

Supplementary table 1. Metabolites listed as in Figure 2A, particle sizes of the lipoproteins and the fold changes of the metabolites vs. serum (after size normalisation).

Metabolite name/Lipoprotein (size, nm)	VLDL	IDL	LDL	HDL2	HDL3
	38	33	25	10	8
Unknown alcohol	-15.96	-15.88	-19.05	-23.59	-17.65
Unknown amino acid	1.27	1.67	-1.23	-1.10	1.18
D-Fructose	-30.27	-37.63	-44.41	-40.73	-49.57
Unknown sugar	-37.31	-48.95	-58.36	-44.06	-61.34
Citric acid	-46.63	-139.09	-206.55	-127.73	-191.05
Myo-Inositol	-44.00	-52.13	-80.01	-98.66	-141.45
L-Proline, 5-oxo	-41.89	-52.36	-85.70	-96.50	-138.30
D-Mannopyranose	-30.81	-26.62	-225.88	-146.86	-538.56
Lactic acid,	-37.38	-46.74	-53.22	-54.99	-85.01
Butanoic acid, 3-hydroxy	-39.59	-63.56	-80.83	-78.08	-171.64
D-Erythrose	-40.78	-58.88	-82.63	-103.95	-207.21
Unknown sugar	-41.04	-50.98	-77.87	-92.50	-199.54
Unknown sugar	-22.58	-26.71	-51.07	-64.17	-134.06
Unknown sugar	-24.23	-23.92	-39.22	-53.83	-120.90
Unknown carboxylic acid	-43.78	-59.16	-97.66	-310.89	-774.72
Unknown carboxylic acid	-28.80	-45.08	-136.71	-207.11	-816.75
Glycine	-36.86	-96.21	-125.31	-268.17	-925.57
Unknown sugar	-34.94	-42.43	-43.60	-52.07	-159.12
Unknown sugar	-37.39	-50.63	-70.12	-145.46	-698.75
Pentitol	-89.76	-72.60	-69.77	-113.17	-737.47
					-
Urea	-35.48	-169.79	-325.33	-12752.85	199776.48
Unknown sugar	-12.24	-8.22	-9.20	-13.31	-891.63
HYDROXYLAMINE	-11.24	-9.13	-13.38	-5.73	-2474.88
Unknown sugar	-112.83	-299.79	-136.91	-363.82	-291.05
Unknown amino acid	-24.83	-38.86	-131.07	-219.37	-175.50
Unknown amino acid	-22.52	-44.59	-120.29	-174.91	-139.93
Unknown sugar	-56.50	-1262.77	-888.21	-3351.95	-2681.56
Fumaric acid	-120.58	-127.12	-144.14	-265.08	-212.07
Unknown sugar	-34.29	-49.66	-93.63	-289.02	-231.22
Unknown amino acid	-32.84	-37.28	-41.27	-111.82	-89.46
Unknown sugar	-52.74	-70.17	-116.88	-511.80	-409.44
Threonic acid	-42.64	-43.75	-84.43	-559.81	-447.85
Unknown carboxylic acid	-44.59	-45.20	-61.95	-353.99	-283.19
Unknown carboxylic acid	-182.51	-117.40	-68.14	-1701.98	-1361.59
Unknown carboxylic acid	-28.57	-20.72	-23.28	-283.48	-226.79
				-	-
Unknown sugar	-42.91	-20.39	-207.65	130279.70	104223.76
Propanoic acid, 2,3-hydroxy	-59.10	-88.41	-131.31	-2347.19	-1877.75
Unknown amino acid	-60.98	-111.19	-145.29	-4476.92	-3581.53
Unknown sugar	-30.10	-54.97	-101.35	-4383.29	-3506.63

Unknown carboxylic acid	-27.45	-19.47	-36.16	-11.72	-8.99
Unknown amino acid	-13.04	-8.11	-15.85	-3.02	-3.06
Unknown amino acid	-52.81	-34.03	-69.92	-27.97	-22.37
Unknown amino acid	-3.56	-2.76	-13.58	-1.30	-1.22
Unknown amino acid	-1.19	1.25	-25.00	2.99	4.01
Unknown carboxylic acid	-10.61	-11.24	-25.00	-10.00	-8.00
Pyruvic acid	-38.85	-38.60	-55.60	-30.48	-25.97
Unknown sugar	-22.77	-32.42	-46.70	-18.68	-14.94
