927987	790663.8	706146.6	724672.3	67898.3	627627.1	1133875	969529.8	980346.3	870279.8	893675.1	-	-	6.97E+01	7.23E+01	7.39E+01	7.80E+01	7.01E+01	0.00	
22	2-(5Z, 8Z, 11Z, 14Z-ekosastenoin)-sn-glycero-3-phosphocholine	LMGP0100021	Phosphocholines	542.3374	9.860726	654202.9	1088208	1419035	2932075	459268.2	1136603	1885686	1945310	2170466	290520	-	-	5.70E+01	5.77E+01	7.39E+01	1.35E+00	1.58E+01	0.57	
22	2-(1Z, 4E-decadienyl)-3-(2E, 4E-decadienyl)-sn-glycero-1-phosphocholine	LMGP0101005	Phosphocholines	556.3183	10.03851	607312.7	1014531	1642650	4016411	801976.8	775604.7	1189946	8897789	3438019	256796.6	-	-	7.78E+01	8.43E+01	8.60E+01	1.17E+01	3.12E+00	0.61	
23	N-butanoyl-1-thiosaccharin lactone	LMFA0001002	Phosphatidylserines	170.0822	6.43643	8872334	1720957	220849.6	6372184	4352.25	38.58.378	217457	296201.6	4756409	3543312	-	-	1.09E+00	7.94E+01	7.64E+01	1.34E+00	1.27E+00	0.30	
23	1-triacyl-sn-glycero-3-phosphoserine	LMGP0300005	Phosphatidylserines	454.2077	6.50079	0	8422.621	10583.41	242800	367039.8	0	8269.867	81785.38	161300.7	293240.4	-	-	#DIV/0!	1.02E+00	1.29E+00	1.50E+00	1.25E+00	0.11	
23	Penicillamin	C03422	Xenobiotics	227.1272	4.20762	5866310	2002124	2625294	2122479	16581.07	7490960	6598118	3124741	5541843	7769112	-	-	7.83E+01	3.03E+00	6.49E+01	5.99E+01	1.85E+00	0.41	
23	Bilirubin	C05060	Hemolysis markers	581.2697	8.058911	61102.2	220515.8	799252	238956.2	167112.5	1248748	516776.6	1560874	35294.4	1315500.9	-	-	6.70E+01	5.12E+00	6.73E+01	6.73E+01	5.90E+01	0.12	
23	Bilirubin	C04886	Hemolysis markers	583.2629	7.699477	9046975.6	1426932	4466598	4435.10	1053392	2477186	1172488	3523683	253908.8	913597.3	-	-	1.65E+01	1.22E+00	1.27E+00	1.75E+00	1.15E+00	0.98	
23	Hemier	C06707	Hemolysis markers	396.229	1.28135	3268.89	32872.48	155309.1	126959.2	24784	5804.718	0	5168.434	10642.04	7377.848	-	-	5.62E+01	#DIV/0!	3.08E+01	1.23E+00	3.38E+01	0.03	
23	2-Methylglucosamine	C02930	Other	143.0342	1.13661	153505.5	120043.5	175817.8	120043.5	150691.9	13547.78	221022.6	13267.4	265338.8	-	-	-	1.13E+00	1.15E+00	7.90E+00	9.06E+01	5.88E+01	0.37	
23	4-Aminobenzoate	C03668	Other	138.0538	1.223529	897412.6	89741.6	9472.66	210257.9	3630.30	62870.1	86036.1	238190	351726.5	329153.2	-	-	9.51E+01	4.71E+01	3.97E+01	5.98E+01	1.10E+00	0.99	
23	Methylmelanin	C06381	Other	133.0722	1.22256	415422.6	4003721	426702.4	3641401	911846.3	24413.26	2664522	321338.8	2282793	620825	-	-	1.70E+00	1.52E+00	1.33E+00	1.60E+00	1.47E+00	0.99	
23	3-Oxobutylate	C01990	Other	204.9969	1.232083	183888.6	0	18544.82	7693.123	23013.92	216660.2	19031.87	188990	292951.8	-	-	-	8.49E+01	0.00E+00	9.84E+02	2.77E+02	6.92E+02	0.02	
24	2-Deoxy-alpha-D-glucoside	C03573	Other	164.6089	1.080861	1686478	3790146	4357662	4814754	3488002	2196795	4676518	5126554	6510654	4223392	-	-	7.68E+01	8.11E+01	8.50E+01	7.40E+01	8.21E+01	0.03	
24	cis-p-Coumarate	C06738	Other	165.0357	1.241479	1249482	961353.7	1705386	1491816	627175.1	1120020	872803.9	1337403	1301343	685311.9	-	-	1.12E+00	1.16E+00	1.28E+00	1.15E+00	9.53E+01	0.99	