Unknown amino acid	-22.97	-37.41	-48.97	-24.88	-30.67
Unknown carboxylic acid	-29.99	-185.29	-2677.22	-37.56	-856.71
Unknown amino acid	-100.94	-272.48	-14804.07	-667.37	-4737.30
Phenylalanine	-73.87	-4750.03	-12098.29	-4839.32	-3871.45
Unknown carboxylic acid	-314.38	-796.31	-2229.98	-891.99	-713.59
Unknown amino acid	-39.40	-79.51	-259.04	-103.62	-82.89
Hippuric acid	-5.19	-9.75	-25.00	-10.00	-8.00
Octanoic acid	-29.39	-42.76	-230.35	-86.56	-81.95
Unknown carboxylic acid	-19.07	-29.79	-128.97	-51.59	-41.27
Unknown amino acid	-20.92	-73.12	-397.31	-158.92	-127.14
Unknown sugar	-35.60	-121.69	-542.72	-217.09	-173.67
Unknown sugar	-44.51	-44.39	-193.68	-77.47	-61.98
Unknown sugar	-215.01	-283.93	-980.45	-392.18	-313.75
Unknown amino acid	-14.69	-13.13	-240.27	-96.11	-6.88
Unknown amino acid	-89.26	-35.20	-492.43	-196.97	-157.58
Unknown amino acid	-1.66	3.27	-25.00	-10.00	-8.00
Unknown amino acid	-19.56	-25.17	-257.02	-102.81	-82.25
Unknown sugar	-27.54	-46.17	-450.73	-180.29	-144.24
Unknown carboxylic acid	-39.71	-115.28	-1445.57	-578.23	-462.58
Unknown amine	-33.47	-174.97	-1726.17	-690.47	-552.38
Unknown sugar	-14.11	-32.46	-269.95	-107.98	-86.39
3,4-Dihydroxybutanoic acid	-39.97	-49.15	-341.24	-136.50	-109.20
Unknown carboxylic acid	-25.55	-39.28	-286.82	-114.73	-91.78
Alpha-ketoglutaric acid	-94.17	-90.25	-779.18	-311.67	-249.34
Fructose derivative	-10.14	-10.14	-92.81	-37.12	-29.70
Tyrosine	-42.29	-317.55	-10315.77	-4126.31	-3301.05
Threonine	-45.54	-589.98	-17924.38	-7169.75	-5735.80
Ornithine	-46.83	-384.60	-10460.05	-4184.02	-3347.22
Unknown amino acid	-31.37	-31.88	-1140.27	-456.11	-364.89
Ethanolamine	-48.21	-71.66	-3057.93	-1223.17	-978.54
Unknown carboxylic acid	-63.28	-100.14	-4107.53	-1643.01	-1314.41
Unknown carboxylic acid	-30.66	-47.39	-1862.47	-744.99	-595.99
Unknown sugar	-31.51	-20.55	-56163.27	-22465.31	-17972.25
Unknown carboxylic acid	-44.68	-70.41	-13035.51	-5214.20	-4171.36
Unknown amino acid	-44.06	-79.52	-19150.55	-7660.22	-6128.18
Unknown amino acid	-8.06	-5.34	-685.19	-274.08	-219.26
Unknown carboxylic acid	-40.01	-34.52	-2615.69	-1046.28	-837.02
Acetic acid, hydroxy	-31.31	-33.22	-1957.56	-783.02	-626.42

Unknown amino acid	-29.89	-32.44	-2799.98	-1119.99	-895.99
Lysine, TMS	-34.93	-62.77	-4855.34	-1942.14	-1553.71
Unknown amino acid	-20.57	-32.79	-2540.23	-1016.09	-812.87
Valine	-35.22	-514.26	-32271.73	-12908.69	-10326.96
Lysine	-84.43	-892.31	-57398.41	-22959.36	-18367.49
Tryptamine	-35.21	-34.96	-667.18	-266.87	-213.50
Galactopyranoside, 1-O-methyl-, beta-	-30.90	-29.97	-691.89	-276.76	-221.41
Alanine [+CO2]	-46.23	-51.32	-1182.89	-473.16	-378.52
Unknown amino acid	-10.79	-11.15	-306.50	-122.60	-98.08
Unknown amine	-38.61	-46.16	-722.72	-289.09	-231.27
Unknown carboxylic acid	-61.22	-76.17	-1004.75	-401.90	-321.52
Unknown amino acid	-23.96	-19.08	-255.94	-102.37	-81.90
Unknown carboxylic acid	-1.86	-1.54	-25.00	-10.00	-8.00
Unknown carboxylic acid	-33.15	-18.91	-452.69	-181.08	-144.86
Unknown sugar	-4.85	-2.30	-71.69	-28.68	-22.94
Gluconic acid-1,4-lactone	1.93	1.40	-25.00	-10.00	-8.00
Unknown amino acid	-28.21	-196.21	-90.99	-136.93	-97.90
Unknown amino acid	-37.12	-633.33	-344.81	-257.21	-173.45
Unknown amino acid	-48.55	-196.82	-221.81	-176.30	-178.76
Unknown amine	20.41	-33.00	-25.00	-10.00	-8.00
Unknown carboxylic acid	-11.84	-23.85	-18.71	-13.23	-7.67
Unknown amino acid	-53.39	-94.49	-98.11	-39.24	-31.39
Unknown amino acid	-2.64	-33.00	-25.00	2.36	-8.00
Unknown carboxylic acid	-40.67	-361.32	-273.73	-109.49	-87.59
Unknown carboxylic acid	-102.80	-1126.46	-853.38	-341.35	-273.08
Unknown amino acid	-74.79	-862.73	-653.58	-261.43	-209.15
Unknown amino acid	-51.81	-603.80	-457.43	-182.97	-146.38
Unknown carboxylic acid	-67.11	-789.72	-598.27	-239.31	-191.45
Unknown carboxylic acid	-44.42	-538.13	-407.67	-163.07	-130.45
Isovaleric acid, 2-oxo-	-169.69	-2868.68	-2173.24	-869.30	-695.44
Unknown amino acid	-41.89	-687.33	-520.70	-208.28	-166.62
Unknown sugar	-23.09	-323.57	-245.13	-98.05	-78.44
Unknown amino acid	-29.28	-386.28	-292.64	-117.05	-93.64
Unknown amino acid	-58.55	-1114.85	-844.58	-337.83	-270.27
Creatinine	-99.75	-2005.83	-1519.56	-607.83	-486.26
Unknown carboxylic acid	-26.95	-535.28	-405.51	-162.21	-129.76
L-Tryptophan	-7.57	-166.35	-126.02	-50.41	-40.33
Unknown carboxylic acid	-46.97	-1076.86	-815.80	-326.32	-261.06
Unknown sugar	-31.06	-705.98	-534.83	-213.93	-171.15
Unknown amine	-87.50	-2204.47	-1670.05	-668.02	-534.42
Unknown amino acid	-22.61	-616.69	-467.19	-186.88	-149.50
Unknown amino acid	-1.18	-33.00	-25.00	-10.00	-8.00
Isoleucine	-67.32	-7228.20	-5475.91	-2190.36	-1752.29
Unknown carboxylic acid	-50.81	-6247.35	-4732.84	-1893.14	-1514.51
Serine	-80.49	-10655.89	-8072.64	-3229.06	-2583.24

Glutamic acid	-94.47	-13421.43	-10167.75	-4067.10	-3253.68
Unknown amino acid	-28.72	-3999.84	-3030.18	-1212.07	-969.66
Unknown amine	-57.75	-12676.43	-9603.36	-3841.34	-3073.07
Unknown carboxylic acid	-42.54	-63773.70	-48313.41	-19325.36	-15460.29
Unknown amino acid	-58.45	-26815.14	-20314.50	-8125.80	-6500.64
Unknown carboxylic acid	-26.26	-19862.44	-15047.30	-6018.92	-4815.14
Alanine	-55.98	-32619.50	-24711.74	-9884.70	-7907.76
Unknown carboxylic acid	-19.47	-6407.30	-4854.02	-1941.61	-1553.29
Leucine	-35.94	-13169.15	-9976.63	-3990.65	-3192.52
Unknown carboxylic acid	-30.21	-11202.78	-8486.95	-3394.78	-2715.82
Unknown amino acid	-37.22	-2249.87	-1704.45	-681.78	-545.42
Unknown sugar	-199.10	-12963.31	-9820.69	-3928.27	-3142.62