24	N-Acyl-D-mannosaminolactone	C03792	Other	395.057	1.118801	271177.6	5031082	292491.2	72428.62	215554.9	43048.33	201431.3	894168.8	228388.1	524121.9	-	-	6.39E+01	2.59E+02	6.03E+00	3.17E+01	4.11E+01	0.24	
24	N6-Methyl-L-lysine	C02728	Other	159.1128	1.378058	174405.5	891591.5	7071403.3	1009427	726846.5	107415.9	143191.5	124774.2	114283.7	132091.8	-	-	1.62E+00	6.92E+00	5.67E+00	8.83E+00	5.52E+00	0.02	
24	Dethiobiotin	C01909	Other	215.139	1.241489	143239.1	359381.4	53934.61	62772.56	312305.3	72875.88	148261.7	85325.75	43005.61	192825.5	-	-	1.97E+00	2.42E+00	6.32E+01	1.46E+00	1.62E+00	0.14	
24	L-2-Aminoisopane	C03956	Other	162.0759	1.236296	207598.2	764990.3	424192.4	499954.1	337087.3	161916.7	304034.1	212960	314816	234123.1	-	-	1.28E+00	2.52E+00	2.01E+01	1.29E+00	1.44E+00	0.07	
24	Threonate	C01620	Other	317.0456	1.237213	81699	1339973	637865.2	507917.8	460722	45696.84	1151578	2138430	1211526	1357292	-	-	1.75E+00	1.07E+00	2.50E+00	4.39E+01	3.96E+01	0.12	
24	Tripeptide	C03316	Other	187.0564	1.075587	483191.2	1094948	1254122	1371900	830737.7	823416.7	1528490	1455443	1829920	1607561	-	-	5.86E+01	7.23E+01	8.62E+01	7.53E+01	7.78E+01	0.00	
24	Catecholamine	C03012	Other	152.6097	1.204103	146833.5	829838.2	117170.2	108520.9	133865.9	206845.3	196609.4	21559.8	96118.09	21195.5	-	-	7.04E+01	4.22E+00	5.18E+01	1.18E+00	6.37E+01	0.59	
24	Ferri gluconate	C13511	Other	196.0583	1.152108	1323338	1429260	3431387	46222.23	8109.001	27507.74	76852.4	34695.82	48777.14	37164.36	-	-	4.81E+01	1.84E+01	9.90E+01	9.48E+01	2.18E+01	0.39	
25	Sodium rhubarb	C13085	Other	215.0146	1.20432	1483050	753995.6	1996821	907895.2	1717988	1070275	806237.6	2081224	881627.7	2609376	-	-	1.37E+00	8.41E+01	9.94E+01	1.03E+00	6.58E+01	0.54	
25	Catechin	C17390	Other	289.0866	1.238157	419111.1	7561230	1626045	5044310	3302962	359007.3	145586.9	340878.8	246611.1	247842.5	-	-	1.19E+00	1.70E+00	4.77E+00	2.05E+01	1.33E+01	0.06	
25	6-Thioxanthine 5-monophosphate	C16618	Other	381.0237	1.169113	1334001	202801.5	54645.19	146147.9	128404	73893.64	108096.5	106473.7	94726.12	632186	-	-	1.81E+01	1.88E+00	5.13E+01	1.54E+00	2.06E+01	0.45	
25	Ferri lactate	C06229	Other	399.6825	1.347247	1808734	3132074	3268370	4503598	9620677	1077829	435934	1649820	2448097	5855516	-	-	1.68E+00	7.20E+01	1.99E+00	1.34E+00	1.54E+00	0.16	
25	Gluconolactone	C17260	Other	316.9766	1.067667	2832988	78449.14	8313049	6229361	55108.25	26491.79	853388	7450541	9109497	77536.66	-	-	1.07E+00	9.19E+01	1.12E+00	6.84E+01	7.11E+01	0.25	
25	alpha-N-Peptidyl-L-glutamate	C0904	Other	316.0834	1.24252	21061.07	32121.07	33581.07	3191E+07	412E+07	1366E+07	137E+07	143E+07	1338E+07	137E+07	-	-	1.54E+00	2.35E+00	2.49E+00	2.94E+00	2.96E+00	0.00	
26	D-Alanyl-L-alanyl-poly(glycerophosphate)	C04457	Other	315.0792	1.24252	194E+08	310E+08	334E+08	366E+08	383E+08	125E+08	129E+08	134E+08	125E+08	135E+08	-	-	1.84E+00	2.35E+00	2.50E+00				