Unknown carboxylic acid	-13.24	-881.30	-667.65	-267.06	-213.65
Unknown carboxylic acid	-69.27	-3488.16	-2642.55	-1057.02	-845.62
Unknown carboxylic acid	-61.32	-3029.14	-2294.80	-917.92	-734.34
Unknown amino acid	-16.05	-835.36	-632.85	-253.14	-202.51
Unknown amino acid	-15.05	-498.23	-377.45	-150.98	-120.78
Unknown amino acid	-15.48	-591.61	-448.19	-179.28	-143.42
Unknown carboxylic acid	-27.83	-1194.16	-904.67	-361.87	-289.49
Noradrenaline	-25.19	-1050.10	-795.53	-318.21	-254.57
Butanoic acid, 2-amino-	-62.16	-2591.60	-1963.33	-785.33	-628.27
Aspartic acid	-284.34	-1325.18	-1003.92	-401.57	-321.25
Unknown amino acid	-115.36	-506.69	-383.85	-153.54	-122.83
Unknown amino acid	-51.35	-328.03	-248.51	-99.40	-79.52
Unknown amino acid	-92.37	-532.90	-403.71	-161.49	-129.19
Unknown sugar	-47.04	-262.76	-199.06	-79.62	-63.70
Unknown amino acid	-112.69	-410.14	-310.71	-124.28	-99.43
Unknown amino acid	-322.52	-1150.21	-871.37	-348.55	-278.84
Unknown carboxylic acid	-97.40	-183.82	-44.56	-68.98	-23.13
Oleic acid	-136.38	-194.05	-60.80	-58.68	-51.53
Arachidonic acid	-132.83	-204.19	-36.82	-36.85	-32.35
Unknown amino acid	-50.01	-92.94	-19.36	-9.85	-10.03
Unknown carboxylic acid	-125.47	-211.42	-57.60	-62.95	-39.56
Unknown carboxylic acid	-194.59	-457.82	-57.21	-63.15	-62.87
Unknown sugar	-149.59	-289.36	-39.17	-59.82	-43.47
Cholesterol	-88.46	-180.15	-12.63	-51.21	-93.57
Unknown carboxylic acid	-403.95	-8933.81	-281.43	-367.48	-2165.77
Unknown carboxylic acid	-220.67	-594.83	-20.04	-17.27	-144.20
Unknown carboxylic acid	-46.17	-117.57	-30.96	-19.43	-18.88
Unknown carboxylic acid	-85.77	-300.92	-14.55	-11.93	-10.59
Unknown carboxylic acid	-214.44	-917.30	-38.90	-66.54	-41.93
Unknown carboxylic acid	-66.43	-277.29	-22.03	-3.73	-7.94
Unknown carboxylic acid	-59.13	-171.98	-33.34	-32.09	-30.62
Undecanoic acid	-50.82	-190.55	-22.25	-19.07	-18.71
Unknown carboxylic acid	-62.60	-211.38	-34.96	-28.37	-23.40
Unknown carboxylic acid	-38.13	-201.67	-17.24	-20.36	-17.20

Unknown carboxylic acid	-66.93	-595.93	-21.10	-28.76	-13.56
Unknown carboxylic acid	-76.02	-756.08	-21.70	-27.32	-19.88
Unknown carboxylic acid	-80.20	-857.73	-20.03	-34.36	-18.46
Unknown carboxylic acid	-70.96	-777.64	-24.69	-36.55	-18.57
Unknown carboxylic acid	-68.29	-689.50	-37.20	-31.83	-65.03
Unknown carboxylic acid	-61.58	-1023.47	-27.51	-37.43	-23.19
Unknown carboxylic acid	-49.80	-817.90	-24.39	-30.04	-23.59
Unknown carboxylic acid	-54.04	-861.93	-27.77	-38.13	-26.18
Unknown carboxylic acid	-65.55	-1532.48	-22.98	-35.26	-17.31
Unknown carboxylic acid	-54.19	-724.24	-29.44	-25.71	-32.15
Unknown carboxylic acid	-59.62	-778.92	-21.24	-15.40	-17.39
Unknown carboxylic acid	-67.36	-683.46	-29.02	-31.00	-30.41
Unknown carboxylic acid	-76.98	-873.40	-26.36	-30.44	-23.73
Unknown carboxylic acid	-53.70	-1424.43	-29.12	-41.15	-32.51
1-Monooleoylglycerol	-69.97	-3271.44	-64.49	-78.37	-68.34
Unknown carboxylic acid	-107.20	-496.58	-28.49	-150.48	-46.96
Unknown carboxylic acid	-93.18	-1105.63	-22.34	-335.04	-58.93
Unknown carboxylic acid	-71.16	-816.93	-35.20	-247.56	-21.91
Unknown carboxylic acid	-93.51	-732.89	-25.71	-222.09	-27.57
Unknown carboxylic acid	-29.78	-226.42	-10.17	-68.61	-5.62
Unknown carboxylic acid	-44.41	-387.97	-28.65	-117.57	-94.05
Succinic acid	-39.67	-1867.41	-68.74	-565.88	-452.71
Unknown carboxylic acid	-71.78	-1259.59	-37.66	-381.69	-305.36
Unknown carboxylic acid	-93.56	-1847.72	-34.82	-559.91	-447.93
Unknown amino acid	-38.00	-33.00	7.79	22.73	-8.00
b-Sitosterol	-31.71	-24.11	-15.64	-11.43	-8.21
Unknown sugar	-29.96	-22.00	-9.13	-7.84	-3.49
Unknown carboxylic acid	-12.27	-6.53	-2.61	-1.77	-1.53
2-Hydroxybutyric acid	-1.46	-2.61	1.50	1.41	2.73
Unknown carboxylic acid	-37.12	-42.91	-22.87	-16.51	-19.83
Hexadecanoic acid	-68.51	-89.79	-36.89	-27.09	-24.40
Stearic acid	-57.94	-71.70	-30.66	-21.51	-19.72
Linoleic acid	-87.17	-97.07	-42.48	-28.26	-26.75
Unknown carboxylic acid	-27.98	-34.05	-15.94	-7.84	-7.27
Unknown carboxylic acid	-5.55	-5.44	-1.77	-1.17	-1.47
Unknown amino acid	-14.78	-15.09	-9.01	-7.39	-5.86
Myristic acid	-180.90	-192.94	-116.59	-86.75	-60.46
Unknown amino acid	-30.24	-32.26	-17.05	-11.29	-8.00
Unknown carboxylic acid	-28.49	-26.35	-16.65	-12.31	-9.62
Heptadecanoic acid	-100.76	-90.91	-50.95	-34.32	-30.93
Unknown carboxylic acid	-450.54	-391.26	-213.89	-118.56	-94.85
Unknown carboxylic acid	-38.00	-33.00	-4.70	1.32	3.17
Unknown carboxylic acid	-195.11	-186.84	-86.52	-74.59	-58.80
Unknown carboxylic acid	-38.00	-33.00	6.99	13.55	23.10
Unknown alcohol	-4723.23	-4101.76	-39.05	-1242.96	-994.37
Unknown carboxylic acid	-38.00	-33.00	1.06	-10.00	-8.00

Unknown sugar	-488.28	-424.03	-71.44	-128.49	-102.80
Unknown alcohol	-259.96	-225.75	-28.37	-68.41	-54.73
Unknown carboxylic acid	-923.29	-801.81	-93.76	-242.97	-194.38
Unknown carboxylic acid	-181.86	-157.93	-16.79	-47.86	-38.29
Unknown carboxylic acid	-1456.49	-1264.85	-127.26	-383.29	-306.63
Unknown carboxylic acid	-713.84	-619.92	-38.78	-187.85	-150.28
Unknown carboxylic acid	-1286.39	-1117.13	-67.96	-338.52	-270.82
Unknown carboxylic acid	-860.96	-747.68	-49.19	-226.57	-181.26
Unknown carboxylic acid	-924.88	-803.19	-45.17	-243.39	-194.71
Unknown carboxylic acid	-1477.16	-1282.79	-66.58	-388.73	-310.98
Unknown carboxylic acid	-788.35	-684.62	-32.35	-207.46	-165.97
Unknown carboxylic acid	-807.32	-701.09	-33.71	-212.45	-169.96
Unknown carboxylic acid	-717.75	-623.31	-54.78	-188.88	-151.10
Malic acid	-424.47	-368.62	-33.39	-111.70	-89.36
Unknown carboxylic acid	-860.86	-747.59	-57.58	-226.54	-181.23
Unknown carboxylic acid	-834.87	-725.02	-55.74	-219.70	-175.76
Unknown carboxylic acid	-888.34	-771.45	-57.08	-233.77	-187.02
Unknown carboxylic acid	-689.49	-598.77	-45.06	-181.44	-145.16
Unknown carboxylic acid	-1864.54	-1619.21	-37.57	-110.39	-72.74
Unknown carboxylic acid	-543.74	-472.20	-12.48	-16.80	-7.35
Unknown carboxylic acid	-38.00	-33.00	1.62	1.11	1.29
n-Pentadecanoic acid	-1310.17	-1137.78	-88.21	-53.15	-35.02
Unknown amino acid	-38.00	-33.00	-2.32	-1.74	1.08
Unknown amino acid	-38.00	-33.00	-1.93	-1.29	1.06
Unknown carboxylic acid	-38.00	-33.00	-4.49	-3.10	-1.39
Unknown carboxylic acid	-38.00	-33.00	-1.93	-3.84	2.20
Unknown carboxylic acid	-38.00	-33.00	2.36	-1.40	2.63
Unknown amino acid	-38.00	-33.00	-3.90	-10.00	-2.22
4-Methyl-2-oxovaleric acid	-141.66	-58.37	-68.08	-64.18	-131.72
Unknown amino acid	-7.84	3.35	2.09	1.29	-1.25
Unknown amino acid	-38.00	1.75	1.88	4.40	-8.00
Unknown carboxylic acid	-25.24	-7.40	-10.41	-5.80	-4.57
Nonanoic acid	-36.78	-18.45	-19.74	-11.65	-10.81
Unknown amino acid	-15.14	-5.95	-7.50	-2.93	-2.79
Unknown amino acid	-38.00	2.33	-1.06	11.21	16.49
Unknown amino acid	-32.08	-10.56	-11.38	-4.96	-3.70
Unknown amino acid	-32.08	-10.56	-11.38	-4.96	-3.70
Unknown amino acid	-28.11	-14.77	-11.28	-5.43	-4.97
Unknown amino acid	-27.99	-10.76	-9.93	-4.33	-3.23
Unknown amino acid	-38.00	5.82	9.42	26.79	32.49
Unknown amino acid	-7.47	1.15	3.18	3.55	6.59
Unknown amino acid	-15.35	-2.15	-2.44	-1.51	1.49
Unknown amino acid	-36.58	-12.63	-8.96	-6.29	-3.30
Unknown alcohol	-38.00	-7.03	-1.81	1.26	3.09
Unknown amino acid	-23.90	-8.48	-2.83	-1.75	-1.74
Unknown amino acid	-38.00	-12.91	-7.56	-4.00	-4.56

Unknown amino acid	-38.00	3.51	5.81	9.78	10.53
Unknown amino acid	-22.16	-3.92	-3.65	-2.22	-1.99
Unknown amino acid	-34.62	-5.25	-4.97	-2.77	-1.35
Unknown carboxylic acid	-38.00	-1.52	-1.59	1.39	3.68
Unknown amino acid	-31.20	-7.98	-7.58	-4.34	-3.39
Unknown amino acid	-38.00	4.57	6.68	13.12	14.78
Unknown amino acid	-38.00	-8.48	-5.98	-2.03	-1.52
Unknown amino acid	-38.00	-5.47	-2.16	-10.00	2.98
Unknown carboxylic acid	-62.71	-12.64	-19.28	-16.50	-13.20
Unknown sugar	-38.00	-9.77	-2.95	-10.00	-8.00
Unknown amino acid	-38.00	5.30	14.35	8.78	5.88
Unknown carboxylic acid	-38.00	1.39	6.61	2.20	2.01
Unknown amino acid	-20.16	-2.36	-2.45	-1.50	-1.24
Unknown carboxylic acid	-227.05	-10.91	-9.92	-12.73	-5.93
Unknown amino acid	-80.91	-5.32	-2.91	-2.68	-1.37
Unknown amino acid	-38.00	3.23	2.96	4.02	4.30
Unknown amino acid	-38.00	-2.32	1.48	1.38	1.19
Unknown amino acid	-38.00	3.61	4.47	3.26	1.68
Unknown amino acid	-38.00	1.10	2.65	2.27	1.03
Homoserine	-38.00	1.80	4.25	3.04	1.91
Unknown carboxylic acid	-38.00	1.20	3.20	2.05	1.26
Unknown carboxylic acid	-38.00	-1.45	-3.94	-1.40	-3.97
Unknown amino acid	-38.00	-1.37	2.81	1.90	-2.74
Unknown sugar	-38.00	-2.92	-1.63	-2.08	-8.00
Unknown amino acid	-38.00	-1.50	-25.00	-10.00	-8.00
Unknown amino acid	-38.00	1.33	-25.00	-10.00	-8.00
Unknown carboxylic acid	-38.00	-3.38	-25.00	-4.06	-8.00
Unknown amino acid	-38.00	-1.59	-25.00	-2.23	-1.28
Unknown amino acid	-38.00	-1.67	-25.00	1.60	1.80
Unknown amino acid	-38.00	-1.51	-25.00	-1.13	2.65
Unknown carboxylic acid	-38.00	-12.51	-25.00	-10.00	-8.06
Unknown amino acid	-20.70	-14.24	-16.81	-8.52	-4.52
Unknown amino acid	-4.11	-3.04	-3.74	-1.76	-1.53
Unknown amine	-23.55	-16.75	-20.62	-10.29	-11.03
Unknown carboxylic acid	-9.69	-6.27	-9.50	-2.87	-3.23
Hexanoic acid	-26.16	-15.14	-17.17	-8.00	-7.62
Unknown amino acid	-59.10	-20.96	-38.88	-8.13	-4.99
Unknown amino acid	-33.12	-17.92	-22.93	-13.58	-12.16
Unknown carboxylic acid	-49.80	-35.53	-28.93	-22.64	-10.78
Unknown amino acid	-30.17	-21.76	-16.86	-8.96	-8.56
Glycine, N-acetyl-	-32.11	-23.74	-19.35	-8.75	-8.22
Unknown sugar	-19.76	-15.82	-14.75	-9.00	-8.62
Unknown carboxylic acid	-3.75	-2.85	-2.81	-1.53	-1.32
Unknown amino acid	-38.00	-33.00	-25.00	4.86	15.40
Unknown carboxylic acid	-253.47	-220.12	-166.76	-66.70	-10.33
Unknown carboxylic acid	-38.00	-33.00	-25.00	-10.00	-5.29

Unknown carboxylic acid	-38.00	24.39	275.87	467.94	796.38
Unknown carboxylic acid	-38.00	-33.00	-25.00	-10.00	5.10
Unknown carboxylic acid	-38.00	-33.00	-25.00	-10.00	6.76
Unknown sugar	-3.75	-3.99	-2.70	-1.54	-1.40
Unknown amino acid	-33.35	-36.69	-29.23	-18.58	-18.05
Unknown amino acid	-432.70	-433.95	-328.75	-131.50	-105.20
Unknown carboxylic acid	-21.84	-22.75	-17.95	-10.15	-9.36
Cystine	-588.61	-617.55	-467.84	-187.14	-149.71
Gulonic acid	-76.19	-69.66	-46.33	-27.35	-34.21
Unknown carboxylic acid	-30.42	-28.32	-20.45	-10.06	-11.50
Unknown sugar	-24.61	-23.46	-18.71	-11.39	-11.18
Unknown carboxylic acid	-32.05	-26.60	-18.84	-11.14	-8.52
Unknown carboxylic acid	-24.03	-21.71	-15.76	-9.14	-8.21
Unknown carboxylic acid	-24.85	-21.88	-16.44	-9.82	-8.38
Unknown carboxylic acid	-25.22	-22.73	-16.78	-10.74	-9.14
Unknown sugar	-24.85	-21.68	-15.42	-9.20	-7.46
Unknown sugar	-24.47	-20.77	-15.82	-8.97	-7.54
Unknown carboxylic acid	-23.83	-20.65	-15.64	-8.65	-7.93
Unknown sugar	-25.52	-22.28	-17.14	-9.90	-8.79
Unknown carboxylic acid	-25.75	-21.92	-17.02	-9.43	-8.92
Unknown carboxylic acid	-25.56	-21.17	-17.85	-9.84	-9.16
Unknown sugar	-24.07	-20.99	-16.95	-9.57	-9.56
Unknown amino acid	-23.10	-20.51	-16.03	-8.80	-7.80
Decanoic acid	-1321.03	-1147.21	-869.10	-347.64	-278.11
Unknown carboxylic acid	-3015.70	-2618.90	-1984.01	-793.61	-634.88
Unknown carboxylic acid	-1858.60	-1614.05	-1222.76	-489.10	-391.28
Unknown carboxylic acid	-1317.51	-1144.16	-866.79	-346.71	-277.37
Unknown sugar	-550.78	-478.31	-362.36	-144.94	-115.95
Unknown sugar	-434.85	-377.63	-286.08	-114.43	-91.55
Unknown carboxylic acid	-1576.23	-1368.83	-1036.99	-414.80	-331.84
Unknown amino acid	-235.47	-204.49	-154.92	-61.97	-49.57
Unknown carboxylic acid	-1067.19	-926.77	-702.10	-280.84	-224.67
Unknown amino acid	-723.24	-628.07	-475.81	-190.33	-152.26
Unknown amino acid	-2427.92	-2108.46	-1597.32	-638.93	-511.14
Unknown carboxylic acid	-3630.00	-3152.37	-2388.16	-955.26	-764.21
Unknown amine	-963.90	-837.07	-634.15	-253.66	-202.93
Unknown carboxylic acid	-402.95	-349.93	-265.10	-106.04	-84.83
Unknown amino acid	-555.49	-482.40	-365.46	-146.18	-116.95
Unknown amino acid	-519.91	-451.50	-342.05	-136.82	-109.46
Unknown carboxylic acid	-466.60	-405.20	-306.97	-122.79	-98.23
Unknown carboxylic acid	-2495.06	-2166.76	-1641.49	-656.59	-525.28
Unknown sugar	-4697.46	-4079.37	-3090.44	-1236.17	-988.94
Unknown carboxylic acid	-966.05	-838.94	-635.56	-254.22	-203.38
Unknown carboxylic acid	-2498.14	-2169.44	-1643.51	-657.40	-525.92
Tryptophan	-716.92	-622.59	-471.66	-188.66	-150.93
Unknown sugar	-37849.51	-32869.31	-24900.99	-9960.40	-7968.32

Unknown amino acid	-2262.43	-1964.74	-1488.44	-595.38	-476.30
	-	-	-		
Unknown sugar	320963.30	278731.30	211160.08	-84464.03	-67571.23
Unknown carboxylic acid	-722.97	-627.84	-475.64	-190.26	-152.20
Lauric acid	-1348.46	-1171.03	-887.15	-354.86	-283.89
Unknown amino acid	-39403.08	-34218.46	-25923.08	-10369.23	-8295.39
Unknown amino acid	-803.41	-697.70	-528.56	-211.42	-169.14
2-OXOISOCAPROIC ACID	-1909.30	-1658.08	-1256.12	-502.45	-401.96
Unknown carboxylic acid	-454.06	-394.31	-298.72	-119.49	-95.59
Methionine	-1089.39	-946.05	-716.70	-286.68	-229.34
Unknown amino acid	-488.20	-423.96	-321.18	-128.47	-102.78
Unknown amino acid	-2663.72	-2313.23	-1752.45	-700.98	-560.78
Unknown sugar	-138.86	-120.59	-91.36	-36.54	-29.23
Unknown amino acid	-904.96	-785.88	-595.37	-238.15	-190.52
Unknown sugar	-496.21	-430.92	-326.46	-130.58	-104.47
Unknown amino acid	-16133.13	-14010.35	-10613.90	-4245.56	-3396.45
Unknown carboxylic acid	-38.00	-33.00	-25.00	-10.00	-8.00
Unknown amino acid	-2612.50	-2268.75	-1718.75	-687.50	-550.00
Unknown amino acid	-758.29	-658.51	-498.87	-6.19	-159.64
Unknown alcohol	-38.00	-33.00	-25.00	69.37	55.25
Unknown carboxylic acid	-38.00	-33.00	-25.00	16.67	17.09
Unknown amine	-33.81	-32.14	-27.59	-14.67	-14.73
Unknown amino acid	-38.00	-33.00	-25.00	1.06	1.68
Unknown amino acid	-38.00	-33.00	-25.00	2.08	1.77
Unknown carboxylic acid	-370.54	-321.78	-243.77	-27.08	-15.20
Unknown amino acid	-310.64	-269.76	-204.37	-25.21	-12.27
Unknown sugar	-38.00	-33.00	-25.00	3.30	6.05
Unknown carboxylic acid	-38.00	-33.00	-25.00	-1.13	1.65
Unknown carboxylic acid	-38.00	-33.00	-25.00	-2.30	1.13